

Full wwPDB X-ray Structure Validation Report (i)

Aug 11, 2021 – 11:31 am BST

PDB ID	:	7A0S
Title	:	50S Deinococcus radiodurans ribosome bounded with mycinamicin I
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Deposited on	:	2020-08-10
$\operatorname{Resolution}$:	3.22 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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

MolProbity	÷	4.02b-467
Mogul		1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 3.22 Å.

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



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R _{free}	130704	1335 (3.24-3.20)
Clashscore	141614	1460(3.24-3.20)
Ramachandran outliers	138981	1437(3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)
RNA backbone	3102	1023 (3.54-2.90)

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

Mol	Chain	Length		Quality of chain		
1	Х	2880	32%	37%	20%	• 6%
2	Y	123	² % 3 5%	41%	21	% ••
3	А	274	56%		38%	5% •
4	В	206	4% 62%		36%	•



Chain Length Quality of chain Mol 6% С 520549% 39% 7% • • 28% D 6 177. . 55% 42% 7% Ε 717161% 36% • 6% \mathbf{G} 8 14346% 47% . .. % 9 Η 13451% 45% • 18% 10Ι 13757% 36% 7% 16% J 11 13653% 38% 7% •• .% Κ 121169% • 59% 32% 19% \mathbf{L} 1310459% 38% . % 14 М 16639% 28% • • 29% .% 15Ν 117 54% 44% • .% Ο 169849% 46% . . 3% Ρ 1713466% 25% . . . 13% 18 \mathbf{Q} 9360% 37% •• 9% R 1911042% 47% 9% • 18% 20 \mathbf{S} 17558% 39% . 15% Т 219152% 27% 19% ••• 14% U 22745%• 51% 42% 10% V 236159% 26% 11% 40% W 245560% 40% Ζ 255857% 34% 5% •• 22% 26491 59% 31% 10% 4% 2274760% 36% •• 33% 28 3 6338% 49% 11% •

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The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-



ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MG	Ι	201	-	-	-	Х
30	MG	K	201	-	-	-	Х
30	MG	Х	2924	-	-	-	Х
30	MG	Х	2953	-	-	-	Х
30	MG	Х	2975	-	-	-	Х
30	MG	Х	2978	-	-	-	Х
30	MG	Х	2983	-	-	-	Х
30	MG	Х	2985	-	-	-	Х
30	MG	Х	3002	-	-	-	Х
30	MG	Х	3023	-	-	-	Х
30	MG	Х	3051	-	-	-	Х
30	MG	Х	3057	-	-	-	Х
30	MG	Х	3065	-	-	-	Х
30	MG	Х	3072	-	-	-	Х
30	MG	Х	3083	-	-	-	Х
30	MG	Х	3086	-	-	-	Х
30	MG	Х	3087	-	_	-	Х
30	MG	Х	3107	-	-	-	Х
30	MG	Х	3110	_	_	-	Х
30	MG	Х	3115	_	_	-	Х
30	MG	Х	3117	-	-	-	Х
30	MG	Х	3120	_	_	-	Х
30	MG	Х	3130	_	_	-	Х
30	MG	Х	3134	-	-	-	Х
30	MG	Х	3143	-	-	-	Х
30	MG	Х	3146	-	-	-	Х
30	MG	Х	3155	-	-	-	Х
30	MG	Х	3176	_	_	-	Х
30	MG	Х	3183	-	_	-	Х
30	MG	Х	3190	_	_	-	Х
30	MG	Х	3196	-	_	-	Х
30	MG	Х	3207	_	_	-	Х
30	MG	Х	3209	-	_	-	Х
30	MG	Х	3210	-	_	-	Х
30	MG	Х	3211	-	_	-	Х
30	MG	Х	3214	-	-	-	Х
30	MG	Х	3224	-	-	-	Х
30	MG	Х	3227	-	-	-	Х
30	MG	Х	3232	-	-	-	X
30	MG	Y	205	-	-	-	Х
30	MG	Y	210	-	-	-	Х
30	MG	Y	213	-	_	-	X



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MG	Y	214	-	-	-	Х
32	MPD	Х	3245	-	-	-	Х

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2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 84486 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a RNA chain called RNA (2732-MER).

Mol	Chain	Residues			Atoms	ZeroOcc	AltConf	Trace		
1	Х	2699	Total 57935	C 25843	N 10696	O 18698	Р 2698	5	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Х	1526	U	С	$\operatorname{conflict}$	GB 1026245073
Х	2779	А	С	$\operatorname{conflict}$	GB 1026245073

• Molecule 2 is a RNA chain called RNA (122-MER).

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		ZeroOcc	AltConf	Trace	
2	Y	122	Total 2598	C 1161	N 476	O 840	Р 121	0	0	0

• Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
3	А	272	Total 2011	C 1248	N 396	O 364	${ m S} { m 3}$	0	0	0

• Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	В	206	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	U	200	1544	968	296	272	8			0

• Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
5	С	196	Total 1479	C 918	N 284	0 274	S 3	0	0	0





• Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
6	D	177	Total 1375	$\begin{array}{c} \mathrm{C} \\ 874 \end{array}$	N 243	0 251	${ m S} 7$	0	0	0

• Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
7	Е	171	Total 1286	C 812	N 237	O 236	S 1	0	0	0

• Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
8	G	142	Total 1110	C 701	N 208	O 198	${ m S} { m 3}$	0	0	0

• Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
9	Н	134	Total 997	C 614	N 198	O 180	S 5	0	0	0
			997	014	198	180	\mathbf{O}			

• Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
10	Ι	137	Total 982	C 603	N 194	0 184	${ m S}$ 1	0	0	0

• Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
11	J	135	Total 1062	C 676	N 197	0 182	S 7	0	0	0

• Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
12	K	115	Total 893	C 549	N 182	O 159	${ m S} { m 3}$	0	0	0

• Molecule 13 is a protein called 50S ribosomal protein L18.



Mol	Chain	Residues		Ato	\mathbf{ms}		ZeroOcc	AltConf	Trace
13	L	104	Total 761	$\begin{array}{c} \mathrm{C} \\ 462 \end{array}$	N 159	O 140	0	0	0

• Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
14	М	118	Total 923	C 578	N 178	О 167	0	0	0

• Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
15	Ν	117	Total 955	$\begin{array}{c} \mathrm{C} \\ 594 \end{array}$	N 203	\mathbf{O} 157	S 1	0	0	0

• Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
16	О	98	Total 736	C 459	N 138	0 138	${ m S}$ 1	0	0	0

• Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
17	Р	129	Total 1014	$\begin{array}{c} \mathrm{C} \\ 640 \end{array}$	N 198	O 174	${ m S} 2$	0	0	0

• Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
18	Q	92	Total 705	$\begin{array}{c} \mathrm{C} \\ 445 \end{array}$	N 131	O 127	${ m S} 2$	0	0	0

• Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
19	R	110	Total 771	C 473	N 147	O 150	S 1	0	0	0

• Molecule 20 is a protein called 50S ribosomal protein L25.



Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
20	S	175	Total 1288	C 809	N 224	O 250	S 5	0	0	0

• Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
21	Т	74	Total 537	С 334	N 105	O 97	S 1	0	0	0

• Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues		Ator	\mathbf{ns}		ZeroOcc	AltConf	Trace
22	U	74	Total 519	C 319	N 106	O 94	0	0	0

• Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues		Ato	\mathbf{ms}			ZeroOcc	AltConf	Trace
23	V	54	Total 438	C 270	N 89	O 78	S 1	0	0	0

• Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues		Atc	\mathbf{ms}			ZeroOcc	AltConf	Trace
24	W	55	Total 424	С 264	N 82	О 76	${ m S} { m 2}$	0	0	0

• Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues		Ato	\mathbf{ms}			ZeroOcc	AltConf	Trace
25	Z	57	Total 448	C 275	N 92	O 76	${ m S}{ m 5}$	0	0	0

• Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues		Aton	ıs		ZeroOcc	AltConf	Trace
26	1	49	Total 314	C 199	N 53	O 62	0	0	0

• Molecule 27 is a protein called 50S ribosomal protein L34.



Mol	Chain	Residues		Atc	\mathbf{ms}			ZeroOcc	AltConf	Trace
27	2	46	Total 383	C 230	N 91	O 60	$\frac{S}{2}$	0	0	0

• Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues		Ato	\mathbf{ms}			ZeroOcc	AltConf	Trace
28	3	63	Total 459	C 288	N 94	0 74	${ m S} { m 3}$	0	0	0

• Molecule 29 is mycinamic in I (three-letter code: QU2) (formula: $C_{37}H_{61}NO_{12}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf
29	Х	1	Total 50	$\begin{array}{c} \mathrm{C} \\ 37 \end{array}$	N 1	О 12	0	0

• Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	Х	335	Total Mg 335 335	0	0
30	Y	17	Total Mg 17 17	0	0
30	А	3	Total Mg 3 3	0	0
30	В	1	Total Mg 1 1	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	Ι	2	TotalMg22	0	0
30	J	1	Total Mg 1 1	0	0
30	К	1	Total Mg 1 1	0	0
30	М	1	Total Mg 1 1	0	0
30	Ν	3	Total Mg 3 3	0	0
30	2	2	TotalMg22	0	0
30	3	1	Total Mg 1 1	0	0

• Molecule 31 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	Х	1	Total C N 10 7 3	0	0
31	Х	1	Total C N 10 7 3	0	0
31	Х	1	$\begin{array}{ccc} {\rm Total} & {\rm C} & {\rm N} \\ 10 & 7 & 3 \end{array}$	0	0
31	Х	1	Total C N 10 7 3	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	1	Total C N	0	0
	Λ	T	10 7 3	0	0
21	v	1	Total C N	0	0
	Λ	T	10 7 3	0	0
21	v	1	Total C N	0	0
101	Λ	T	10 7 3	0	0
21	v	1	Total C N	0	0
	Λ	I	10 7 3	0	0

• Molecule 32 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	Х	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 8 6 2 \end{array}$	0	0
32	Х	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 8 & 6 & 2 \end{array}$	0	0
32	Х	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 8 6 2 \end{array}$	0	0
32	Х	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 8 6 2 \end{array}$	0	0

• Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	Х	1	Total Na 1 1	0	0



• Molecule 34 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).



Mol	Chain	Residues	Ate	oms		ZeroOcc	AltConf
34	Х	1	Total 3	${ m C} 2$	O 1	0	0

• Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	Х	5	Total Ca 5 5	0	0

• Molecule 36 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	Х	1	Total K 1 1	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: RNA (2732-MER)



G738 G739 A740	6741 6742 4743	G746	A/4/ A748 C749	C750 6751	G752 U753	G754 C755	C756 U757	G758 C759	0160 0761	A762	A764	A766	G772	6774	0775 6776	A777 G778	0779 11780	6781 1700	0/02 6783	A787	G788 G789	A790 G791	U792 G793	A794 A795	A796 A797	6798 6798	U800	A801 A802	C804 C804
<mark>G805</mark> A806 A807	U810 0811	6812 A813	4815 A815 U816	A817 G818	<mark>C8 19</mark> U820	<mark>4821</mark> G822	<mark>U823</mark> U824	C825 U826	C827	C830	4832 4832	A834 11025	0030 6836 11027	u83/ <u>4838</u>	U839 U840	6841 4842	<mark>6843</mark>	A846	4848	G849 C850	<mark>C851</mark> U852	<mark>C853</mark> G854	1857	G858 U859	U860	C863	U868	C869 C870	08/1 6872
G875 A876	G877 C878 4870	4883 4883	0004 A885 A886	G887	U890 A891	5 5	00	50	o o n	• ⊲ t	סט⊲	¢ تۍ ر	יםנ	∩ ¥	00	A911 A912	A913	1917	OTA	A922 A923	C924	<mark>6928</mark> A929	A930	<u>A936</u> C937	<mark>6938</mark> (939	6940 6940	U942	0943 A944	0945 0946
C947 C948 G949	A952 2053	0954 0955	6957 (958	<mark>C959</mark>	<mark>C962</mark>	6967 0968	U969 A970	<mark>A971</mark> C972	0973 0974	C975	<mark>6977</mark>	6983 *004	4904 (985	A986 G987	<mark>6988</mark>	A9 <mark>9</mark> 1 A992	C993 A004	A995		A1001	01005 01006	A1007 G1008	C1009	G1013	C1016 C1017	C1018	41020	A1021 A1022	01023 61024
A1025 U1026 C1027	G1028 C1029 IT1030	C1031 A1032	61035 01034 61035	G1036 U1037	U1038	A1043 U1044	<mark>G1045</mark> U1046	<mark>G1047</mark> U1048	C1049 G1050	U1051	G1053 C1054	A1055	A1057	G1058 A1059	C1060 A1061	G1062 C1063	C1064	61066 61066	A1068	G1069 G1070	U1071 U1072	G1073 G1074	C1075 U1076	U1077 • A1078	G1079 A1080	A1081	G1083	A1084 G1085	C1086 C1087
1089 1090	1091 1092 1093	1095	1097	1099 1100	1101 1102	1103 1104	1105 1106	1107	1110	1112	1114 1115	1116	1118	<mark>1121</mark>	1122 1123	1124	1127 1128	1129		1133 1134	1135 1136	1137 1138	1139 1140	1141 1142	1143 1144	1145	1147	1148 1149	1152
54 0 0 0 0 0 0 0 0			54 54 55	36 G	71 72 6	73 74	75 76	۲ <mark>0</mark>	000				<u> </u>	0	91 92 6	93 94	2			0 0 0	22 2	10 1 1	12 (3 A	2 [2	18 19 0		5 5 5 7	23 24 6	5 20
A115 A115 A115 G115	U115	A116		A116	A117 U117	G117 G117	A117 U117	A117	A118	U118	611 0) ^ლ «	द ⊲द र	50	G119 A119	G119 U119			0120	A120	G120	G121 G121	U121 U121	U121	C121 C121	G122	G122	6122 A122	6122 A122
A1227 G1228 C1229	C1234	61241 A1242	<mark>61246</mark> 01247	<mark>61248</mark> 61249	A1250 G1251	C1252 C1253	<mark>G1254</mark> A1255	C1256 U1257	G1258	<mark>61261</mark>	C1264	G 1266 6 1266 A 1727	01268 01268	G1270	C1271 G1272	A1275	U1276 01277	A1278 A1278	U1280	A1281 A1282	C1283 G1284	A1285 U1286	A1287 A1288	A1289 A1290	G1291 A1292		G1298	A1299 A1300	01301 C1302
U1303 U1304 C1305	U1306 U1307 C1308	61309 61310 61310	01311 61312 01313	A1314 A1315	G1316	A1321 G1322	<mark>G1323</mark> G1324	U1325 U1326	01329	G1330	61332 61332	41334	G1336 G1336 G1336	G1337 G1338	U1339 C1340	G1341 U1342	C1343	61345 61345	C1347 C1347	C1348 A1349	G1350 G1351	G1352 A1353	A1354 A1355	G1356 U1357	C1358 G1359		41366 A1366	A1367 G1368	G1369 U1370
61371 <mark>A1372</mark> 61373	61377 61377 61378	A1379 C1380	G1385	A1386	A1391 U1392	<mark>G1393</mark>	<mark>A13</mark> 97 G1398	C1399 A1400	G1401 G1402	U1403	41408	01409	C1411 C1411	C1412 U1413	C1418	G1419	C1422	01424	01426 U1426	<mark>G1427</mark> G1428	A1429 G1430	U1431 G1432	A1433 U1434	G1435 G1436	A1437 G1438	G 1439	61440 A1441	C1442 C1443	C1444 A1445
U1 446 U1 447 A1 448	C1451 114 452	A1453 U1454 M1454	61460	A1463	<mark>A1464</mark> G1465	C1466 U1467	A1468 U1469	G1470 G1471	C1472 U1473	A1474	G1476 G1476 C1477	U1478	6/#T9	01482 61483	G1484 U1485	A1486 C1487	G1488 C1480	067-100 01460	G1495	G1496 C1497	G1498 A1499	U1500 C1501	<mark>G1502</mark> G1503	G1504 U1505	C1506	A1509	A1511 A1511	A1512 U1513	
C1517 C1518 C1519 G1519	61520 U1521 C1523	4 U -	A U1526	U1530 C1531	G1536	U1537 A1538	U1539 C1540	<mark>G1541</mark> G1542	G1543 A1544	G1545		000	זמנ	5 5	G A	₽ G	C1558 C1558	A1560	61562	01563 01564	G1571	C1572 G1573	A1574 C1575	C1581	A1582 A1583	G1584	A1586	A1587 A1588	U1592
C1593 U1594 A1595	U1601 01600	A1604	A1607 01608	<mark>61609</mark> A1610	G1622	C1623 A1624	A1625 A1626	<mark>C1627</mark> C1628	61629 A1630	V169A	61635 61635		61042 A1643	<mark>61644</mark> U1645	G1646 U1647	C1648 A1649	A1650 111651	G1652	A1654	C1655 U1656	A1657 A1658	<mark>G1659</mark> G1660	<mark>C1661</mark> G1662	C1663 G1664	C1665 G1666	A1667	41669	G1670 A1671	C1673
C1674 C1675 U1676	C1677 G1678 111679	01680 41681	A1002 G1683 G1684	A1685 A1686	C1687 U1688	U1689 U1690	G1691 C1692	A1693 A1694	U1695 C1696	U1697	A1699	C1701		01/05 A1706	A1707 C1708	U1709 U1710	C1711 C1712	G1713 61713	A1/ 1 4 A17 15	G1716 A1717	A1718 G1719	U1723	C1724	C1727 A1728	<mark>C1729</mark>	U1732	0 0	G1735 C1736	G1/3/ U1738



G1739	G 17 40	C1743	G1744 C1745	A1746	G 17 47	01/48 G1749	A1750	A1751 11752	A1753	G1754	G1755 C1756	C1757		G1761 G1761	C1762	A1764	C1765	01/66 G1767	U1768	01770	A1771	C1772 C1773	A1774	A1775 A1776	A1777 114770	C1779	A1780 C1781	A1782	A1785	C1786 U1787	C1788	01/89 G1790	C1791	A1793	A1794 C1795	A1796	61798	A1799 A1800	C1801
A1802	G1803 U1804	<mark>G 1805</mark>	G1806 A1807	C1808	G1809	01810 A1811	U1812	A1813	G1816	U1817	G1818 111810	61820	A1821	01822 01823	C1824	U1826	G1827	C1830	G 1831	01834	C1835	C1836	A1839	A1840	U1843	010 71 A1845	A1846	G1850	61852	G1855	U1856	16819	C1865	41867	U1870	G1871	A1873	G1874	G1882
A1883	A1884 C1885	<mark>G1886</mark>	G1887	G1889	G1890	C C C C	5 5	D	A A	U I	D	a D	A	G ₽	5 5	9.0	G 21000	01908 01909	A1910	A1911 61912	G1913	01914	G1918	A1919 A1920	A1921	77610	01925 01926	U1927	07679	61931 61932	G1933	01934 01935	A1936	01938 U1938	U1939	A1943	01946	G1947 C1948	A1949
C1950	A1953	A1954	G 1955	G1958	U1959	G1963	A1964	U1965		G1970	C1971 61972	C1973	U1974	01976 U1976	C1977 111078	C1979	A1980	A1981 C1982	G1983	A1984 G1985	G1986	G1987 A1988	C1989	01990 C1991	G1992	01994	G1995 A1996	A1997	01999	U2000	A2002	A2003 U2004	U2005	G2007	C2008	U2011	A2012 A2013	A2014 G2015	A2016
U2017	62018 C2019	<mark>62020</mark>	62021	C2023	U2024	G2026	C2027	C2028	U2030	A2031	G2032 C2033	A2034	G2035	C2038	G2039	A2041	A2042	62044	A2045	C2046 C2047	C2048	G2052		G2055 C2056	U2057	00070	A2063 U2064	A2065	02067 U2067	C2068 U2069	G2070	A2073	U2074	G2076	G2077 G2078	A2079	U2081	C2082 G2083	<mark>G2084</mark>
G2085	U2086 U2087	U2088	C2089	C C C C C C C C C C C C C C C C C C C	D C	5 0) (n	4 5	5	A 11	A	5 5	ם פ	55 5	5 13	Ą	5 0	G	ם ט	00	54	A	G A	D	5 55	00	D	o D	ם פו		.5 55	n	J 15	5 D	. ლ. ი	P C	5 5	Ð
A	C P	IJ	5 11	o 13	A	A A	n	٩	0 0	Ā	טנ	00	n	ы А2165	G2166	A2168	A2169	U2171	U2172	G2173 G2174	A2175	U2176 U2177	U2178	C2179 U2180	A2181	<mark>G2186</mark>	A2187 A2188	A2189	A2191	U2192 C2193	A2194	U2195 U2196	U2197	C2199	G 2200	A2204		U2208 G2209	-
U2212	G2213	G2217	G2218 117240	A2220	G2221	U2223 U2223	U2224	G2225 A7776	C2227	U2228	(2229 (2223)	G2231	G2232	G2234 G2234	G2235	C2237	G2238	C2240	U2241	C2242 C2243	C2244	A2245 A2246	A2247	U2251		G2255	<mark>(2256</mark>	(12259	G2261	02262 02263	C2264	A2260 A2266	A2267	62269 62269	U2270 C2271	A2272	02274	U2275 C2276	A2277
A2278	G2279 A2280	<mark>C2281</mark>	G2282	u2284	U2285	G2280 G2287	A2288	A2289	U2291	C2292	G2293 112204	C2295	U2296	6229/ U2298	A2299	A2301		G2304 C2305	A2306	A2307 A2308	G 2309	<mark>62310</mark> U2311	A2312	G2313 A2314	A2315	62317	U2318	U2322 110202	62324	A2325 C2326	U2327	62328 C2329	G2330	62332	A2333	G2336	A2331 C2338	A2339	G2344
	A2348	G2 <mark>351</mark>	A2352	G2354	A2355	A2350 A2357	C2358	U2359 77360	G2361	G2362	G2363 C2364	±00770	A2367	62.368 U2.369	G2370	A2372	C2373	62375		G2378 G2370		C2382	U2385	G2386 U2387	G2388	42.309	A2391 (2392	G2393	62395 C2395	U2.398	C2399	42400 42401	U2402 40403	02404 A2404	A2405 C2406	G2407	62408 A2409	U2410 A2411	A2412
-	G2415 U2416	U2417	A2418	C2420	C2421	G2423	G2424	62425 01/176	A2 427	U2428	A2429 A2430	C2431	A2432	G2434 G2434	C2435	62437	A2438	02440 C2440	U2441	C2442	02446	G2447 A2448		02452 C2453	C2454	U2456	A2457 U2458	C2459	62461 62461	62464	G2465	42460 A2467	G2468	u2470 U2470	U2471 U2472	G2473	G2475 C2475	A2476 C2477	C2478
U2479	C2480 G2481	A2482	U2483	42404 U2485	C2486	G248/ G2488	C2489	U2490	G2492	U2493	C2494 C2495	G2496	A2497	02498 C2499	C2500 117501	10020	U2507	G2509 A2509	A2510	62511 42512	A2513	G2514 G2515	U2516	C2517	A2520	62522	G2523 G252 4	U2525 110506	02527 G2527	G2528 G2529	C2530	02031 62532	U2533 112524	02034 C2535	C2538	C2539	A2040 U2541	U2542 A2543	A2544
A2545	62546 C2547	G2548	G2549 C2550	A2551	C2552	G2554	G2555	A2556 C7557	C2558	U2559	G2560 C2561	62562	U2563	02565 C2565	A2566	A2568	A2569 40570	0.755 / 0	G2578	A2579 C2580	A2581	G2582 U2583		G2586 G2587	U2588	U2590	C2591 U2592	A2593	02595	C2596 G2597	C2598	42600	C2601	62603 62603	G2604 C2605	G2606	6200/ A2608	<mark>62609</mark>	A2613
	U2616	G2621	(12622 A7673	62624 G2624	U2625 10000	02625 G2627	C2628	U2629 17630	C2631	U2632	A2633 C2634	E 0075	A2639	G2040 A2641	G2642		U2651	62002	C2655	G2656 G2657	A2658	C2659 C2660	G2661	C2662 U2663	G2664	u2666	C2667 U2668	C2669	C2671	U2672 G2673	C2674	02676 G2676	U2677	G2679	U2680 A2681	C2682	C2083 A2684	A2685 C2686	<mark>G2687</mark>









 \bullet Molecule 5: 50S ribosomal protein L4













• Molecule 22: 50S ribosomal protein L28







4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	170.00Å 410.74Å 697.78Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{B}_{\mathrm{ascolution}}(\mathbf{A})$	49.67 - 3.22	Depositor
Resolution (A)	49.67 - 3.22	EDS
% Data completeness	99.1 (49.67-3.22)	Depositor
(in resolution range)	99.2(49.67-3.22)	EDS
R_{merge}	0.18	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.14 (at 3.19 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R R.	0.224 , 0.253	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.225 , 0.231	DCC
R_{free} test set	19448 reflections (5.00%)	wwPDB-VP
Wilson B-factor ($Å^2$)	93.5	Xtriage
Anisotropy	0.672	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.17, 30.9	EDS
L-test for $twinning^2$	$ < L >=0.46, < L^2>=0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	84486	wwPDB-VP
Average B, all atoms $(Å^2)$	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, EOH, K, CA, NA, MPD, SPD, QU2

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

Mol Chain		Bo	ond lengths	Bond angles		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	Х	0.85	58/64872~(0.1%)	1.51	1153/101178~(1.1%)	
2	Y	0.61	1/2904~(0.0%)	1.25	15/4525~(0.3%)	
3	А	0.42	0/2050	0.70	1/2772~(0.0%)	
4	В	0.66	0/1572	0.88	1/2112~(0.0%)	
5	С	0.57	0/1502	0.84	1/2035~(0.0%)	
6	D	0.36	0/1393	0.62	0/1873	
7	Ε	0.36	0/1308	0.59	0/1771	
8	G	0.59	1/1134~(0.1%)	0.77	0/1535	
9	Н	0.75	0/1007	0.96	1/1352~(0.1%)	
10	Ι	0.54	0/994	0.92	3/1338~(0.2%)	
11	J	0.59	0/1085	0.84	1/1451~(0.1%)	
12	Κ	0.79	2/901~(0.2%)	1.07	5/1208~(0.4%)	
13	L	0.40	0/767	0.69	0/1027	
14	М	0.74	0/936	0.93	1/1257~(0.1%)	
15	Ν	0.63	0/971	0.95	3/1296~(0.2%)	
16	0	0.52	0/743	0.83	1/995~(0.1%)	
17	Р	0.70	1/1027~(0.1%)	0.94	5/1375~(0.4%)	
18	Q	0.52	0/716	0.76	1/963~(0.1%)	
19	R	0.51	0/781	0.74	0/1062	
20	S	0.34	0/1313	0.59	0/1796	
21	Т	0.52	0/543	0.76	0/722	
22	U	0.43	0/524	0.71	0/707	
23	V	0.44	0/441	0.59	0/586	
24	W	0.44	0/426	0.75	0/568	
25	Ζ	0.72	0/460	1.12	1/618~(0.2%)	
26	1	0.46	0/317	0.70	0/434	
27	2	0.46	0/387	0.81	0/509	
28	3	0.50	0/464	0.83	0/611	
All	All	0.77	63/91538~(0.1%)	1.37	$11\overline{93}/137676~(0.9\%)$	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if



the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	А	0	2
4	В	0	2
5	С	0	2
8	G	0	3
10	Ι	0	4
11	J	0	6
12	Κ	0	1
14	М	0	1
16	0	0	1
17	Р	0	2
19	R	0	3
20	S	0	1
21	Т	0	1
22	U	0	1
25	Ζ	0	2
28	3	0	4
All	All	0	36

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	Х	1278	А	N3-C4	-7.98	1.30	1.34
1	Х	827	С	N1-C6	-7.37	1.32	1.37
1	Х	2795	А	C6-N1	6.95	1.40	1.35
1	Х	537	С	N1-C2	6.69	1.46	1.40
1	Х	1283	С	N3-C4	-6.59	1.29	1.33
1	Х	1288	А	C5-C6	-6.47	1.35	1.41
1	Х	1468	А	C8-N7	-6.38	1.27	1.31
1	Х	699	G	N9-C4	-6.37	1.32	1.38
1	Х	540	G	C2-N3	6.36	1.37	1.32
1	Х	1669	А	N9-C4	-6.13	1.34	1.37
1	Х	1655	С	N1-C6	-6.08	1.33	1.37
1	Х	2598	С	N3-C4	-6.05	1.29	1.33
1	Х	540	G	C5-C6	-6.04	1.36	1.42
1	Х	2564	U	C2-N3	5.99	1.42	1.37
1	Х	1333	G	N9-C8	5.93	1.42	1.37
1	X	1666	G	C5-C4	-5.92	1.34	1.38
1	Х	2660	С	N1-C6	-5.91	1.33	1.37
1	Х	1688	U	C4-O4	5.89	1.28	1.23
2	Y	14	С	N1-C6	5.84	1.40	1.37



(Å)			
7			
7			
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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Х	2480	С	N1-C6	5.84	1.40	1.37
1	Х	2823	G	N9-C8	-5.82	1.33	1.37
1	Х	759	С	N3-C4	5.79	1.38	1.33
1	Х	1753	А	N9-C4	5.76	1.41	1.37
1	Х	1278	А	N9-C4	-5.71	1.34	1.37
1	Х	90	G	N9-C4	5.69	1.42	1.38
1	Х	2795	А	C5-C4	5.67	1.42	1.38
1	Х	1992	G	C5-C4	-5.66	1.34	1.38
1	Х	2530	С	N1-C6	-5.66	1.33	1.37
1	Х	756	С	N3-C4	-5.66	1.29	1.33
1	Х	2567	G	N7-C5	-5.65	1.35	1.39
1	Х	787	А	N9-C4	-5.62	1.34	1.37
1	Х	1468	А	N7-C5	-5.61	1.35	1.39
12	Κ	43	GLU	CG-CD	5.58	1.60	1.51
1	Х	2003	А	N9-C4	5.57	1.41	1.37
1	Х	928	G	N7-C5	-5.54	1.35	1.39
1	Х	756	С	N1-C6	-5.53	1.33	1.37
1	Х	1333	G	C5-C4	5.53	1.42	1.38
1	Х	1666	G	N1-C2	-5.49	1.33	1.37
1	Х	1667	А	C5-C6	-5.48	1.36	1.41
1	Х	1278	А	N7-C5	-5.40	1.36	1.39
1	Х	2488	G	N1-C2	-5.40	1.33	1.37
1	Х	1665	С	N3-C4	-5.39	1.30	1.33
1	Х	1991	С	N3-C4	-5.39	1.30	1.33
1	Х	1743	C	N1-C6	-5.38	1.33	1.37
1	Х	2686	C	N1-C6	-5.32	1.33	1.37
1	Х	841	G	N9-C4	-5.31	1.33	1.38
1	Х	2685	A	N7-C5	5.30	1.42	1.39
1	Х	1677	C	N3-C4	-5.29	1.30	1.33
1	Х	1468	A	N9-C4	5.29	1.41	1.37
12	K	114	GLU	CG-CD	5.28	1.59	1.51
1	Х	540	G	N7-C5	-5.28	1.36	1.39
8	G	140	GLN	CG-CD	-5.26	1.39	1.51
1	Х	1682	A	N7-C5	-5.25	1.36	1.39
1	X	173	A	N3-C4	-5.21	1.31	1.34
1	X	759	C	C4-C5	5.16	1.47	1.43
1	X	2014	A	N9-C4	5.15	1.41	1.37
17	P	55	ASP	CB-CG	5.10	1.62	1.51
	X	1981	A	N7-C5	-5.08	1.36	1.39
	X	542	A	N9-C4	-5.07	1.34	1.37
1	X	1981	A	N9-C4	-5.07	1.34	1.37
1	X	1282	A	P-OP2	5.03	1.57	1.49



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Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	Х	2530	С	N3-C4	-5.02	1.30	1.33
1	Х	1976	U	C2-N3	-5.01	1.34	1.37

All (1193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	Х	540	G	C6-C5-N7	-20.38	118.17	130.40
1	Х	1468	A	C8-N9-C4	-19.09	98.16	105.80
1	Х	540	G	C4-C5-N7	17.19	117.68	110.80
1	Х	540	G	N1-C6-O6	17.00	130.10	119.90
1	Х	540	G	C5-C6-O6	-16.48	118.71	128.60
1	Х	1467	U	C6-N1-C2	16.05	130.63	121.00
1	Х	537	С	N1-C2-O2	14.55	127.63	118.90
1	Х	537	С	N3-C2-O2	-14.27	111.91	121.90
1	Х	1467	U	N1-C2-N3	-14.22	106.37	114.90
1	Х	2580	С	C6-N1-C2	-14.07	114.67	120.30
1	Х	1333	G	N3-C4-N9	-13.51	117.90	126.00
1	Х	1468	А	N7-C8-N9	12.96	120.28	113.80
1	Х	2478	С	C6-N1-C2	-12.88	115.15	120.30
1	Х	1675	С	O5'-P-OP1	-12.38	94.56	105.70
1	Х	1278	А	N1-C2-N3	12.06	135.33	129.30
1	Х	1746	A	O5'-P-OP1	-11.90	94.99	105.70
1	Х	1278	А	C2-N3-C4	-11.62	104.79	110.60
1	Х	2491	С	C6-N1-C2	-11.61	115.66	120.30
1	Х	1973	С	C6-N1-C2	-11.57	115.67	120.30
1	Х	2692	A	O5'-P-OP2	-11.56	95.30	105.70
1	Х	343	A	O4'-C1'-N9	11.45	117.36	108.20
1	Х	540	G	C5-N7-C8	-11.40	98.60	104.30
1	Х	2423	G	O5'-P-OP2	-11.19	95.63	105.70
1	Х	540	G	N3-C4-N9	11.17	132.70	126.00
1	Х	2025	A	N1-C6-N6	11.11	125.26	118.60
1	Х	2408	G	O5'-P-OP1	-11.03	95.78	105.70
1	Х	1333	G	C2-N3-C4	-10.90	106.45	111.90
1	Х	1665	С	O5'-P-OP1	-10.87	95.92	105.70
1	Х	699	G	C5-N7-C8	-10.86	98.87	104.30
1	Х	540	G	N9-C4-C5	-10.80	101.08	105.40
1	Х	699	G	C4-C5-N7	10.77	115.11	110.80
1	Х	2845	С	C6-N1-C2	-10.72	116.01	120.30
1	Х	542	A	N1-C2-N3	10.68	134.64	129.30
1	Х	1989	С	O5'-P-OP2	10.59	123.41	110.70
1	Х	1989	С	O5'-P-OP1	-10.53	96.22	105.70
1	X	1333	G	N3-C4-C5	10.49	133.85	128.60



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	1278	А	N7-C8-N9	10.49	119.04	113.80
1	Х	2795	А	N1-C6-N6	10.42	124.85	118.60
1	Х	2478	С	C5-C6-N1	10.37	126.19	121.00
1	Х	1288	А	N1-C6-N6	10.36	124.82	118.60
1	Х	1770	U	C5-C6-N1	-10.12	117.64	122.70
1	Х	1288	А	O4'-C1'-N9	10.11	116.28	108.20
1	Х	1288	А	C4-C5-N7	10.10	115.75	110.70
1	Х	542	А	C2-N3-C4	-10.02	105.59	110.60
1	Х	928	G	N1-C6-O6	10.02	125.91	119.90
1	Х	760	U	O5'-P-OP2	-10.00	96.70	105.70
1	Х	1278	А	C8-N9-C4	-9.95	101.82	105.80
1	Х	1682	A	C8-N9-C4	-9.88	101.85	105.80
1	Х	2484	G	O5'-P-OP1	-9.79	96.89	105.70
1	Х	954	U	O5'-P-OP1	-9.77	96.91	105.70
1	Х	243	G	C8-N9-C4	-9.74	102.50	106.40
1	Х	689	А	C2-N3-C4	-9.68	105.76	110.60
1	Х	699	G	N3-C4-C5	9.64	133.42	128.60
1	Х	243	G	C5-C6-O6	-9.63	122.82	128.60
1	Х	343	А	N7-C8-N9	9.59	118.60	113.80
1	Х	243	G	N1-C6-O6	9.58	125.65	119.90
1	Х	2668	U	N1-C2-N3	9.55	120.63	114.90
1	Х	1988	A	C8-N9-C4	9.47	109.59	105.80
1	Х	2494	С	N3-C4-C5	-9.41	118.14	121.90
1	Х	1652	G	C4-C5-N7	9.37	114.55	110.80
1	Х	1966	С	O5'-P-OP1	-9.36	97.28	105.70
1	Х	1663	С	N1-C2-O2	9.33	124.50	118.90
10	Ι	56	LEU	CA-CB-CG	9.29	136.68	115.30
1	Х	1467	U	C4-C5-C6	-9.28	114.13	119.70
1	Х	1679	U	C5-C6-N1	-9.24	118.08	122.70
1	Х	2667	С	N3-C4-C5	9.23	125.59	121.90
1	X	$26\overline{62}$	C	N1-C2-O2	9.21	124.43	118.90
1	X	928	G	C6-C5-N7	-9.18	124.89	130.40
1	X	343	A	N1-C2-N3	9.18	133.89	129.30
1	X	1288	A	C5-N7-C8	-9.13	99.34	103.90
1	Х	1278	A	C6-C5-N7	-9.08	125.95	132.30
1	X	661		C6-N1-C2	-9.07	116.67	120.30

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105.80

110.80

103.90

132.30

128.60

111.90

102.17

114.41

99.39

125.99

123.19

107.41



-9.07

9.03

-9.02

-9.02

-9.02

-8.98

C8-N9-C4

C4-C5-N7

C5-N7-C8

C6-C5-N7

C5-C6-O6

C2-N3-C4

А

G

А

А

G

G

343

2624

1278

1288

928

699

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	343	А	C2-N3-C4	-8.94	106.13	110.60
1	Х	1278	А	O4'-C1'-N9	8.93	115.35	108.20
1	Х	1989	С	C5-C6-N1	8.92	125.46	121.00
1	Х	540	G	C4-C5-C6	8.92	124.15	118.80
1	Х	2550	С	C6-N1-C2	-8.87	116.75	120.30
15	Ν	50	ARG	CB-CG-CD	-8.88	88.53	111.60
1	Х	689	А	N7-C8-N9	8.86	118.23	113.80
1	Х	689	А	C5-N7-C8	-8.85	99.47	103.90
1	Х	2025	А	C5-C6-N6	-8.83	116.64	123.70
1	Х	841	G	C5-N7-C8	-8.82	99.89	104.30
1	Х	1667	А	C5-C6-N6	-8.79	116.67	123.70
1	Х	2782	G	C6-C5-N7	-8.74	125.15	130.40
1	Х	2867	G	N1-C6-O6	8.74	125.14	119.90
1	Х	540	G	N7-C8-N9	8.73	117.47	113.10
1	Х	26	G	C8-N9-C4	-8.71	102.91	106.40
1	Х	522	G	N1-C6-O6	8.69	125.11	119.90
1	Х	2408	G	C8-N9-C4	-8.68	102.93	106.40
1	Х	803	С	N1-C2-O2	8.67	124.10	118.90
1	Х	2670	С	C6-N1-C2	-8.65	116.84	120.30
1	Х	661	С	C5-C6-N1	8.61	125.31	121.00
1	Х	774	A	C4-C5-C6	-8.61	112.69	117.00
1	Х	30	G	C8-N9-C4	-8.60	102.96	106.40
1	Х	833	A	N1-C6-N6	8.58	123.75	118.60
1	Х	2795	A	N9-C4-C5	-8.58	102.37	105.80
1	Х	1976	U	N3-C2-O2	-8.54	116.22	122.20
1	Х	1468	A	N1-C6-N6	-8.48	113.51	118.60
1	Х	537	С	C2-N1-C1'	8.47	128.12	118.80
1	Х	2691	С	O4'-C1'-N1	8.43	114.94	108.20
1	Х	957	G	N1-C6-O6	-8.42	114.85	119.90
1	Х	1333	G	C5-C6-N1	-8.39	107.30	111.50
1	Х	841	G	C2-N3-C4	-8.36	107.72	111.90
1	Х	2481	G	C4-C5-N7	8.36	114.14	110.80
1	Х	1696	С	N3-C2-O2	-8.34	116.06	121.90
1	Х	2044	G	N3-C4-C5	-8.34	124.43	128.60
1	Х	2782	G	N1-C6-O6	8.33	124.90	119.90
1	X	1468	A	N9-C4-C5	8.32	109.13	105.80
1	X	2668	U	C2-N3-C4	-8.32	122.01	127.00
1	Х	1989	C	C6-N1-C2	-8.30	116.98	120.30
1	X	2534	U	C5-C4-O4	-8.28	120.93	125.90
1	Х	537	C	C6-N1-C1'	-8.27	110.87	120.80
1	Х	1681	A	C2-N3-C4	-8.27	106.47	110.60
2	Y	39	С	C2-N1-C1'	8.25	127.88	118.80



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	1770	U	O4'-C1'-N1	8.24	114.80	108.20
1	Х	543	G	O5'-P-OP1	-8.23	98.30	105.70
1	Х	1391	А	P-O3'-C3'	8.22	129.56	119.70
1	Х	649	G	N3-C4-N9	-8.20	121.08	126.00
1	Х	1278	А	C4-C5-C6	8.19	121.09	117.00
1	Х	2553	G	C4-C5-N7	8.17	114.07	110.80
1	Х	841	G	N3-C4-C5	8.16	132.68	128.60
1	Х	2567	G	C8-N9-C4	-8.15	103.14	106.40
1	Х	1474	А	N1-C6-N6	-8.14	113.72	118.60
1	Х	977	G	C8-N9-C4	8.12	109.65	106.40
1	Х	2044	G	C8-N9-C4	-8.12	103.15	106.40
1	Х	955	G	N9-C4-C5	-8.09	102.16	105.40
1	Х	134	G	N3-C4-C5	-8.09	124.56	128.60
1	Х	1626	A	N1-C6-N6	8.06	123.44	118.60
1	Х	661	С	N1-C2-O2	8.02	123.71	118.90
1	Х	2667	С	C2-N3-C4	-8.01	115.90	119.90
1	Х	541	С	C6-N1-C2	7.95	123.48	120.30
1	Х	2371	А	C8-N9-C4	-7.93	102.63	105.80
1	Х	2854	G	N7-C8-N9	7.90	117.05	113.10
1	Х	822	G	N3-C4-C5	-7.90	124.65	128.60
1	Х	1468	A	C2-N3-C4	7.90	114.55	110.60
1	Х	559	С	C2-N1-C1'	7.89	127.48	118.80
1	Х	2035	G	O5'-P-OP1	-7.88	98.61	105.70
2	Y	14	С	C6-N1-C2	-7.85	117.16	120.30
1	Х	2843	А	N1-C6-N6	-7.84	113.90	118.60
1	Х	343	A	C6-C5-N7	-7.82	126.83	132.30
1	Х	1691	G	C4-C5-N7	7.80	113.92	110.80
1	Х	1696	С	C6-N1-C2	-7.80	117.18	120.30
1	Х	2274	С	C2-N1-C1'	7.79	127.36	118.80
1	Х	1283	С	N3-C4-C5	-7.77	118.79	121.90
1	X	$16\overline{47}$	U	C6-N1-C2	-7.77	116.34	121.00
1	X	646	C	C6-N1-C2	-7.73	117.21	120.30
1	Х	1343	C	N3-C4-C5	7.73	124.99	121.90
1	Х	1392	U	C5-C6-N1	7.73	126.56	122.70
1	Х	1678	G	C8-N9-C4	7.72	109.49	106.40
1	X	2782	G	O4'-C1'-N9	7.72	114.37	108.20
1	X	2854	G	C5-N7-C8	-7.71	100.44	104.30
1	Х	928	G	C4-C5-N7	7.70	113.88	110.80
1	X	1282	A	N1-C6-N6	7.70	123.22	118.60
1	Х	2469	G	C8-N9-C4	-7.69	103.32	106.40
1	Х	2668	U	N3-C2-O2	-7.69	116.82	122.20
1	Х	2857	C	C6-N1-C2	-7.68	117.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	2624	G	C6-C5-N7	-7.67	125.80	130.40
1	Х	2564	U	C5-C6-N1	7.67	126.53	122.70
1	Х	343	А	C5-C6-N1	-7.67	113.87	117.70
1	Х	1692	С	N3-C4-C5	-7.66	118.84	121.90
10	Ι	93	LEU	CA-CB-CG	7.64	132.88	115.30
1	Х	2867	G	C4-C5-N7	7.64	113.86	110.80
1	Х	2544	А	C2-N3-C4	7.63	114.41	110.60
1	Х	2700	U	O5'-P-OP1	-7.63	98.84	105.70
1	Х	824	U	N1-C2-N3	7.62	119.47	114.90
1	Х	1468	А	C5-C6-N1	7.62	121.51	117.70
1	Х	2698	G	N3-C4-C5	-7.61	124.79	128.60
1	Х	833	А	C4-C5-N7	7.60	114.50	110.70
1	Х	134	G	N3-C4-N9	7.60	130.56	126.00
1	Х	2478	С	N3-C4-N4	7.58	123.31	118.00
1	Х	1920	А	P-O3'-C3'	7.58	128.80	119.70
1	Х	968	С	N1-C2-O2	7.57	123.44	118.90
1	Х	134	G	C4-N9-C1'	7.56	136.33	126.50
1	Х	343	А	C4-C5-C6	7.55	120.78	117.00
1	Х	456	С	N1-C2-O2	-7.55	114.37	118.90
1	Х	1643	А	N9-C4-C5	-7.54	102.78	105.80
1	Х	542	А	C8-N9-C4	-7.52	102.79	105.80
1	Х	1333	G	C8-N9-C4	-7.51	103.39	106.40
1	Х	244	С	N3-C4-N4	7.50	123.25	118.00
1	Х	1336	G	C4-C5-N7	7.50	113.80	110.80
1	Х	833	А	C5-C6-N6	-7.49	117.71	123.70
1	Х	2558	С	O5'-P-OP2	-7.49	98.96	105.70
1	Х	796	А	C2-N3-C4	-7.48	106.86	110.60
1	Х	1282	A	N9-C4-C5	-7.47	102.81	105.80
1	Х	1671	A	O5'-P-OP2	-7.47	98.97	105.70
1	Х	1674	С	OP1-P-O3'	7.47	121.63	105.20
1	Х	90	G	N3-C4-C5	-7.46	124.87	128.60
1	Х	2590	U	C6-N1-C2	-7.45	116.53	121.00
1	Х	2590	U	N3-C2-O2	-7.44	116.99	122.20
1	Х	2561	G	N1-C6-O6	-7.43	115.44	119.90
1	Х	537	С	C2-N3-C4	-7.42	116.19	119.90
1	X	822	G	C8-N9-C4	-7.41	103.44	106.40
1	X	1333	G	C5-C6-O6	7.41	$1\overline{33.05}$	128.60
1	X	$16\overline{83}$	G	N3-C4-N9	-7.41	121.56	126.00
1	X	1976	U	N1-C2-N3	7.38	119.33	114.90
1	X	849	G	C8-N9-C4	-7.38	103.45	106.40
1	X	$24\overline{81}$	G	C5-N7-C8	-7.37	100.61	104.30
1	X	1972	G	C8-N9-C4	-7.37	103.45	106.40



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	1211	G	O5'-P-OP2	-7.37	99.07	105.70
1	Х	2408	G	N3-C4-C5	-7.37	124.92	128.60
1	Х	1288	А	N9-C4-C5	-7.36	102.85	105.80
1	Х	1344	С	N1-C2-O2	7.36	123.32	118.90
1	Х	1288	А	C4-N9-C1'	7.36	139.54	126.30
1	Х	841	G	N3-C4-N9	-7.35	121.59	126.00
1	Х	1628	С	O5'-P-OP2	-7.34	99.09	105.70
1	Х	330	С	C6-N1-C2	-7.34	117.36	120.30
1	Х	1283	С	C4-C5-C6	7.34	121.07	117.40
1	Х	30	G	N3-C4-C5	-7.34	124.93	128.60
1	Х	522	G	C6-C5-N7	-7.34	126.00	130.40
1	Х	1280	U	N3-C2-O2	-7.33	117.07	122.20
1	Х	2521	А	N1-C6-N6	-7.33	114.20	118.60
1	Х	788	G	P-O3'-C3'	7.31	128.47	119.70
1	Х	1765	С	N1-C2-O2	7.29	123.28	118.90
1	Х	1683	G	N9-C4-C5	7.29	108.32	105.40
1	Х	583	С	N3-C2-O2	7.28	127.00	121.90
1	Х	983	G	C8-N9-C4	-7.27	103.49	106.40
1	Х	1982	С	C5-C6-N1	-7.26	117.37	121.00
1	Х	501	G	N3-C4-N9	-7.26	121.64	126.00
1	Х	2478	С	C2-N1-C1'	7.25	126.78	118.80
1	Х	2018	G	O5'-P-OP2	-7.25	99.18	105.70
1	Х	2782	G	C8-N9-C1'	-7.24	117.58	127.00
1	Х	1777	А	N1-C6-N6	7.23	122.94	118.60
1	Х	2815	С	C6-N1-C2	7.23	123.19	120.30
1	Х	1683	G	C6-C5-N7	7.23	134.74	130.40
1	Х	501	G	N3-C2-N2	-7.23	114.84	119.90
1	Х	519	С	C6-N1-C2	-7.22	117.41	120.30
1	Х	2561	G	C5-C6-N1	7.21	115.11	111.50
1	Х	1683	G	C4-C5-N7	-7.21	107.92	110.80
1	Х	2815	С	C5-C6-N1	-7.21	117.40	121.00
1	Х	2043	A	N1-C6-N6	7.20	122.92	118.60
1	Х	2876	С	C2-N3-C4	-7.18	116.31	119.90
1	Х	1770	U	C4-C5-C6	7.17	124.00	119.70
1	Х	1977	С	N1-C2-O2	7.16	123.20	118.90
1	Х	2624	G	C5-N7-C8	-7.15	100.72	104.30
1	Х	563	U	C6-N1-C2	7.15	125.29	121.00
17	Р	25	PHE	CB-CG-CD1	7.13	125.79	120.80
1	Х	700	С	C6-N1-C2	-7.13	117.45	120.30
1	Х	1288	A	N9-C1'-C2'	7.13	123.26	114.00
1	Х	2538	С	C6-N1-C2	-7.12	117.45	120.30
1	Х	1333	G	N9-C4-C5	7.11	108.24	105.40

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	1468	А	N3-C4-C5	-7.10	121.83	126.80
1	Х	2624	G	N1-C6-O6	7.10	124.16	119.90
1	Х	797	А	P-O3'-C3'	7.09	128.21	119.70
1	Х	1288	А	C1'-O4'-C4'	-7.07	104.24	109.90
1	Х	689	А	N1-C6-N6	7.07	122.84	118.60
1	Х	540	G	N1-C2-N2	-7.07	109.84	116.20
1	Х	1992	G	N7-C8-N9	-7.06	109.57	113.10
1	Х	579	G	C5-C6-O6	7.04	132.83	128.60
1	Х	2273	С	C6-N1-C2	-7.04	117.48	120.30
1	Х	2491	С	C5-C6-N1	7.03	124.52	121.00
2	Y	39	С	N1-C2-O2	7.03	123.12	118.90
1	Х	2371	A	N7-C8-N9	7.03	117.31	113.80
1	Х	1919	A	N1-C6-N6	7.01	122.81	118.60
1	Х	1712	G	N3-C4-N9	7.01	130.20	126.00
1	Х	955	G	N3-C4-N9	7.00	130.20	126.00
1	Х	2671	С	C6-N1-C2	-7.00	117.50	120.30
1	Х	2530	С	N3-C4-C5	-7.00	119.10	121.90
1	Х	1284	G	N3-C2-N2	7.00	124.80	119.90
1	Х	2487	G	C5-C6-N1	6.99	114.99	111.50
1	Х	136	A	N7-C8-N9	6.98	117.29	113.80
1	Х	2699	G	C5-C6-N1	-6.97	108.02	111.50
1	Х	1698	С	N1-C2-O2	-6.96	114.72	118.90
1	Х	175	С	C5-C6-N1	6.96	124.48	121.00
1	Х	2018	G	O4'-C1'-N9	6.95	113.76	108.20
1	Х	2550	С	C5-C6-N1	6.95	124.47	121.00
1	Х	2314	A	N1-C6-N6	-6.94	114.44	118.60
1	Х	824	U	O5'-P-OP1	-6.93	99.46	105.70
1	Х	243	G	N7-C8-N9	6.93	116.57	113.10
1	Х	2043	A	C8-N9-C4	-6.93	103.03	105.80
1	Х	1819	U	C6-N1-C2	-6.92	116.85	121.00
1	Х	1142	G	C8-N9-C4	6.92	109.17	106.40
1	Х	2697	G	C2-N3-C4	6.91	115.36	111.90
1	Х	1288	A	C8-N9-C1'	-6.91	115.27	127.70
1	Х	2688	G	C8-N9-C4	6.91	109.16	106.40
1	Х	236	С	N1-C2-O2	6.90	123.04	118.90
1	Х	1885	С	N1-C2-O2	6.88	123.03	118.90
1	X	2479	U	N1-C2-O2	6.88	127.61	122.80
1	Х	841	G	N7-C8-N9	6.87	116.54	113.10
1	X	1775	A	C5-N7-C8	6.87	107.34	103.90
1	Х	2700	U	C6-N1-C2	-6.87	116.88	121.00
1	Х	660	G	N3-C2-N2	-6.87	115.09	119.90
1	X	2032	G	C8-N9-C4	6.87	109.15	106.40

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	2558	С	OP1-P-O3'	6.86	120.30	105.20
1	Х	2662	С	C2-N3-C4	6.86	123.33	119.90
1	Х	660	G	N3-C4-N9	-6.86	121.89	126.00
1	Х	243	G	C2-N3-C4	6.86	115.33	111.90
1	Х	2492	G	N3-C4-C5	-6.86	125.17	128.60
1	Х	2043	А	N7-C8-N9	6.85	117.23	113.80
1	Х	1678	G	N7-C8-N9	-6.84	109.68	113.10
1	Х	501	G	N9-C4-C5	6.84	108.14	105.40
1	Х	2867	G	C5-N7-C8	-6.83	100.89	104.30
1	Х	2782	G	C4-N9-C1'	6.82	135.37	126.50
1	Х	2854	G	C4-C5-N7	6.82	113.53	110.80
1	Х	649	G	N3-C4-C5	6.81	132.00	128.60
1	Х	661	С	C2-N1-C1'	6.80	126.28	118.80
1	Х	2256	G	C8-N9-C4	-6.80	103.68	106.40
1	Х	243	G	N3-C4-C5	-6.79	125.20	128.60
1	Х	2467	A	N1-C6-N6	-6.79	114.52	118.60
1	Х	2827	G	N3-C4-N9	6.79	130.08	126.00
1	Х	1667	А	N1-C6-N6	6.79	122.67	118.60
1	Х	1800	А	OP1-P-O3'	6.79	120.14	105.20
1	Х	968	С	C2-N1-C1'	6.79	126.27	118.80
1	Х	2543	А	C8-N9-C4	-6.77	103.09	105.80
1	Х	2553	G	C5-N7-C8	-6.76	100.92	104.30
1	Х	1473	U	C6-N1-C2	-6.75	116.95	121.00
1	Х	797	А	N1-C6-N6	-6.74	114.55	118.60
1	Х	875	G	N3-C4-C5	-6.74	125.23	128.60
1	Х	2017	U	C2-N1-C1'	6.73	125.78	117.70
1	Х	2580	С	N3-C2-O2	-6.73	117.19	121.90
1	Х	343	А	C5-N7-C8	-6.73	100.53	103.90
1	Х	25	U	C6-N1-C2	-6.72	116.97	121.00
1	Х	1686	А	C8-N9-C4	-6.72	103.11	105.80
1	Х	2698	G	C2-N3-C4	6.72	115.26	111.90
_ 1	X	649	G	N3-C2-N2	-6.72	115.20	119.90
1	Х	2481	G	N3-C2-N2	6.70	124.59	119.90
1	Х	343	A	C4-N9-C1'	6.70	138.35	126.30
1	Х	824	U	N1-C2-O2	-6.70	118.11	122.80
1	Х	1991	С	OP2-P-O3'	6.69	119.92	105.20
1	Х	1665	С	C6-N1-C2	6.69	122.98	120.30
1	Х	2524	G	C5-C6-N1	6.69	114.84	111.50
1	Х	1665	С	C5-C6-N1	-6.69	117.66	121.00
1	Х	1778	U	N3-C2-O2	-6.68	117.52	122.20
1	Х	2844	G	OP1-P-OP2	-6.68	109.58	119.60
1	Х	1324	G	O4'-C1'-N9	6.68	113.54	108.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	542	А	N7-C8-N9	6.67	117.14	113.80
1	Х	699	G	N1-C6-O6	6.67	123.90	119.90
1	Х	1037	U	N1-C2-O2	6.67	127.47	122.80
1	Х	1684	G	C5-C6-O6	-6.67	124.60	128.60
1	Х	1222	G	N3-C4-C5	-6.67	125.27	128.60
1	Х	2484	G	N1-C6-O6	-6.67	115.90	119.90
1	Х	796	А	C5-C6-N1	-6.66	114.37	117.70
1	Х	2857	С	N3-C4-C5	-6.66	119.24	121.90
1	Х	2019	С	O5'-P-OP2	-6.65	99.71	105.70
1	Х	580	А	N1-C6-N6	6.65	122.59	118.60
1	Х	1992	G	C8-N9-C4	6.65	109.06	106.40
1	Х	754	G	C8-N9-C4	-6.64	103.74	106.40
1	Х	2700	U	OP2-P-O3'	6.64	119.81	105.20
1	Х	689	А	N1-C2-N3	6.64	132.62	129.30
1	Х	2032	G	N7-C8-N9	-6.63	109.78	113.10
1	Х	1308	С	C6-N1-C2	-6.63	117.65	120.30
1	Х	1297	А	C2-N3-C4	-6.62	107.29	110.60
1	Х	236	С	N3-C2-O2	-6.62	117.27	121.90
1	Х	1466	С	C6-N1-C2	-6.62	117.65	120.30
1	Х	2230	G	N3-C2-N2	-6.61	115.27	119.90
1	Х	90	G	N3-C4-N9	6.61	129.97	126.00
1	Х	2580	С	C5-C4-N4	6.60	124.82	120.20
1	Х	338	G	C8-N9-C4	-6.60	103.76	106.40
1	Х	751	G	O5'-P-OP2	-6.60	99.76	105.70
1	Х	1666	G	N7-C8-N9	-6.60	109.80	113.10
1	Х	1686	А	N7-C8-N9	6.60	117.10	113.80
1	Х	2480	С	N3-C4-N4	-6.60	113.38	118.00
1	Х	2694	G	OP2-P-O3'	6.59	119.71	105.20
1	Х	2849	С	O5'-P-OP1	-6.59	99.77	105.70
1	Х	1682	А	N9-C4-C5	6.59	108.43	105.80
1	Х	2664	G	N3-C2-N2	-6.58	115.29	119.90
1	Х	362	С	N1-C2-O2	6.58	122.85	118.90
1	Х	42	G	C8-N9-C4	-6.57	103.77	106.40
1	Х	756	С	C6-N1-C2	-6.57	117.67	120.30
1	Х	2025	А	C6-C5-N7	-6.57	127.70	132.30
1	Х	1278	А	C4-N9-C1'	6.56	138.10	126.30
1	X	2043	A	OP2-P-O3'	6.56	119.62	105.20
1	X	2417	U	N3-C2-O2	-6.56	117.61	122.20
1	X	1574	A	O4'-C1'-N9	6.55	113.44	108.20
1	X	1006	C	N3-C2-O2	-6.55	117.31	121.90
1	X	516	G	C4-C5-N7	6.54	113.42	110.80
12	K	92	GLY	C-N-CA	-6.54	108.57	122.30



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	1280	U	N1-C2-O2	6.54	127.38	122.80
1	Х	1289	A	N1-C6-N6	6.53	122.52	118.60
1	Х	2795	А	C5-C6-N6	-6.53	118.47	123.70
1	Х	1932	G	O5'-P-OP1	-6.53	99.83	105.70
1	Х	2564	U	C2-N1-C1'	6.52	125.53	117.70
1	Х	689	А	C5-C6-N1	-6.52	114.44	117.70
1	Х	344	G	C8-N9-C4	-6.51	103.80	106.40
1	Х	1980	А	OP1-P-OP2	6.51	129.37	119.60
1	Х	2656	G	O5'-P-OP1	6.51	118.51	110.70
1	Х	2667	С	OP1-P-O3'	6.51	119.52	105.20
1	Х	525	А	C2-N3-C4	6.50	113.85	110.60
1	Х	660	G	C8-N9-C4	-6.50	103.80	106.40
1	Х	869	С	C5-C6-N1	6.50	124.25	121.00
1	Х	343	А	N9-C1'-C2'	6.50	122.45	114.00
1	Х	589	С	N3-C4-C5	-6.49	119.30	121.90
1	Х	1626	А	C5-C6-N6	-6.49	118.51	123.70
1	Х	646	С	C2-N1-C1'	6.49	125.93	118.80
12	Κ	64	ARG	CG-CD-NE	6.48	125.41	111.80
1	Х	483	А	P-O3'-C3'	6.48	127.48	119.70
1	Х	25	U	C2-N1-C1'	6.48	125.47	117.70
1	Х	985	G	C4-C5-N7	6.48	113.39	110.80
1	Х	2700	U	O5'-P-OP2	6.47	118.47	110.70
1	Х	2385	U	O4'-C1'-N1	6.47	113.38	108.20
1	Х	469	G	O4'-C1'-N9	6.47	113.37	108.20
1	Х	689	A	C6-C5-N7	-6.46	127.78	132.30
1	Х	27	G	O4'-C1'-N9	6.46	113.37	108.20
1	Х	556	A	N1-C6-N6	6.46	122.47	118.60
1	Х	869	С	C6-N1-C2	-6.45	117.72	120.30
1	Х	1466	С	N3-C2-O2	-6.45	117.38	121.90
1	Х	2371	A	C6-C5-N7	-6.45	127.78	132.30
1	Х	2867	G	C5-C6-O6	-6.45	124.73	128.60
1	X	2487	G	C6-C5-N7	6.44	134.27	130.40
1	X	526	C	C6-N1-C2	-6.44	117.72	120.30
1	Х	1713	G	N1-C6-O6	-6.44	116.04	119.90
1	X	2546	G	N3-C4-C5	-6.44	125.38	128.60
1	X	$28\overline{54}$	G	C5-C6-O6	-6.44	124.74	128.60
1	X	2555	G	C8-N9-C4	6.43	108.97	106.40
1	X	438	G	N1-C6-O6	$6.4\overline{2}$	123.75	119.90
1	X	1475	U	N3-C2-O2	-6.42	117.70	122.20
1	Х	689	A	O4'-C1'-N9	6.42	113.33	108.20
1	X	$249\overline{5}$	G	C5-C6-N1	$6.4\overline{1}$	$114.7\overline{1}$	111.50
1	Х	684	C	C6-N1-C2	-6.40	117.74	120.30


Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	757	U	C5-C6-N1	-6.40	119.50	122.70
1	Х	1467	U	N3-C4-C5	6.40	118.44	114.60
1	Х	1801	С	O5'-P-OP1	-6.39	99.94	105.70
1	Х	699	G	N7-C8-N9	6.39	116.30	113.10
1	Х	484	G	C8-N9-C4	-6.39	103.84	106.40
1	Х	774	А	N1-C6-N6	-6.39	114.77	118.60
1	Х	2465	G	C8-N9-C4	-6.38	103.85	106.40
1	Х	2488	G	C5-C6-N1	6.38	114.69	111.50
1	Х	2823	G	C4-C5-N7	-6.38	108.25	110.80
1	Х	2025	А	C4-C5-N7	6.38	113.89	110.70
1	Х	2543	А	N9-C4-C5	6.38	108.35	105.80
1	Х	954	U	N1-C2-O2	-6.37	118.34	122.80
1	Х	765	С	N3-C4-C5	6.37	124.45	121.90
1	Х	928	G	N9-C4-C5	-6.37	102.85	105.40
1	Х	962	С	N3-C2-O2	-6.37	117.44	121.90
1	Х	259	U	P-O3'-C3'	6.37	127.34	119.70
1	Х	2693	U	N3-C2-O2	-6.36	117.75	122.20
1	Х	1474	А	C5-C6-N6	6.36	128.79	123.70
1	Х	1652	G	C5-N7-C8	-6.35	101.12	104.30
1	Х	518	А	N1-C6-N6	6.34	122.41	118.60
1	Х	2696	А	C5-C6-N1	6.34	120.87	117.70
1	Х	1647	U	N3-C4-C5	-6.34	110.80	114.60
1	Х	1984	А	O5'-P-OP2	-6.33	100.00	105.70
15	Ν	50	ARG	CA-CB-CG	6.31	127.29	113.40
1	Х	1467	U	N3-C2-O2	6.31	126.61	122.20
1	Х	2045	А	N1-C6-N6	-6.31	114.82	118.60
1	Х	600	G	P-O3'-C3'	6.30	127.26	119.70
1	Х	834	А	C8-N9-C4	-6.30	103.28	105.80
1	Х	1652	G	C6-C5-N7	-6.30	126.62	130.40
1	Х	654	А	N1-C6-N6	-6.30	114.82	118.60
1	Х	1993	G	N1-C6-O6	6.30	123.68	119.90
1	Х	2546	G	N3-C4-N9	6.29	129.78	126.00
2	Y	83	С	N1-C2-O2	6.29	122.68	118.90
1	Х	1662	G	N3-C4-N9	6.29	129.78	126.00
1	Х	1475	U	P-O3'-C3'	6.29	127.24	119.70
1	Х	2817	А	C2-N3-C4	-6.28	107.46	110.60
1	X	492	G	O4'-C1'-N9	6.28	113.22	108.20
1	X	1287	A	OP1-P-O3'	6.26	118.98	105.20
1	X	$2\overline{560}$	G	C8-N9-C4	-6.26	103.89	106.40
1	X	2825	A	N1-C6-N6	6.26	122.36	118.60
1	X	1338	G	C8-N9-C4	-6.26	103.90	106.40
1	Х	686	С	N1-C2-O2	-6.25	115.15	118.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	2043	А	C6-C5-N7	-6.25	127.93	132.30
1	Х	2678	С	C2-N3-C4	-6.25	116.78	119.90
1	Х	525	А	C8-N9-C4	-6.24	103.30	105.80
1	Х	540	G	C4-N9-C1'	6.24	134.62	126.50
1	Х	2330	G	P-O3'-C3'	6.24	127.19	119.70
1	Х	2704	U	N3-C4-O4	6.24	123.77	119.40
1	Х	2316	G	C4-C5-N7	6.24	113.30	110.80
1	Х	2700	U	N3-C4-O4	6.23	123.76	119.40
1	Х	134	G	C8-N9-C1'	-6.23	118.90	127.00
1	Х	2322	U	P-O3'-C3'	6.23	127.18	119.70
1	Х	2823	G	C5-C6-O6	6.23	132.34	128.60
1	Х	563	U	C5-C6-N1	-6.23	119.59	122.70
1	Х	699	G	C6-C5-N7	-6.23	126.66	130.40
1	Х	456	С	O5'-P-OP2	-6.22	100.10	105.70
2	Y	84	G	C8-N9-C4	6.22	108.89	106.40
1	Х	1660	G	C4-C5-N7	-6.22	108.31	110.80
1	Х	14	А	C8-N9-C4	-6.21	103.31	105.80
1	Х	1775	А	O5'-P-OP1	-6.21	100.11	105.70
1	Х	849	G	N7-C8-N9	6.21	116.20	113.10
1	Х	2432	А	C8-N9-C4	-6.21	103.32	105.80
1	Х	765	С	N1-C2-O2	6.20	122.62	118.90
1	Х	2534	U	N3-C4-O4	6.20	123.74	119.40
2	Y	14	С	C5-C6-N1	6.20	124.10	121.00
1	Х	89	A	C8-N9-C4	-6.20	103.32	105.80
1	Х	1684	G	N1-C6-O6	6.20	123.62	119.90
2	Y	39	С	C6-N1-C1'	-6.20	113.36	120.80
1	Х	579	G	C4-C5-N7	-6.20	108.32	110.80
1	Х	542	А	C5-N7-C8	-6.19	100.81	103.90
1	Х	2795	A	P-O3'-C3'	6.18	127.12	119.70
1	Х	2597	G	N3-C4-C5	-6.18	125.51	128.60
1	Х	833	A	C5-N7-C8	-6.18	100.81	103.90
1	Х	2590	U	C2-N1-C1'	6.18	125.11	117.70
1	Х	686	С	C2-N1-C1'	-6.16	112.02	118.80
1	Х	1970	G	N3-C4-C5	-6.16	125.52	128.60
1	Х	2813	G	C8-N9-C4	6.16	108.86	106.40
1	X	2876	С	N1-C2-O2	-6.16	115.20	118.90
1	X	1278	A	O5'-P-OP2	-6.16	100.16	105.70
1	X	581	A	N1-C6-N6	-6.15	114.91	118.60
1	X	1356	G	C4-N9-C1'	6.15	134.49	126.50
1	X	522	G	N9-C4-C5	-6.15	102.94	105.40
1	X	2782	G	C4-C5-N7	6.15	113.26	110.80
1	Х	174	A	C6-N1-C2	-6.15	114.91	118.60

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	460	U	N1-C2-N3	6.14	118.58	114.90
1	Х	524	A	O5'-P-OP2	-6.14	100.17	105.70
1	Х	1278	А	C5-C6-N1	-6.14	114.63	117.70
1	Х	1326	U	C2-N1-C1'	6.14	125.06	117.70
1	Х	1288	А	C5-C6-N6	-6.13	118.79	123.70
1	Х	1304	U	C5-C6-N1	-6.13	119.63	122.70
1	Х	649	G	N1-C2-N2	6.13	121.71	116.20
5	С	127	ASP	CB-CG-OD1	6.13	123.81	118.30
1	Х	1919	А	C2-N3-C4	-6.12	107.54	110.60
1	Х	2473	G	N3-C4-C5	-6.12	125.54	128.60
1	Х	2480	С	N3-C4-C5	6.12	124.35	121.90
1	Х	2867	G	C2-N3-C4	-6.12	108.84	111.90
1	Х	1288	А	N7-C8-N9	6.12	116.86	113.80
1	Х	2554	С	C5-C6-N1	6.12	124.06	121.00
1	Х	689	А	C8-N9-C4	-6.11	103.36	105.80
1	Х	2705	А	P-O3'-C3'	6.11	127.04	119.70
1	Х	1163	С	C6-N1-C2	-6.11	117.86	120.30
1	Х	1712	G	N3-C4-C5	-6.11	125.55	128.60
1	Х	1970	G	C2-N3-C4	6.11	114.95	111.90
1	Х	2820	С	C6-N1-C2	6.11	122.74	120.30
1	Х	1304	U	C6-N1-C2	6.09	124.65	121.00
1	Х	1333	G	N7-C8-N9	6.09	116.14	113.10
1	Х	2230	G	N1-C6-O6	6.09	123.55	119.90
1	Х	2326	С	O5'-P-OP2	-6.09	100.22	105.70
1	Х	540	G	N3-C2-N2	6.08	124.16	119.90
1	Х	2057	U	C6-N1-C2	-6.08	117.35	121.00
1	Х	762	A	C4-C5-N7	6.08	113.74	110.70
1	Х	1203	A	N1-C6-N6	6.08	122.25	118.60
1	Х	2025	A	N9-C4-C5	-6.08	103.37	105.80
1	Х	2666	U	N3-C4-C5	-6.08	110.95	114.60
1	Х	2766	U	C5-C6-N1	-6.08	119.66	122.70
1	Х	2593	A	OP1-P-O3'	6.08	118.58	105.20
1	Х	1687	С	C4-C5-C6	6.07	120.44	117.40
1	Х	1939	U	N3-C2-O2	-6.07	117.95	122.20
1	Х	1692	С	C4-C5-C6	6.07	120.43	117.40
1	Х	2524	G	N3-C4-C5	-6.06	125.57	128.60
1	X	1690	U	N3-C4-C5	6.06	118.24	114.60
1	X	2441	U	N3-C2-O2	-6.05	117.96	122.20
1	X	1751	A	C5-C6-N1	6.05	120.72	117.70
1	Х	2685	A	N1-C6-N6	-6.04	114.97	118.60
1	Х	1009	C	C6-N1-C1'	-6.04	113.55	120.80
1	Х	1691	G	N9-C4-C5	-6.04	102.98	105.40



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	796	A	N7-C8-N9	6.04	116.82	113.80
1	Х	2627	G	C8-N9-C4	-6.04	103.98	106.40
16	0	38	LEU	CA-CB-CG	6.04	129.19	115.30
1	Х	2668	U	C5-C6-N1	-6.04	119.68	122.70
1	Х	2530	С	C4-C5-C6	6.03	120.42	117.40
1	Х	1037	U	N3-C2-O2	-6.03	117.98	122.20
1	Х	1749	G	O4'-C1'-N9	6.03	113.03	108.20
1	Х	2858	А	N3-C4-C5	-6.03	122.58	126.80
1	Х	957	G	C2-N3-C4	6.02	114.91	111.90
1	Х	2798	A	N1-C6-N6	6.02	122.21	118.60
1	Х	1032	A	C2-N3-C4	-6.02	107.59	110.60
1	Х	1683	G	C8-N9-C1'	6.02	134.82	127.00
1	Х	2559	U	C5-C4-O4	-6.02	122.29	125.90
1	Х	1669	A	N1-C6-N6	6.01	122.21	118.60
1	Х	2858	А	C2-N3-C4	6.01	113.61	110.60
1	Х	1338	G	N3-C4-C5	-6.01	125.59	128.60
1	Х	2484	G	C5-C6-O6	6.01	132.21	128.60
1	Х	2790	С	O5'-P-OP2	-6.00	100.30	105.70
1	Х	2850	U	O5'-P-OP1	-6.00	100.30	105.70
1	Х	2027	С	C2-N1-C1'	6.00	125.40	118.80
1	Х	2820	С	N3-C4-C5	6.00	124.30	121.90
1	Х	1342	U	C5-C4-O4	5.99	129.50	125.90
1	Х	1467	U	N1-C2-O2	5.99	127.00	122.80
1	Х	2045	A	C4-C5-C6	-5.99	114.00	117.00
2	Y	17	A	O4'-C1'-N9	5.99	112.99	108.20
1	Х	1020	A	C2-N3-C4	5.99	113.59	110.60
1	Х	2854	G	N1-C6-O6	5.99	123.49	119.90
1	Х	858	G	P-O3'-C3'	5.98	126.88	119.70
1	Х	1974	U	C6-N1-C2	-5.98	117.41	121.00
1	Х	518	А	C5-C6-N6	-5.98	118.91	123.70
1	Х	1338	G	C2-N3-C4	5.98	114.89	111.90
1	Х	2521	А	C2-N3-C4	5.98	113.59	110.60
1	Х	1288	A	C5'-C4'-C3'	5.98	125.56	116.00
1	Х	136	А	C8-N9-C4	-5.97	103.41	105.80
1	Х	1356	G	C8-N9-C1'	-5.97	119.24	127.00
1	Х	1757	С	N3-C4-C5	5.97	124.29	121.90
1	Х	2041	A	N1-C6-N6	5.97	122.18	118.60
1	Х	2570	С	C6-N1-C2	-5.96	117.92	120.30
1	Х	2682	С	C2-N1-C1'	5.96	125.36	118.80
1	Х	1337	G	C5-C6-N1	5.96	114.48	111.50
1	Х	1345	G	C6-C5-N7	-5.96	126.83	130.40
1	Х	1984	A	C8-N9-C4	5.96	108.18	105.80



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	596	С	N3-C4-C5	-5.95	119.52	121.90
1	Х	746	G	N1-C6-O6	5.95	123.47	119.90
1	Х	1707	А	O5'-P-OP1	-5.95	100.34	105.70
1	Х	1775	А	N7-C8-N9	-5.95	110.83	113.80
1	Х	2017	U	C6-N1-C2	-5.95	117.43	121.00
1	Х	2480	С	O4'-C1'-N1	5.95	112.96	108.20
1	Х	1765	С	N3-C2-O2	-5.95	117.74	121.90
1	Х	2523	G	C8-N9-C4	-5.95	104.02	106.40
1	Х	527	С	C2-N1-C1'	5.95	125.34	118.80
1	Х	974	U	N3-C4-O4	5.94	123.56	119.40
1	Х	958	G	C5-C6-N1	5.94	114.47	111.50
1	Х	1269	G	C4-C5-N7	5.94	113.17	110.80
1	Х	1469	U	N1-C2-N3	5.94	118.46	114.90
12	К	90	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	Х	1469	U	N3-C2-O2	-5.93	118.05	122.20
1	Х	2854	G	C8-N9-C4	-5.93	104.03	106.40
1	Х	683	А	O4'-C1'-N9	-5.93	103.45	108.20
1	Х	1468	А	C6-N1-C2	-5.93	115.04	118.60
1	Х	1661	С	N3-C4-C5	5.93	124.27	121.90
1	Х	1919	А	C4-C5-N7	5.93	113.67	110.70
1	Х	2855	С	C5-C6-N1	5.92	123.96	121.00
1	Х	559	С	C6-N1-C1'	-5.92	113.69	120.80
1	Х	1312	G	C2-N3-C4	-5.92	108.94	111.90
1	Х	1312	G	C6-C5-N7	-5.92	126.85	130.40
1	Х	1582	А	N1-C6-N6	-5.92	115.05	118.60
1	Х	1687	С	N1-C2-N3	5.92	123.34	119.20
1	Х	1790	G	P-O3'-C3'	5.92	126.80	119.70
1	Х	1667	А	C5-C6-N1	5.91	120.66	117.70
1	Х	2246	A	N1-C6-N6	-5.91	115.05	118.60
1	Х	2371	A	C5-N7-C8	-5.91	100.94	103.90
1	Х	2586	G	C6-C5-N7	-5.91	126.85	130.40
1	X	1562	G	N3-C4-N9	-5.91	122.46	126.00
1	X	2559	U	C2-N1-C1'	5.91	124.79	117.70
1	X	2698	G	N3-C4-N9	5.90	129.54	126.00
1	X	2524	G	C6-N1-C2	-5.90	121.56	125.10
1	Х	1282	А	C8-N9-C4	5.90	108.16	105.80
1	X	1987	G	C8-N9-C4	-5.89	104.04	106.40
1	X	2669	C	N3-C4-C5	-5.89	119.54	121.90
1	X	1009	C	N1-C2-O2	5.88	122.43	118.90
1	X	2017	U	O5'-P-OP1	-5.88	100.41	105.70
9	Н	57	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	Х	537	С	N3-C4-C5	5.87	124.25	121.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	136	A	O5'-P-OP1	-5.86	100.42	105.70
1	Х	969	U	OP2-P-O3'	5.86	118.10	105.20
1	Х	1684	G	N9-C4-C5	-5.85	103.06	105.40
1	Х	2691	С	C2-N3-C4	-5.85	116.97	119.90
1	Х	462	G	C5-C6-N1	-5.85	108.58	111.50
1	Х	850	С	C2-N1-C1'	5.85	125.23	118.80
1	Х	854	G	N3-C4-N9	-5.85	122.49	126.00
1	Х	2535	C	C6-N1-C2	5.85	122.64	120.30
1	Х	1009	С	C2-N1-C1'	5.85	125.23	118.80
1	Х	1626	A	C4-C5-N7	5.85	113.62	110.70
1	Х	2495	G	N3-C4-C5	-5.84	125.68	128.60
1	Х	26	G	N3-C4-C5	-5.84	125.68	128.60
1	Х	2045	A	C5-C6-N1	5.84	120.62	117.70
1	Х	655	A	C4-C5-C6	-5.84	114.08	117.00
1	Х	2688	G	O5'-P-OP1	5.84	117.70	110.70
1	Х	380	С	N1-C2-O2	5.83	122.40	118.90
1	Х	841	G	C4-C5-N7	5.82	113.13	110.80
1	Х	2434	G	N3-C4-C5	-5.82	125.69	128.60
1	Х	1713	G	N3-C4-C5	-5.82	125.69	128.60
1	Х	2222	U	N3-C2-O2	-5.82	118.13	122.20
1	Х	2325	A	N1-C6-N6	5.82	122.09	118.60
1	Х	2751	С	N3-C4-C5	5.81	124.23	121.90
1	Х	1981	A	N1-C6-N6	5.81	122.09	118.60
1	Х	522	G	C4-C5-N7	5.81	113.12	110.80
1	Х	1662	G	C5-C6-N1	5.81	114.41	111.50
1	Х	2409	A	C5-C6-N6	-5.81	119.05	123.70
1	Х	1037	U	C2-N1-C1'	5.81	124.67	117.70
1	Х	2858	A	N9-C4-C5	5.80	108.12	105.80
1	Х	2254	С	N1-C2-O2	-5.80	115.42	118.90
1	Х	2579	A	C8-N9-C4	5.80	108.12	105.80
1	Х	673	G	C8-N9-C4	5.80	108.72	106.40
1	X	2481	G	N7-C8-N9	5.80	116.00	113.10
1	Х	2858	A	N1-C6-N6	-5.80	115.12	118.60
1	Х	2867	G	N3-C4-C5	5.80	131.50	128.60
1	Х	1662	G	N3-C4-C5	-5.79	125.70	128.60
1	Х	2607	C	N1-C2-O2	5.79	122.38	118.90
1	Х	2677	U	C5-C4-O4	5.79	129.38	125.90
1	Х	2819	G	N3-C4-N9	5.79	129.48	126.00
1	Х	2868	G	C8-N9-C4	-5.79	104.08	106.40
1	Х	968	C	C5-C6-N1	5.79	123.89	121.00
1	Х	1279	G	N3-C2-N2	5.79	123.95	119.90
1	Х	2468	G	N1-C6-O6	-5.79	116.43	119.90

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	1270	С	N3-C4-C5	-5.79	119.59	121.90
1	Х	1283	С	N1-C2-O2	-5.79	115.43	118.90
1	Х	1712	G	C4-N9-C1'	5.79	134.02	126.50
1	Х	527	С	N1-C2-O2	5.78	122.37	118.90
1	Х	2421	С	C6-N1-C2	-5.78	117.99	120.30
1	Х	1766	U	C5-C4-O4	-5.78	122.43	125.90
1	Х	344	G	N7-C8-N9	5.78	115.99	113.10
1	Х	2487	G	N1-C6-O6	-5.77	116.44	119.90
1	Х	1724	С	C6-N1-C2	5.77	122.61	120.30
1	Х	1687	С	C2-N3-C4	-5.76	117.02	119.90
1	Х	1688	U	N3-C4-C5	-5.76	111.14	114.60
1	Х	2410	U	C5-C6-N1	5.76	125.58	122.70
1	Х	1541	G	N1-C6-O6	-5.76	116.44	119.90
1	Х	2432	А	N7-C8-N9	5.76	116.68	113.80
1	Х	2593	А	N7-C8-N9	5.76	116.68	113.80
1	Х	2876	С	N1-C2-N3	5.76	123.23	119.20
1	Х	617	U	N3-C2-O2	-5.75	118.17	122.20
1	Х	833	А	N9-C4-C5	-5.75	103.50	105.80
1	Х	746	G	C6-C5-N7	-5.75	126.95	130.40
1	Х	2243	С	C2-N1-C1'	5.75	125.12	118.80
1	Х	1810	U	P-O3'-C3'	5.74	126.59	119.70
1	Х	460	U	C6-N1-C2	-5.73	117.56	121.00
1	Х	746	G	N3-C4-N9	5.73	129.44	126.00
1	Х	170	U	C5-C4-O4	5.72	129.34	125.90
1	Х	1675	С	O5'-P-OP2	5.72	117.56	110.70
1	Х	2432	А	C6-N1-C2	5.72	122.03	118.60
1	Х	2492	G	O5'-P-OP2	-5.72	100.55	105.70
1	Х	438	G	C4-C5-N7	5.72	113.09	110.80
1	Х	1777	А	O5'-P-OP2	-5.72	100.55	105.70
1	Х	2032	G	C5-C6-N1	5.72	114.36	111.50
1	Х	2482	А	OP1-P-OP2	-5.72	111.03	119.60
1	Х	2604	G	C4-C5-N7	-5.72	108.51	110.80
1	Х	955	G	C8-N9-C1'	-5.71	119.57	127.00
1	Х	1666	G	C8-N9-C4	5.71	108.69	106.40
1	Х	1988	А	N7-C8-N9	-5.71	110.94	113.80
1	Х	1286	U	N3-C2-O2	-5.70	118.21	122.20
1	Х	2625	U	C5-C4-O4	-5.70	122.48	125.90
1	Х	2868	G	N9-C4-C5	5.70	107.68	105.40
1	Х	1679	U	C2-N3-C4	-5.70	123.58	127.00
1	X	219	G	P-O3'-C3'	5.70	126.54	119.70
1	X	1647	U	N1-C2-N3	5.70	118.32	114.90
1	Х	957	G	N3-C4-C5	-5.70	125.75	128.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	1688	U	N3-C4-O4	5.70	123.39	119.40
1	Х	2664	G	OP1-P-O3'	5.70	117.73	105.20
1	Х	2559	U	N1-C2-N3	-5.69	111.48	114.90
1	Х	484	G	N7-C8-N9	5.69	115.95	113.10
1	Х	940	G	C4-N9-C1'	-5.69	119.10	126.50
1	Х	2468	G	OP2-P-O3'	5.69	117.72	105.20
1	Х	2846	G	O4'-C1'-N9	5.69	112.75	108.20
1	Х	1919	А	C5-N7-C8	-5.69	101.06	103.90
1	Х	2530	С	C6-N1-C2	-5.69	118.03	120.30
1	Х	1345	G	C4-C5-N7	5.68	113.07	110.80
1	Х	1630	A	O5'-P-OP1	5.68	117.52	110.70
1	Х	1819	U	N3-C4-C5	-5.68	111.19	114.60
1	Х	2228	U	N3-C4-O4	5.68	123.38	119.40
1	Х	822	G	N9-C4-C5	5.68	107.67	105.40
1	Х	1212	U	O5'-P-OP2	-5.68	100.59	105.70
1	Х	2586	G	N3-C4-N9	5.67	129.40	126.00
1	Х	1652	G	N1-C6-O6	5.67	123.30	119.90
1	Х	1757	С	C2-N3-C4	-5.67	117.06	119.90
1	Х	2423	G	C5-C6-N1	5.67	114.33	111.50
1	Х	2687	G	C8-N9-C4	5.67	108.67	106.40
1	Х	501	G	C2-N3-C4	-5.67	109.07	111.90
1	Х	686	С	O5'-P-OP1	-5.67	100.60	105.70
1	Х	2757	G	C8-N9-C4	5.66	108.67	106.40
1	Х	1312	G	N1-C6-O6	5.66	123.30	119.90
1	Х	1683	G	C5-C6-O6	5.66	131.99	128.60
1	Х	1340	С	N1-C2-O2	-5.65	115.51	118.90
1	Х	2434	G	C4-N9-C1'	5.65	133.85	126.50
1	Х	2251	U	N3-C4-C5	5.65	117.99	114.60
1	Х	2410	U	C6-N1-C2	-5.65	117.61	121.00
1	Х	112	U	C2-N1-C1'	5.65	124.48	117.70
1	Х	2818	G	O5'-P-OP2	-5.65	100.62	105.70
1	Х	2580	С	N1-C2-N3	5.64	123.15	119.20
1	Х	2559	U	C6-N1-C1'	-5.64	113.30	121.20
1	Х	957	G	C5-C6-N1	5.64	114.32	111.50
1	Х	1269	G	C6-C5-N7	-5.64	127.02	130.40
1	Х	1340	С	OP1-P-OP2	-5.64	111.14	119.60
1	Х	2274	С	C6-N1-C1'	-5.63	114.04	120.80
1	Х	2827	G	N3-C2-N2	5.63	123.84	119.90
1	Х	484	G	C6-C5-N7	-5.63	127.02	130.40
1	Х	957	G	C4-C5-N7	-5.63	108.55	110.80
1	Х	803	С	C2-N1-C1'	5.63	124.99	118.80
1	Х	2554	С	O5'-P-OP1	-5.63	100.64	105.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	1702	С	C6-N1-C2	5.63	122.55	120.30
1	Х	1933	G	C2-N3-C4	5.63	114.71	111.90
1	Х	1667	А	C4-C5-N7	5.62	113.51	110.70
1	Х	2766	U	C6-N1-C2	5.62	124.37	121.00
1	Х	1982	С	C2-N3-C4	-5.62	117.09	119.90
1	Х	2580	С	N3-C4-C5	-5.62	119.65	121.90
1	Х	2423	G	N1-C6-O6	-5.61	116.53	119.90
1	Х	995	А	O5'-P-OP2	-5.61	100.65	105.70
1	Х	2747	С	C6-N1-C2	5.61	122.55	120.30
1	Х	2843	А	C2-N3-C4	5.61	113.41	110.60
1	Х	2052	G	C4-N9-C1'	5.61	133.79	126.50
1	Х	173	А	N1-C2-N3	5.61	132.10	129.30
1	Х	1679	U	C6-N1-C2	5.61	124.36	121.00
1	Х	527	С	C5-C6-N1	5.60	123.80	121.00
1	Х	1277	G	C8-N9-C4	5.60	108.64	106.40
1	Х	1699	А	C5-C6-N1	-5.60	114.90	117.70
1	Х	2867	G	C6-C5-N7	-5.60	127.04	130.40
1	Х	1336	G	N9-C4-C5	-5.60	103.16	105.40
1	Х	2408	G	N7-C8-N9	5.60	115.90	113.10
1	Х	519	С	C5-C6-N1	5.59	123.80	121.00
1	Х	2544	А	N1-C2-N3	-5.59	126.50	129.30
1	Х	2796	А	C5-C6-N1	5.59	120.50	117.70
1	Х	1963	G	N3-C4-C5	-5.59	125.81	128.60
1	Х	124	А	C8-N9-C4	-5.59	103.56	105.80
1	Х	2426	G	C4-C5-N7	5.59	113.03	110.80
1	Х	2479	U	O4'-C1'-N1	5.59	112.67	108.20
1	Х	1277	G	N1-C6-O6	-5.58	116.55	119.90
1	Х	2432	А	N1-C2-N3	-5.58	126.51	129.30
1	Х	2700	U	N3-C4-C5	-5.57	111.26	114.60
1	Х	50	G	C4-N9-C1'	5.57	133.74	126.50
1	Х	2022	С	C6-N1-C2	-5.57	118.07	120.30
1	X	1287	A	N1-C6-N6	-5.57	115.26	118.60
1	Х	2338	С	C6-N1-C2	-5.57	118.07	120.30
1	Х	266	U	C5-C6-N1	5.57	125.48	122.70
1	X	438	G	N9-C4-C5	-5.56	103.17	105.40
1	X	1624	A	05'-P-OP2	-5.56	100.70	105.70
17	Р	96	TYR	CB-CG-CD2	-5.56	117.66	121.00
1	X	2819	G	C5-C6-O6	-5.56	125.27	128.60
1	X	2865	G	N1-C6-O6	-5.56	116.57	119.90
1	X	2242	C	O5'-P-OP1	-5.56	100.70	105.70
1	X	236	C	C6-N1-C2	-5.55	118.08	120.30
1	Х	787	A	N1-C6-N6	5.55	121.93	118.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	774	А	C6-C5-N7	5.55	136.19	132.30
1	Х	859	U	N1-C2-O2	-5.55	118.91	122.80
1	Х	521	U	N1-C2-O2	-5.55	118.92	122.80
1	Х	787	A	C2-N3-C4	-5.55	107.83	110.60
1	Х	1142	G	N7-C8-N9	-5.55	110.33	113.10
1	Х	2597	G	C4-N9-C1'	5.54	133.71	126.50
1	Х	2256	G	N7-C8-N9	5.54	115.87	113.10
1	Х	2489	С	N3-C4-C5	-5.54	119.68	121.90
1	Х	1326	U	O4'-C1'-N1	5.54	112.63	108.20
1	Х	859	U	P-O3'-C3'	5.54	126.35	119.70
1	Х	1670	G	C6-N1-C2	-5.54	121.78	125.10
1	Х	2692	А	N1-C6-N6	5.54	121.92	118.60
1	Х	928	G	N3-C4-N9	5.54	129.32	126.00
1	Х	2492	G	C8-N9-C4	-5.53	104.19	106.40
1	Х	1985	G	N7-C8-N9	5.53	115.87	113.10
1	Х	2551	A	N7-C8-N9	-5.53	111.03	113.80
1	Х	2782	G	N9-C4-C5	-5.52	103.19	105.40
1	Х	2033	С	C6-N1-C2	-5.52	118.09	120.30
1	Х	796	A	C5-N7-C8	-5.51	101.14	103.90
1	Х	940	G	C8-N9-C1'	5.51	134.17	127.00
1	Х	540	G	P-O3'-C3'	5.51	126.31	119.70
1	Х	762	А	N1-C2-N3	-5.51	126.55	129.30
1	Х	2616	U	N3-C2-O2	5.51	126.06	122.20
1	Х	30	G	N7-C8-N9	5.51	115.85	113.10
1	Х	803	С	C5-C6-N1	5.51	123.75	121.00
1	Х	803	С	N3-C2-O2	-5.50	118.05	121.90
1	Х	739	G	N1-C2-N3	5.50	127.20	123.90
2	Y	2	С	C5-C6-N1	5.50	123.75	121.00
1	Х	525	А	C5-C6-N1	5.50	120.45	117.70
1	Х	2553	G	C8-N9-C4	-5.50	104.20	106.40
1	Х	661	С	N3-C2-O2	-5.50	118.05	121.90
2	Y	4	С	C5-C6-N1	5.50	123.75	121.00
1	Х	2665	G	C4-C5-N7	5.50	113.00	110.80
1	Х	1981	А	OP1-P-OP2	5.50	127.85	119.60
1	Х	968	С	C6-N1-C1'	-5.49	114.21	120.80
1	Х	2821	G	OP1-P-O3'	5.49	117.29	105.20
1	Х	344	G	C4-N9-C1'	5.49	133.63	126.50
1	Х	463	С	O5'-P-OP1	-5.49	100.76	105.70
1	Х	1932	G	O5'-P-OP2	5.49	117.28	110.70
1	Х	2542	U	C5-C4-O4	5.49	129.19	125.90
1	Х	2314	A	N9-C4-C5	5.49	107.99	105.80
1	Х	2822	U	N3-C4-O4	5.49	123.24	119.40



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	1666	G	OP1-P-OP2	-5.48	111.38	119.60
1	Х	541	С	O5'-P-OP2	-5.48	100.77	105.70
1	Х	686	С	C5-C6-N1	-5.48	118.26	121.00
1	Х	2478	С	N3-C4-C5	-5.47	119.71	121.90
1	Х	757	U	OP2-P-O3'	5.47	117.24	105.20
1	Х	1001	А	C8-N9-C4	-5.47	103.61	105.80
1	Х	2710	С	N1-C2-O2	5.47	122.18	118.90
1	Х	1991	С	C5-C6-N1	-5.47	118.27	121.00
1	Х	2626	U	N3-C4-C5	5.47	117.88	114.60
1	Х	2655	С	C6-N1-C2	5.47	122.49	120.30
1	Х	525	А	N1-C6-N6	-5.47	115.32	118.60
1	Х	2598	С	C5-C6-N1	-5.46	118.27	121.00
1	Х	2371	А	N1-C6-N6	5.46	121.88	118.60
1	Х	1729	С	C6-N1-C2	-5.46	118.12	120.30
1	Х	1984	А	O5'-P-OP1	5.46	117.25	110.70
1	Х	2032	G	C5-N7-C8	5.46	107.03	104.30
1	Х	1223	G	N7-C8-N9	5.45	115.83	113.10
1	Х	1283	С	C5-C6-N1	-5.45	118.27	121.00
1	Х	2792	С	C5-C6-N1	-5.45	118.27	121.00
1	Х	469	G	OP1-P-O3'	5.45	117.19	105.20
1	Х	958	G	C2-N3-C4	5.45	114.63	111.90
1	Х	1478	U	N3-C2-O2	-5.45	118.39	122.20
1	Х	939	С	C5-C6-N1	5.45	123.72	121.00
1	Х	1767	G	C5-C6-N1	5.44	114.22	111.50
1	Х	2052	G	N3-C4-N9	5.44	129.26	126.00
1	Х	2659	С	C6-N1-C2	-5.44	118.12	120.30
1	Х	2057	U	N3-C4-O4	5.44	123.21	119.40
1	Х	522	G	C8-N9-C1'	-5.44	119.93	127.00
15	N	50	ARG	CG-CD-NE	5.44	123.22	111.80
1	Х	456	С	C6-N1-C1'	5.43	127.32	120.80
1	Х	1284	G	N1-C2-N2	-5.43	111.31	116.20
1	Х	1141	U	C5-C6-N1	-5.43	119.98	122.70
1	Х	682	G	C2-N3-C4	5.43	114.61	111.90
1	Х	2402	U	P-O3'-C3'	5.43	126.21	119.70
1	Х	2681	A	N1-C6-N6	5.42	121.85	118.60
2	Y	67	C	C6-N1-C2	-5.42	118.13	120.30
1	X	555	U	C5-C6-N1	-5.42	119.99	122.70
1	X	$242\overline{2}$	C	$C2-N1-\overline{C1'}$	$5.4\overline{2}$	124.77	118.80
1	X	$24\overline{91}$	C	C2-N1-C1'	5.42	124.77	118.80
1	X	18	U	N3-C2-O2	-5.42	118.41	122.20
1	X	975	C	N1-C2-O2	-5.42	115.65	118.90
1	X	1344	C	N3-C4-C5	5.42	124.07	121.90

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	438	G	C5-C6-O6	-5.42	125.35	128.60
1	Х	850	С	C6-N1-C2	-5.42	118.13	120.30
1	Х	2034	А	C5-C6-N6	-5.42	119.37	123.70
1	Х	2676	G	C8-N9-C4	5.42	108.57	106.40
1	Х	2586	G	N3-C4-C5	-5.41	125.89	128.60
1	Х	573	С	C6-N1-C2	5.41	122.46	120.30
1	Х	868	U	C6-N1-C2	-5.41	117.75	121.00
1	Х	1283	С	N1-C2-N3	5.41	122.99	119.20
1	Х	2034	А	C5-C6-N1	5.41	120.40	117.70
1	Х	1931	G	C8-N9-C4	-5.40	104.24	106.40
1	Х	381	С	C2-N1-C1'	5.40	124.74	118.80
1	Х	2245	А	N1-C6-N6	-5.40	115.36	118.60
1	Х	2856	U	C5-C6-N1	5.39	125.40	122.70
1	Х	1333	G	C5-N7-C8	-5.39	101.60	104.30
1	Х	796	А	C8-N9-C4	-5.39	103.64	105.80
1	Х	1253	С	C4-C5-C6	5.39	120.09	117.40
1	Х	2239	С	C6-N1-C2	-5.39	118.15	120.30
1	Х	1757	С	C5-C6-N1	-5.38	118.31	121.00
1	Х	2495	G	C2-N3-C4	5.38	114.59	111.90
1	Х	757	U	N1-C2-N3	5.38	118.13	114.90
14	М	28	ARG	C-N-CD	-5.38	108.77	120.60
1	Х	2669	С	C4-C5-C6	5.38	120.09	117.40
1	Х	485	G	N3-C4-C5	-5.37	125.91	128.60
1	Х	1825	С	C2-N1-C1'	5.37	124.71	118.80
2	Y	14	С	P-O3'-C3'	5.37	126.14	119.70
1	Х	2045	А	C6-C5-N7	5.37	136.06	132.30
1	Х	1990	U	N3-C2-O2	-5.37	118.44	122.20
1	Х	656	U	N3-C2-O2	5.36	125.95	122.20
1	Х	2602	G	C8-N9-C4	-5.36	104.25	106.40
1	Х	754	G	N7-C8-N9	5.36	115.78	113.10
1	Х	994	A	C6-N1-C2	-5.36	115.38	118.60
1	X	1316	G	N3-C4-C5	-5.36	125.92	128.60
1	Х	2039	G	C4-C5-N7	5.36	112.94	110.80
1	Х	754	G	N1-C2-N3	5.36	127.11	123.90
1	X	1810	U	<u>OP2-P-O3</u> '	5.36	116.98	105.20
1	X	508	G	C4-C5-N7	5.35	112.94	110.80
1	Х	2699	G	C4-C5-N7	-5.35	108.66	110.80
1	X	2796	A	C6-N1-C2	-5.35	115.39	118.60
1	X	594	G	N1-C6-O6	-5.35	116.69	119.90
1	Х	1279	G	OP1-P-O3'	5.35	116.97	105.20
1	X	2534	U	C2-N1-C1'	5.35	124.12	117.70
1	Х	859	U	C2-N1-C1'	-5.35	111.28	117.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	2043	A	C5-N7-C8	-5.35	101.23	103.90
1	Х	2652	G	C8-N9-C4	-5.35	104.26	106.40
1	Х	804	С	C5-C6-N1	-5.34	118.33	121.00
1	Х	2316	G	C5-C6-O6	-5.34	125.39	128.60
1	Х	485	G	C8-N9-C4	-5.34	104.26	106.40
1	Х	2540	А	C2-N3-C4	5.34	113.27	110.60
1	Х	2843	A	C5-C6-N1	5.34	120.37	117.70
1	Х	788	G	C5-C6-N1	5.34	114.17	111.50
1	Х	242	A	C8-N9-C4	-5.33	103.67	105.80
1	Х	540	G	C8-N9-C1'	-5.33	120.07	127.00
1	Х	228	A	N1-C6-N6	-5.33	115.40	118.60
1	Х	1473	U	N3-C4-C5	-5.33	111.40	114.60
2	Y	14	С	OP2-P-O3'	5.33	116.92	105.20
1	Х	1258	G	C8-N9-C4	-5.33	104.27	106.40
1	Х	2540	А	OP1-P-OP2	5.32	127.58	119.60
1	Х	242	А	C2-N3-C4	5.32	113.26	110.60
1	Х	685	U	N1-C2-O2	-5.32	119.08	122.80
1	Х	1009	С	N3-C2-O2	-5.32	118.18	121.90
1	Х	16	G	C8-N9-C4	5.32	108.53	106.40
1	Х	2593	А	C8-N9-C4	-5.32	103.67	105.80
1	Х	1683	G	C4-N9-C1'	-5.31	119.59	126.50
1	Х	689	А	C4-C5-N7	5.31	113.36	110.70
1	Х	974	U	OP1-P-OP2	-5.31	111.64	119.60
1	Х	2690	A	P-O3'-C3'	5.31	126.07	119.70
1	Х	2317	G	O5'-P-OP1	-5.30	100.93	105.70
1	Х	2409	A	C4-C5-N7	5.30	113.35	110.70
1	Х	2660	С	C4-C5-C6	5.30	120.05	117.40
1	Х	747	A	N1-C6-N6	5.30	121.78	118.60
1	Х	100	G	P-O3'-C3'	5.29	126.05	119.70
1	X	583	C	C2-N3-C4	5.29	122.55	119.90
1	X	975	C	N1-C2-N3	5.29	122.90	119.20
1	X	759	C	P-O3'-C3'	5.29	126.04	119.70
1	X	2587	G	C6-C5-N7	-5.29	127.23	130.40
1	X	1690	U	O4'-C1'-N1	5.29	112.43	108.20
1	Х	501	G	C5-C6-O6	5.28	131.77	128.60
1	X	173	A	$C2-N\overline{3-C4}$	-5.28	107.96	110.60
1	X	518	A	P-O3'-C3'	5.28	126.04	119.70
1	X	1702	C	C5-C6-N1	-5.28	118.36	121.00
1	X	2492	G	N1-C6-O6	-5.28	116.73	119.90
1	X	848	A	C2-N3-C4	5.28	113.24	110.60
1	X	26	G	N7-C8-N9	5.28	115.74	113.10
1	X	$13\overline{4}$	G	C2-N3-C4	5.28	114.54	111.90



Mol	Chain	Res	Type	Atoms Z Obs		$Observed(^{o})$	$Ideal(^{o})$
1	Х	924	С	C2-N1-C1'	5.28	124.60	118.80
1	Х	2528	G	OP1-P-O3'	5.28	116.81	105.20
1	Х	2596	С	O5'-P-OP1	-5.28	100.95	105.70
1	Х	2652	G	N7-C8-N9	5.28	115.74	113.10
1	Х	2598	С	N3-C4-C5	5.27	124.01	121.90
1	Х	2687	G	C6-N1-C2	-5.27	121.94	125.10
1	Х	1662	G	N1-C6-O6	-5.27	116.74	119.90
1	Х	2399	С	C6-N1-C2	5.27	122.41	120.30
11	J	93	TYR	CA-CB-CG	5.27	123.42	113.40
1	Х	582	G	OP2-P-O3'	5.27	116.79	105.20
2	Y	26	G	C8-N9-C4	-5.27	104.29	106.40
1	Х	739	G	C6-N1-C2	-5.26	121.94	125.10
1	Х	699	G	N3-C4-N9	-5.26	122.84	126.00
1	Х	985	G	C5-N7-C8	-5.26	101.67	104.30
1	Х	2338	С	C5-C6-N1	5.26	123.63	121.00
1	Х	2433	G	C6-C5-N7	5.26	133.56	130.40
1	Х	1820	G	C8-N9-C4	-5.26	104.30	106.40
1	Х	1990	U	N3-C4-C5	-5.25	111.45	114.60
1	Х	482	A	C8-N9-C4	-5.25	103.70	105.80
1	Х	557	U	N1-C2-O2	-5.25	119.12	122.80
1	Х	2316	G	N3-C4-N9	5.25	129.15	126.00
1	Х	2809	А	C2-N3-C4	5.25	113.23	110.60
1	Х	2022	С	N3-C4-C5	-5.25	119.80	121.90
1	Х	2694	G	N7-C8-N9	5.25	115.73	113.10
1	Х	2041	А	C4-C5-N7	5.25	113.33	110.70
17	Р	36	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	Х	698	А	C2-N3-C4	5.24	113.22	110.60
1	Х	2557	G	OP1-P-O3'	5.24	116.72	105.20
1	Х	2712	G	C8-N9-C4	5.24	108.49	106.40
1	Х	14	A	N7-C8-N9	5.23	116.42	113.80
1	Х	1656	U	O5'-P-OP1	-5.23	101.00	105.70
1	Х	2256	G	O5'-P-OP2	5.23	116.97	110.70
1	Х	2330	G	OP2-P-O3'	5.23	116.70	105.20
1	Х	2492	G	OP1-P-O3'	5.22	116.69	105.20
1	Х	2017	U	C5-C6-N1	5.22	125.31	122.70
1	X	2033	С	C2-N1-C1'	5.22	124.55	118.80
1	Х	574	С	C5-C6-N1	5.22	123.61	121.00
12	K	10	LEU	CA-CB-CG	-5.22	103.29	115.30
1	X	2039	G	C5-C6-N1	5.22	114.11	111.50
1	X	1819	U	N3-C2-O2	-5.22	118.55	122.20
1	X	1890	G	N3-C4-N9	5.22	129.13	126.00
1	X	1660	G	N1-C6-O6	-5.21	116.77	119.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	609	U	C6-N1-C2	5.21	124.13	121.00
1	Х	984	A	N1-C6-N6	5.21	121.73	118.60
1	Х	1217	U	C5-C6-N1	-5.21	120.09	122.70
1	Х	1990	U	C6-N1-C2	-5.21	117.87	121.00
1	Х	2040	А	N1-C6-N6	5.21	121.73	118.60
1	Х	2531	U	N3-C2-O2	-5.21	118.55	122.20
1	Х	501	G	C4-C5-N7	-5.21	108.72	110.80
1	Х	655	А	C4-N9-C1'	-5.21	116.92	126.30
1	Х	519	С	O5'-P-OP2	-5.21	101.01	105.70
1	Х	2409	А	N1-C6-N6	5.21	121.72	118.60
1	Х	2553	G	O5'-P-OP2	-5.21	101.01	105.70
1	Х	2692	А	C5-N7-C8	-5.21	101.30	103.90
1	Х	2686	С	C2-N1-C1'	5.21	124.53	118.80
1	Х	2851	G	C6-C5-N7	-5.21	127.28	130.40
1	Х	1264	С	N1-C2-O2	5.20	122.02	118.90
1	Х	1333	G	C6-N1-C2	5.20	128.22	125.10
1	Х	2876	С	C2-N1-C1'	-5.20	113.08	118.80
1	Х	766	А	C8-N9-C4	5.19	107.88	105.80
1	Х	2551	A	C8-N9-C4	5.19	107.88	105.80
1	Х	2665	G	N9-C4-C5	-5.19	103.32	105.40
1	Х	690	А	C8-N9-C4	5.19	107.88	105.80
1	Х	2046	С	C4-C5-C6	5.19	120.00	117.40
1	Х	2481	G	C8-N9-C4	-5.19	104.32	106.40
1	Х	2666	U	C6-N1-C2	-5.19	117.89	121.00
1	Х	2868	G	C4-C5-N7	-5.19	108.72	110.80
1	Х	565	A	C2-N3-C4	-5.19	108.01	110.60
1	Х	2046	С	N3-C4-C5	-5.19	119.83	121.90
1	Х	2473	G	N3-C4-N9	5.19	129.11	126.00
1	Х	506	G	OP2-P-O3'	5.18	116.61	105.20
1	Х	1626	А	C5-N7-C8	-5.18	101.31	103.90
1	Х	1683	G	N1-C2-N2	5.18	120.87	116.20
1	Х	2033	С	O5'-P-OP2	-5.18	101.03	105.70
1	Х	753	U	O5'-P-OP2	5.18	116.92	110.70
1	Х	89	А	N7-C8-N9	5.18	116.39	113.80
1	Х	822	G	C2-N3-C4	5.18	114.49	111.90
1	Х	1241	G	N3-C4-C5	-5.18	126.01	128.60
1	Х	1682	A	C6-N1-C2	-5.18	115.49	118.60
1	Х	1712	G	C8-N9-C1'	-5.18	120.27	127.00
1	Х	2041	A	N9-C4-C5	-5.18	103.73	105.80
1	Х	1652	G	C5-C6-O6	-5.18	125.49	128.60
1	Х	2692	A	C5-C6-N6	-5.18	119.56	123.70
18	Q	91	LEU	CA-CB-CG	5.17	127.20	115.30



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	1299	А	N9-C4-C5	N9-C4-C5 5.17		105.80
1	Х	559	С	N1-C2-O2	5.17	122.00	118.90
1	Х	2433	G	N1-C6-O6	-5.17	116.80	119.90
1	Х	2624	G	C2-N3-C4	-5.17	109.31	111.90
1	Х	2827	G	C8-N9-C1'	-5.17	120.28	127.00
1	Х	1339	U	OP2-P-O3'	5.16	116.56	105.20
3	А	215	LEU	CA-CB-CG	-5.16	103.43	115.30
1	Х	1139	А	N1-C6-N6	5.16	121.70	118.60
1	Х	448	С	N1-C2-O2	5.16	122.00	118.90
1	Х	1765	С	C6-N1-C2	5.16	122.36	120.30
1	Х	1933	G	C5-C6-N1	5.16	114.08	111.50
1	Х	2045	А	C4-N9-C1'	-5.16	117.02	126.30
1	Х	594	G	C5-C6-O6	5.15	131.69	128.60
1	Х	1696	С	N1-C2-N3	5.15	122.81	119.20
1	Х	1279	G	C8-N9-C4	5.15	108.46	106.40
1	Х	1663	С	C6-N1-C1'	-5.15	114.62	120.80
1	Х	2817	А	C5-N7-C8	-5.15	101.33	103.90
17	Р	105	ARG	NE-CZ-NH1	-5.15	117.73	120.30
1	Х	2000	U	N1-C2-O2	-5.15	119.20	122.80
1	Х	528	G	C8-N9-C4	-5.14	104.34	106.40
10	Ι	77	LEU	CA-CB-CG	5.14	127.13	115.30
1	Х	1668	G	N3-C2-N2	-5.14	116.30	119.90
1	Х	2662	С	N3-C4-C5	-5.14	119.84	121.90
1	Х	1013	G	N1-C6-O6	-5.14	116.82	119.90
1	Х	2691	С	C5-C6-N1	-5.14	118.43	121.00
1	Х	1990	U	C4-C5-C6	5.14	122.78	119.70
1	Х	2228	U	N3-C4-C5	-5.14	111.52	114.60
1	Х	501	G	N1-C2-N3	5.13	126.98	123.90
1	Х	24	G	O5'-P-OP1	-5.13	101.08	105.70
1	Х	988	G	O5'-P-OP1	-5.13	101.08	105.70
1	Х	1443	G	C4-C5-N7	5.13	112.85	110.80
1	Х	1918	G	N1-C6-O6	-5.13	116.82	119.90
1	Х	923	A	N1-C6-N6	5.13	121.68	118.60
1	Х	460	U	N3-C2-O2	-5.13	118.61	122.20
1	Х	2409	A	C5-N7-C8	-5.13	101.34	103.90
25	Z	56	GLN	CG-CD-OE1	5.13	131.86	121.60
1	Х	1223	G	C4-N9-C1'	5.13	133.17	126.50
1	Х	2298	U	N1-C2-O2	5.13	126.39	122.80
1	Х	2474	G	C2-N3-C4	5.13	114.46	111.90
1	Х	2521	A	N9-C4-C5	5.13	107.85	105.80
1	Х	2820	С	C5-C6-N1	-5.12	118.44	121.00
1	Х	2369	U	C5-C6-N1	5.12	125.26	122.70

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	2600	А	C5-C6-N1	5.12	120.26	117.70
17	Р	96	TYR	CA-CB-CG	5.11	123.11	113.40
1	Х	1764	А	C8-N9-C4	-5.11	103.76	105.80
1	Х	1625	A	N1-C6-N6	5.11	121.67	118.60
1	Х	2487	G	C4-C5-C6	-5.11	115.73	118.80
1	Х	2044	G	OP1-P-O3'	5.11	116.44	105.20
1	Х	2474	G	C5-C6-N1	5.11	114.05	111.50
4	В	58	LYS	CD-CE-NZ	5.11	123.44	111.70
1	Х	25	U	C5-C6-N1	5.10	125.25	122.70
1	Х	1292	А	C8-N9-C4	5.10	107.84	105.80
1	Х	2482	А	C2-N3-C4	5.10	113.15	110.60
1	Х	2658	А	O5'-P-OP2	-5.10	101.11	105.70
1	Х	2825	А	C5-C6-N6	-5.10	119.62	123.70
1	Х	1032	А	N1-C2-N3	5.10	131.85	129.30
1	Х	2300	G	C8-N9-C4	-5.10	104.36	106.40
1	Х	393	U	C6-N1-C2	-5.09	117.94	121.00
1	Х	1466	С	C2-N1-C1'	5.09	124.41	118.80
1	Х	2408	G	C2-N3-C4	5.09	114.45	111.90
1	Х	1666	G	C5-N7-C8	5.09	106.85	104.30
1	Х	1683	G	N1-C6-O6	-5.09	116.84	119.90
1	Х	1770	U	C2-N1-C1'	-5.09	111.59	117.70
1	Х	2750	G	N3-C4-C5	-5.09	126.06	128.60
1	Х	2847	G	P-O3'-C3'	5.09	125.81	119.70
1	Х	1023	U	P-O3'-C3'	5.09	125.81	119.70
1	Х	2587	G	C4-C5-N7	5.09	112.83	110.80
1	Х	1681	A	C5-C6-N1	-5.09	115.16	117.70
1	Х	2564	U	N3-C4-O4	5.08	122.96	119.40
1	Х	2003	А	C2-N3-C4	5.08	113.14	110.60
1	Х	2265	A	O4'-C1'-N9	5.08	112.27	108.20
1	Х	2484	G	N3-C2-N2	5.08	123.46	119.90
1	X	1912	G	C8-N9-C4	-5.08	104.37	106.40
1	X	2323	U	C5-C6-N1	5.08	125.24	122.70
1	X	580	A	C5-C6-N6	-5.08	119.64	123.70
1	Х	1253	С	N3-C4-C5	-5.08	119.87	121.90
1	X	545	С	C2-N1-C1'	-5.08	113.22	118.80
1	X	508	G	C5-C6-O6	-5.07	125.56	128.60
1	X	1291	G	C8-N9-C4	5.07	108.43	106.40
1	X	1471	G	C5-C6-N1	5.07	114.04	111.50
1	X	1285	A	C5-C6-N1	-5.07	115.16	117.70
1	X	805	G	04'-C1'-N9	-5.07	104.14	108.20
12	K	22	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	Х	756	C	N3-C4-C5	-5.07	119.87	121.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	977	G	N7-C8-N9	-5.07	110.56	113.10
1	Х	2033	С	OP1-P-O3'	5.07	116.35	105.20
1	Х	2698	G	C4-N9-C1'	5.07	133.09	126.50
1	Х	538	A	C8-N9-C4	-5.07	103.77	105.80
1	Х	1775	А	C8-N9-C4	5.07	107.83	105.80
1	Х	2402	U	N3-C2-O2	-5.07	118.65	122.20
1	Х	1646	G	C2-N3-C4	-5.07	109.37	111.90
1	Х	1692	С	OP1-P-O3'	5.07	116.34	105.20
1	Х	1882	G	C2-N3-C4	-5.07	109.37	111.90
1	Х	2559	U	C5-C6-N1	5.07	125.23	122.70
1	Х	660	G	N9-C4-C5	5.06	107.42	105.40
1	Х	2487	G	C2-N3-C4	5.06	114.43	111.90
1	Х	863	С	C6-N1-C2	-5.06	118.28	120.30
1	Х	574	С	C6-N1-C2	-5.06	118.28	120.30
1	Х	757	U	C4-C5-C6	5.06	122.73	119.70
1	Х	2468	G	C5-C6-N1	5.06	114.03	111.50
1	Х	175	С	N3-C4-N4	5.06	121.54	118.00
1	Х	822	G	N1-C6-O6	-5.06	116.86	119.90
1	Х	957	G	C5-N7-C8	5.05	106.83	104.30
1	Х	1333	G	N3-C2-N2	-5.05	116.36	119.90
1	Х	1336	G	N3-C2-N2	5.05	123.44	119.90
1	Х	2229	G	O5'-P-OP2	-5.05	101.15	105.70
2	Y	4	С	N1-C2-O2	5.05	121.93	118.90
1	Х	1973	С	N3-C2-O2	-5.05	118.36	121.90
1	Х	2232	G	C5-C6-O6	-5.05	125.57	128.60
1	Х	2670	С	N3-C4-C5	-5.05	119.88	121.90
1	Х	2044	G	C4-C5-N7	-5.05	108.78	110.80
1	Х	2553	G	N7-C8-N9	5.05	115.62	113.10
1	Х	456	С	C2-N1-C1'	-5.04	113.25	118.80
1	Х	1623	С	N1-C2-O2	5.04	121.93	118.90
1	Х	2235	G	C5-C6-O6	-5.04	125.57	128.60
1	Х	1953	А	C8-N9-C4	-5.04	103.78	105.80
1	Х	2795	A	C8-N9-C4	5.04	107.82	105.80
1	Х	1978	U	C5-C6-N1	5.04	125.22	122.70
1	Х	1761	G	N3-C4-C5	-5.04	126.08	128.60
1	Х	2438	A	N1-C2-N3	5.04	131.82	129.30
1	Х	595	A	OP2-P-O3'	5.04	116.28	105.20
1	Х	875	G	C8-N9-C4	-5.04	104.39	106.40
1	Х	972	С	C6-N1-C2	-5.04	118.28	120.30
1	Х	2325	A	C5-C6-N6	-5.04	119.67	123.70
1	Х	2604	G	N9-C4-C5	5.04	107.42	105.40
1	Х	2489	С	C4-C5-C6	5.03	119.92	117.40



Mol	Chain	Res	Type	Atoms Z		$Observed(^{o})$	$Ideal(^{o})$
1	Х	2843	А	OP2-P-O3'	5.03	116.27	105.20
1	Х	457	С	O5'-P-OP2	-5.03	101.17	105.70
1	Х	1474	А	N9-C4-C5	5.03	107.81	105.80
1	Х	522	G	C5-C6-O6	-5.03	125.58	128.60
1	Х	2555	G	N3-C4-C5	5.03	131.12	128.60
1	Х	2609	G	C8-N9-C4	-5.03	104.39	106.40
1	Х	2792	С	C6-N1-C2	5.03	122.31	120.30
1	Х	2475	С	C6-N1-C2	-5.03	118.29	120.30
1	Х	1660	G	C5-N7-C8	5.02	106.81	104.30
1	Х	2430	А	N1-C2-N3	5.02	131.81	129.30
1	Х	2482	А	N3-C4-C5	-5.02	123.28	126.80
1	Х	1770	U	C5-C4-O4	5.02	128.91	125.90
1	Х	2235	G	N9-C4-C5	-5.02	103.39	105.40
1	Х	265	U	C5-C6-N1	5.01	125.20	122.70
1	Х	2327	U	C5-C6-N1	5.01	125.20	122.70
1	Х	924	С	N3-C2-O2	-5.01	118.39	121.90
1	Х	344	G	N3-C4-C5	-5.01	126.10	128.60
1	Х	1622	G	C8-N9-C4	5.01	108.40	106.40
1	Х	2868	G	N3-C4-C5	-5.01	126.10	128.60
1	Х	136	A	C4-N9-C1'	5.00	135.31	126.30
1	Х	9	U	N3-C2-O2	-5.00	118.70	122.20
1	Х	1306	U	N1-C2-O2	-5.00	119.30	122.80
1	Х	2847	G	O4'-C1'-N9	-5.00	104.20	108.20

There are no chirality outliers.

\mathbf{Mol}	Chain	\mathbf{Res}	Type	Group
28	3	14	ILE	Peptide
28	3	16	ILE	Peptide
28	3	26	LYS	Peptide
28	3	34	THR	Peptide
3	А	210	GLY	Peptide
3	А	271	VAL	Peptide
4	В	132	LYS	Peptide
4	В	146	THR	Peptide
5	С	49	ALA	Peptide
5	С	55	GLY	Peptide
8	G	115	ALA	Peptide
8	G	36	ASN	Peptide
8	G	95	LEU	Peptide
10	Ι	20	GLY	Peptide



Mol	Chain	\mathbf{Res}	Type	Group
10	Ι	38	LYS	Peptide
10	Ι	40	ARG	Peptide
10	Ι	57	ILE	Peptide
11	J	12	LYS	Peptide
11	J	26	ASP	Peptide
11	J	28	VAL	Peptide
11	J	71	PRO	Peptide
11	J	81	GLU	Peptide
11	J	91	VAL	Peptide
12	K	8	ARG	Peptide
14	М	28	ARG	Peptide
16	0	13	ARG	Peptide
17	Р	132	GLY	Peptide
17	Р	45	ILE	Peptide
19	R	60	PRO	Peptide
19	R	81	VAL	Peptide
19	R	86	PRO	Peptide
20	S	32	PHE	Peptide
21	Т	68	VAL	Peptide
22	U	47	HIS	Peptide
25	Ζ	52	TYR	Peptide
25	Ζ	53	ASP	Peptide

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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	Х	57935	0	29196	1261	0
2	Y	2598	0	1328	75	0
3	А	2011	0	2012	124	0
4	В	1544	0	1605	86	0
5	С	1479	0	1488	111	0
6	D	1375	0	1433	67	0
7	Е	1286	0	1336	58	0
8	G	1110	0	1133	80	0
9	Н	997	0	1046	68	0
10	Ι	982	0	973	62	0
11	J	1062	0	1067	56	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	К	893	0	944	39	0
13	L	761	0	776	47	0
14	М	923	0	942	56	0
15	Ν	955	0	974	57	0
16	0	736	0	735	42	0
17	Р	1014	0	1085	48	0
18	Q	705	0	717	38	0
19	R	771	0	740	50	0
20	S	1288	0	1237	63	0
21	Т	537	0	537	21	0
22	U	519	0	501	35	0
23	V	438	0	456	13	0
24	W	424	0	470	17	0
25	Ζ	448	0	448	32	0
26	1	314	0	249	16	0
27	2	383	0	414	19	0
28	3	459	0	486	55	0
29	Х	50	0	0	0	0
30	2	2	0	0	0	0
30	3	1	0	0	0	0
30	А	3	0	0	0	0
30	В	1	0	0	0	0
30	Ι	2	0	0	0	0
30	J	1	0	0	0	0
30	Κ	1	0	0	0	0
30	М	1	0	0	0	0
30	Ν	3	0	0	0	0
30	Х	335	0	0	0	0
30	Y	17	0	0	0	0
31	Х	80	0	124	18	0
32	X	32	0	55	2	0
33	X	1	0	0	0	0
34	X	3	0	6	0	0
35	X	5	0	0	0	0
36	X	1	0	0	0	0
All	All	84486	0	54513	2385	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 17.

All (2385) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom 2	Interatomic	Clash
	Atom-2	distance (Å)	overlap (Å)
4:B:143:GLN:HB2	4:B:147:PRO:HG3	1.30	1.10
1:X:243:G:H2'	1:X:244:C:H5'	1.32	1.07
18:Q:89:GLU:HB2	18:Q:91:LEU:HD22	1.38	1.06
15:N:66:ASN:HB3	15:N:76:TYR:HB2	1.38	1.05
1:X:566:U:O3'	8:G:140:GLN:NE2	1.88	1.04
21:T:68:VAL:HG12	21:T:80:SER:H	1.23	1.04
1:X:1277:G:OP1	25:Z:19:ARG:NH2	1.94	1.00
1:X:1673:C:H5"	4:B:136:ARG:HB3	1.43	0.99
3:A:28:ARG:HE	3:A:29:PRO:HD2	1.29	0.97
8:G:35:LYS:HD3	8:G:37:ASP:H	1.29	0.97
1:X:1201:G:OP1	16:O:82:ARG:NH1	1.99	0.95
3:A:252:LYS:HD2	3:A:253:PRO:HD3	1.45	0.95
9:H:125:LYS:HD3	9:H:125:LYS:H	1.30	0.93
2:Y:32:C:H1'	2:Y:59:A:H61	1.33	0.92
28:3:16:ILE:HG21	28:3:63:PRO:HB3	1.46	0.92
5:C:56:ARG:HG2	5:C:57:LYS:H	1.33	0.92
1:X:699:G:H1	27:2:12:ARG:HD2	1.33	0.91
8:G:55:ALA:HB1	8:G:134:MET:HE1	1.53	0.90
1:X:545:C:H1'	15:N:53:LYS:HE3	1.52	0.89
1:X:386:U:HO2'	1:X:387:A:H8	0.95	0.89
3:A:69:ARG:HD2	3:A:130:ALA:HB2	1.55	0.89
28:3:5:LYS:HE2	28:3:62:LEU:HB3	1.50	0.88
1:X:70:A:H4'	1:X:71:A:H5"	1.54	0.88
1:X:1979:C:OP1	9:H:43:ARG:NH1	2.07	0.88
9:H:56:LYS:HD3	9:H:57:ASP:HB2	1.56	0.88
10:I:55:ARG:H	10:I:55:ARG:CZ	1.87	0.88
18:Q:10:PRO:HA	18:Q:27:PHE:HB3	1.56	0.87
5:C:6:VAL:HG12	5:C:118:VAL:HG21	1.54	0.87
3:A:244:ARG:O	3:A:252:LYS:NZ	2.08	0.86
17:P:25:PHE:HB2	17:P:127:ILE:HG12	1.57	0.86
5:C:148:VAL:HG12	5:C:185:ARG:HB2	1.57	0.86
1:X:689:A:H8	1:X:2052:G:H21	1.24	0.86
1:X:938:G:H4'	1:X:939:C:H5"	1.56	0.86
17:P:58:ARG:HH21	25:Z:39:LYS:HD3	1.40	0.86
4:B:132:LYS:HG2	4:B:133:LYS:H	1.39	0.85
11:J:74:PRO:HB3	11:J:91:VAL:HG11	1.59	0.85
9:H:99:ILE:HD12	9:H:103:GLY:HA2	1.59	0.84
14:M:2:GLN:HG2	14:M:3:THR:H	1.41	0.84
1:X:1542:G:H22	1:X:1562:G:H1	1.24	0.84
1:X:1173:G:H4'	16:O:22:VAL:HG22	1.58	0.84
1:X:1466:C:H2'	1:X:1467:U:H1'	1.57	0.84
10:I:83:LEU:HD21	10:I:99:VAL:HG11	1.59	0.84



A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
25:Z:51:TYR:HE1	25:Z:55:ARG:HG2	1.42	0.84
1:X:967:G:O6	11:J:17:ARG:NH1	2.10	0.83
10:I:101:ARG:H	10:I:118:VAL:HG22	1.43	0.83
5:C:6:VAL:HG13	5:C:7:ILE:H	1.43	0.83
20:S:6:LYS:HB3	20:S:31:SER:HB2	1.60	0.83
1:X:1882:G:H21	1:X:1885:C:H41	1.27	0.83
9:H:75:VAL:HG12	9:H:118:LEU:HD21	1.58	0.83
14:M:82:PRO:HG2	14:M:85:SER:HB2	1.59	0.83
5:C:127:ASP:OD1	5:C:128:ALA:N	2.12	0.83
1:X:1745:C:OP1	14:M:101:ARG:NH2	2.11	0.82
1:X:2281:C:H42	1:X:2293:G:H1	1.27	0.82
1:X:1919:A:H2	1:X:1926:U:H3	1.24	0.82
1:X:492:G:HO2'	1:X:517:A:N6	1.77	0.82
28:3:61:MET:N	28:3:61:MET:SD	2.52	0.82
1:X:1919:A:N6	1:X:1946:U:H3	1.76	0.82
5:C:176:ASN:HB3	5:C:179:ASP:HB2	1.61	0.82
1:X:304:A:N6	1:X:356:A:N7	2.28	0.81
9:H:105:PRO:HG3	9:H:126:ILE:HG12	1.61	0.81
1:X:243:G:H2'	1:X:244:C:C5'	2.09	0.81
20:S:11:LYS:HG2	20:S:12:GLN:H	1.45	0.81
1:X:652:C:H42	1:X:657:A:H61	1.26	0.81
3:A:63:ARG:O	3:A:88:ARG:NH2	2.13	0.81
10:I:103:ASN:HD21	10:I:121:HIS:HB2	1.44	0.81
1:X:841:G:H2'	1:X:842:A:C8	2.16	0.81
3:A:145:LEU:HB3	3:A:155:LEU:HB2	1.62	0.81
6:D:101:GLU:O	6:D:105:ASN:HB2	1.80	0.81
7:E:88:GLU:HG2	7:E:130:ARG:HG2	1.61	0.81
18:Q:60:GLY:HA3	18:Q:73:ASN:H	1.46	0.80
12:K:52:ILE:HD11	12:K:94:TYR:CG	2.16	0.80
7:E:97:LYS:HG3	7:E:98:LEU:H	1.46	0.80
10:I:73:GLU:OE2	10:I:81:GLN:NE2	2.15	0.80
1:X:1009:C:OP1	15:N:84:LYS:NZ	2.15	0.80
1:X:1006:C:O2	8:G:31:THR:OG1	1.99	0.79
24:W:25:LEU:HD22	24:W:30:ASP:HB3	1.64	0.79
20:S:7:PRO:HB3	20:S:11:LYS:HD2	1.65	0.79
1:X:476:G:H4'	27:2:16:HIS:HD2	1.48	0.79
3:A:76:ASN:OD1	3:A:118:ASN:ND2	2.16	0.79
1:X:1846:A:H62	1:X:1871:G:H8	1.31	0.79
1:X:1377:G:N7	22:U:6:TYR:N	2.31	0.78
1:X:244:C:N3	1:X:438:G:N1	2.31	0.78
1:X:244:C:N4	1:X:438:G:O6	2.15	0.78



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:X:2078:G:N2	1:X:2178:U:O2	2.17	0.78
1:X:2040:A:H2'	1:X:2041:A:C8	2.19	0.78
1:X:2271:C:OP2	13:L:18:ARG:NH2	2.15	0.78
5:C:118:VAL:HG22	5:C:120:VAL:H	1.49	0.78
7:E:165:VAL:HG23	7:E:166:GLY:H	1.48	0.78
19:R:22:VAL:HG11	19:R:80:LYS:HD3	1.65	0.78
1:X:1058:G:H2'	1:X:1121:G:H1	1.48	0.77
21:T:73:GLY:HA3	21:T:76:ALA:HB3	1.66	0.77
1:X:2418:A:H4'	1:X:2419:C:H5"	1.66	0.77
12:K:56:LYS:NZ	12:K:87:TYR:O	2.16	0.77
14:M:41:GLU:HG3	14:M:46:ARG:HE	1.48	0.77
17:P:36:ARG:CZ	25:Z:20:ARG:HH12	1.97	0.77
1:X:793:G:H21	1:X:796:A:H62	1.30	0.77
1:X:1468:A:H5"	1:X:1468:A:H8	1.47	0.77
1:X:1947:G:O2'	1:X:1950:C:OP2	2.02	0.77
16:O:66:GLY:O	16:O:87:ARG:NH1	2.16	0.77
1:X:1270:C:H4'	5:C:77:PHE:CE1	2.20	0.77
1:X:2318:U:H4'	2:Y:43:G:H22	1.49	0.77
1:X:1850:G:O2'	1:X:1866:G:N2	2.18	0.77
19:R:15:HIS:CD2	19:R:82:ALA:HB2	2.19	0.76
3:A:252:LYS:HD2	3:A:253:PRO:CD	2.15	0.76
9:H:90:ARG:NH1	14:M:78:GLU:OE1	2.18	0.76
3:A:72:LYS:NZ	3:A:99:ASP:OD2	2.18	0.76
4:B:60:ASN:HB3	4:B:62:PRO:HD2	1.67	0.76
14:M:90:GLN:HG2	14:M:91:VAL:H	1.50	0.76
21:T:23:VAL:HA	21:T:38:VAL:HG23	1.66	0.76
7:E:127:GLU:HG2	7:E:129:THR:H	1.50	0.76
1:X:699:G:H1	27:2:12:ARG:CD	1.98	0.76
17:P:103:LEU:HB3	17:P:105:ARG:HH12	1.50	0.76
1:X:2737:A:H2'	1:X:2738:A:H5"	1.66	0.76
22:U:14:VAL:HG12	22:U:15:VAL:H	1.51	0.76
4:B:31:CYS:HB3	4:B:49:ILE:HG12	1.67	0.76
5:C:34:GLN:OE1	5:C:176:ASN:ND2	2.17	0.76
9:H:85:ASP:OD1	9:H:87:SER:N	2.15	0.76
11:J:27:TYR:OH	11:J:136:GLU:N	2.19	0.76
12:K:92:GLY:HA2	12:K:94:TYR:CZ	2.19	0.76
1:X:1079:G:H22	1:X:1106:A:H2'	1.51	0.76
2:Y:107:C:O2'	20:S:25:ASN:O	2.04	0.76
1:X:817:A:OP2	10:I:40:ARG:NH2	2.18	0.75
1:X:1745:C:P	14:M:101:ARG:HH22	2.08	0.75
1:X:2291:U:OP2	6:D:71:LYS:NZ	2.19	0.75



	A + 0	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
4:B:91:VAL:HG12	4:B:93:VAL:H	1.51	0.75
1:X:544:U:H2'	1:X:545:C:C6	2.21	0.75
11:J:15:ARG:HD3	11:J:73:LYS:HG3	1.69	0.75
1:X:492:G:O2'	1:X:517:A:N6	2.18	0.75
2:Y:14:C:H5"	21:T:72:LYS:HG2	1.69	0.75
1:X:537:C:C5	1:X:2759:U:H2'	2.22	0.75
1:X:1278:A:H2	1:X:1997:A:H62	1.32	0.75
2:Y:12:C:O2	2:Y:113:G:N2	2.13	0.75
3:A:4:LYS:HB2	3:A:18:THR:HG23	1.68	0.75
16:O:50:ASP:O	16:O:53:LYS:NZ	2.19	0.75
28:3:5:LYS:HD2	28:3:5:LYS:N	2.02	0.75
7:E:8:PRO:O	7:E:69:ARG:NH1	2.20	0.75
21:T:68:VAL:HG12	21:T:80:SER:N	1.99	0.75
1:X:2191:A:H5"	1:X:2192:U:H5	1.51	0.74
1:X:2266:A:N6	1:X:2323:U:H3	1.84	0.74
1:X:2399:C:N4	28:3:31:HIS:O	2.20	0.74
9:H:116:ARG:H	9:H:134:LEU:HD21	1.52	0.74
1:X:476:G:H4'	27:2:16:HIS:CD2	2.21	0.74
9:H:2:ILE:HB	9:H:45:ALA:HB3	1.69	0.74
1:X:265:U:HO2'	1:X:266:U:H6	1.35	0.74
1:X:1687:C:H42	1:X:1691:G:H5'	1.52	0.74
1:X:243:G:H3'	1:X:243:G:N3	2.03	0.74
1:X:2563:U:H2'	1:X:2564:U:H2'	1.70	0.74
8:G:75:ILE:HD12	8:G:147:ARG:HE	1.52	0.74
9:H:47:VAL:HA	9:H:74:VAL:HG23	1.70	0.73
1:X:2292:C:O4'	6:D:37:ASN:ND2	2.21	0.73
19:R:15:HIS:HD2	19:R:82:ALA:HB2	1.53	0.73
1:X:649:G:H22	1:X:660:G:N2	1.87	0.73
1:X:2225:G:H2'	1:X:2226:A:H8	1.51	0.73
2:Y:45:C:O2	6:D:92:ARG:NH2	2.22	0.73
2:Y:67:C:H2'	2:Y:111:C:H41	1.54	0.73
9:H:134:LEU:HD12	14:M:38:LYS:HE3	1.71	0.73
1:X:654:A:H2'	1:X:655:A:H5'	1.70	0.73
1:X:1468:A:H5"	1:X:1468:A:C8	2.23	0.73
20:S:27:GLU:HG3	20:S:28:ASN:H	1.53	0.73
1:X:309:G:N2	1:X:352:G:O6	2.22	0.73
1:X:1105:U:H2'	1:X:1106:A:H5"	1.69	0.73
1:X:1816:G:OP1	3:A:52:ARG:HD3	1.88	0.73
1:X:2533:U:H2'	1:X:2534:U:C6	2.23	0.73
17:P:58:ARG:NH2	25:Z:39:LYS:HD3	2.03	0.73
24:W:36:ASP:OD1	24:W:41:ARG:NH1	2.22	0.73



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:X:1475:U:O2'	1:X:1476:G:OP1	2.07	0.72
9:H:85:ASP:OD1	9:H:86:GLY:N	2.22	0.72
18:Q:11:VAL:HG23	18:Q:27:PHE:HA	1.70	0.72
28:3:36:LYS:HG2	28:3:37:SER:H	1.54	0.72
8:G:116:ARG:HG3	8:G:118:ALA:H	1.53	0.72
15:N:42:ALA:O	15:N:46:GLU:HG3	1.89	0.72
1:X:2191:A:OP1	1:X:2193:C:N4	2.22	0.72
1:X:1270:C:H4'	5:C:77:PHE:CD1	2.24	0.72
3:A:6:TYR:CD2	3:A:13:ARG:HD2	2.24	0.72
1:X:320:A:N3	1:X:340:G:O2'	2.21	0.72
1:X:1670:G:H5'	12:K:2:ARG:HD2	1.72	0.72
1:X:2015:G:H21	4:B:146:THR:HB	1.52	0.72
1:X:2594:U:H2'	1:X:2595:C:C6	2.24	0.72
4:B:132:LYS:HA	4:B:134:TRP:CD1	2.25	0.72
5:C:2:ALA:H	5:C:14:THR:HB	1.54	0.72
5:C:72:ARG:HA	5:C:77:PHE:CE2	2.25	0.72
1:X:2318:U:H4'	2:Y:43:G:N2	2.05	0.72
3:A:34:THR:O	3:A:36:ALA:N	2.22	0.72
4:B:7:THR:HG21	14:M:5:ILE:HD11	1.70	0.72
6:D:4:LEU:HD11	6:D:97:TYR:HB3	1.72	0.72
1:X:259:U:O2'	1:X:260:U:OP2	2.07	0.71
5:C:2:ALA:HB2	5:C:14:THR:HG22	1.71	0.71
1:X:661:C:H2'	1:X:662:G:C8	2.25	0.71
1:X:2314:A:O2'	1:X:2316:G:N7	2.23	0.71
1:X:318:G:H21	1:X:341:A:H62	1.35	0.71
1:X:640:C:H4'	1:X:660:G:H21	1.56	0.71
1:X:826:U:H2'	1:X:827:C:C6	2.25	0.71
1:X:1399:C:OP2	1:X:1409:U:N3	2.21	0.71
5:C:56:ARG:CG	5:C:57:LYS:H	2.03	0.71
4:B:128:SER:OG	4:B:129:HIS:N	2.22	0.71
8:G:146:THR:O	8:G:149:LYS:NZ	2.23	0.71
1:X:1981:A:OP2	4:B:136:ARG:NH1	2.24	0.71
1:X:2085:G:N2	1:X:2171:U:O2'	2.24	0.70
1:X:2279:G:H2'	1:X:2280:A:H8	1.55	0.70
1:X:1693:A:C2	1:X:1976:U:H5'	2.26	0.70
5:C:45:THR:HG21	5:C:85:GLY:HA3	1.73	0.70
7:E:23:VAL:HG13	7:E:36:PRO:HA	1.72	0.70
25:Z:36:CYS:HB2	25:Z:49:CYS:SG	2.31	0.70
1:X:244:C:O2'	1:X:245:C:O4'	2.06	0.70
22:U:21:ARG:HE	22:U:23:LYS:HE3	1.57	0.70
1:X:1995:G:H4'	17:P:117:ILE:HD11	1.74	0.70



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	$distance ({ m \AA})$	overlap (Å)
1:X:957:G:H2'	1:X:958:G:H8	1.58	0.69
1:X:1673:C:C5'	4:B:136:ARG:HB3	2.20	0.69
1:X:567:G:P	8:G:140:GLN:HE21	2.15	0.69
1:X:652:C:O2'	1:X:2329:C:OP1	2.09	0.69
1:X:1437:A:H2'	1:X:1438:G:H8	1.56	0.69
11:J:20:GLY:O	11:J:99:LYS:HG3	1.91	0.69
6:D:19:GLN:HG3	6:D:20:PHE:H	1.56	0.69
15:N:5:LYS:HG3	15:N:7:GLY:H	1.55	0.69
1:X:168:A:H2'	1:X:169:C:C6	2.27	0.69
1:X:1662:G:H5"	1:X:1663:C:H5'	1.74	0.69
7:E:18:ASN:HB3	7:E:25:LYS:HB3	1.74	0.69
8:G:70:PHE:O	15:N:64:ARG:NH1	2.26	0.69
19:R:72:ARG:NH1	19:R:73:GLU:O	2.25	0.69
5:C:137:ALA:HB1	5:C:142:LEU:HB2	1.75	0.69
6:D:117:ILE:HG13	6:D:118:ASN:H	1.55	0.69
18:Q:64:ARG:HD3	18:Q:67:ARG:HA	1.75	0.69
6:D:43:SER:OG	6:D:150:ARG:NH2	2.25	0.69
11:J:43:ILE:HD12	11:J:98:VAL:HG21	1.75	0.69
21:T:38:VAL:HG12	21:T:59:LEU:HG	1.75	0.69
22:U:10:LYS:HG2	22:U:12:ASN:HB3	1.74	0.69
23:V:14:PHE:HD2	23:V:57:LYS:HD3	1.57	0.69
28:3:8:LYS:O	28:3:12:ARG:HD3	1.92	0.69
1:X:1467:U:O2'	1:X:1468:A:OP1	2.11	0.69
1:X:1836:C:H5'	3:A:254:THR:HG22	1.72	0.69
1:X:38:G:H1	1:X:453:U:H3	1.39	0.69
1:X:1448:A:H61	1:X:1574:A:H61	1.40	0.69
8:G:44:VAL:HG11	8:G:54:LEU:HD11	1.74	0.69
8:G:104:THR:HG22	8:G:109:GLY:HA3	1.74	0.69
1:X:1418:C:H2'	1:X:1419:G:H8	1.54	0.68
8:G:110:LEU:O	8:G:112:THR:N	2.26	0.68
9:H:81:ILE:HD11	9:H:117:GLU:HG3	1.75	0.68
1:X:358:C:H2'	1:X:359:G:H5'	1.76	0.68
1:X:2843:A:H5'	1:X:2844:G:OP2	1.94	0.68
5:C:54:THR:OG1	5:C:73:SER:HB3	1.92	0.68
5:C:57:LYS:HD2	5:C:58:MET:H	1.58	0.68
22:U:21:ARG:HE	22:U:23:LYS:CE	2.06	0.68
1:X:2040:A:H2'	1:X:2041:A:H8	1.56	0.68
8:G:35:LYS:HD3	8:G:37:ASP:N	2.07	0.68
1:X:405:C:H2'	1:X:406:G:H8	1.58	0.68
1:X:2393:G:H21	10:I:59:ARG:HH11	1.42	0.68
17:P:103:LEU:HB3	17:P:105:ARG:NH1	2.09	0.68



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
22:U:9:GLY:O	22:U:11:LYS:N	2.26	0.68
1:X:2672:U:H2'	1:X:2673:G:H8	1.58	0.68
8:G:68:PRO:HB2	8:G:70:PHE:CE1	2.29	0.68
15:N:49:ASP:O	15:N:53:LYS:HG2	1.93	0.68
1:X:171:G:H2'	1:X:172:A:O4'	1.94	0.68
1:X:1418:C:H2'	1:X:1419:G:C8	2.28	0.68
1:X:2437:G:O2'	1:X:2439:U:O4	2.10	0.68
3:A:17:THR:HB	3:A:205:VAL:H	1.59	0.68
7:E:172:LYS:HG2	7:E:173:ALA:H	1.59	0.68
1:X:814:G:O4'	5:C:48:ARG:NH2	2.26	0.68
1:X:2691:C:O2'	1:X:2692:A:OP2	2.10	0.68
3:A:134:ARG:HB2	3:A:187:SER:HB2	1.76	0.68
7:E:154:PRO:HA	7:E:160:LYS:O	1.93	0.68
8:G:95:LEU:O	8:G:97:ASP:N	2.27	0.68
1:X:318:G:N1	1:X:321:A:OP2	2.26	0.68
1:X:797:A:C5	3:A:229:VAL:HG21	2.29	0.68
1:X:1856:U:OP1	1:X:2389:G:O2'	2.10	0.67
13:L:36:LYS:HG2	13:L:64:LYS:HB2	1.76	0.67
1:X:618:A:H2'	1:X:619:A:C8	2.28	0.67
1:X:1024:G:H2'	1:X:1025:A:H8	1.58	0.67
1:X:2287:G:O2'	1:X:2289:A:OP2	2.11	0.67
4:B:132:LYS:HG2	4:B:133:LYS:N	2.03	0.67
10:I:54:SER:HB3	10:I:55:ARG:NH1	2.09	0.67
11:J:15:ARG:HE	11:J:73:LYS:NZ	1.91	0.67
1:X:1468:A:C8	1:X:1468:A:OP2	2.48	0.67
19:R:77:HIS:O	19:R:79:SER:N	2.24	0.67
1:X:2237:C:O2'	1:X:2406:C:OP2	2.13	0.67
19:R:52:ASN:OD1	19:R:73:GLU:HA	1.95	0.67
1:X:1005:U:H3'	15:N:54:LYS:HE3	1.76	0.67
18:Q:38:ILE:O	18:Q:42:ILE:HG12	1.95	0.67
18:Q:88:ILE:HD12	18:Q:90:ALA:H	1.59	0.67
1:X:2708:U:H2'	1:X:2709:C:C6	2.29	0.67
15:N:7:GLY:O	15:N:8:ILE:HG12	1.95	0.67
15:N:10:ARG:HG2	15:N:14:HIS:CD2	2.30	0.67
1:X:2594:U:H2'	1:X:2595:C:H6	1.60	0.67
1:X:38:G:H2'	1:X:39:C:C6	2.30	0.67
1:X:649:G:H22	1:X:660:G:H22	1.42	0.67
1:X:2579:A:N7	3:A:237:GLU:HG3	2.10	0.67
11:J:92:GLU:O	11:J:93:TYR:HD1	1.78	0.67
17:P:87:GLU:HA	17:P:90:LEU:HG	1.77	0.67
20:S:17:SER:OG	20:S:35:ASP:OD1	2.10	0.67



		Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
3:A:251:GLY:H	3:A:255:LYS:NZ	1.92	0.67
5:C:58:MET:HE1	5:C:69:HIS:HB3	1.77	0.67
10:I:56:LEU:HB3	28:3:12:ARG:HG2	1.75	0.67
3:A:245:VAL:HA	3:A:252:LYS:HZ1	1.60	0.66
11:J:106:GLU:N	11:J:106:GLU:OE1	2.28	0.66
19:R:52:ASN:HB3	19:R:72:ARG:O	1.94	0.66
1:X:651:C:H2'	1:X:652:C:H6	1.60	0.66
11:J:100:PRO:HB2	20:S:74:ARG:HG2	1.77	0.66
1:X:2616:U:H5"	4:B:82:ARG:NH1	2.10	0.66
1:X:1428:G:N2	1:X:1602:G:H5'	2.11	0.66
11:J:31:GLY:HA2	11:J:108:ALA:HB2	1.76	0.66
1:X:1793:A:H2'	1:X:1794:A:C8	2.31	0.66
1:X:2186:G:H2'	1:X:2187:A:C8	2.30	0.66
10:I:54:SER:HB3	10:I:55:ARG:HH12	1.61	0.66
18:Q:88:ILE:HD12	18:Q:90:ALA:N	2.10	0.66
1:X:2043:A:H1'	1:X:2481:G:H1'	1.76	0.66
1:X:2173:G:H2'	1:X:2174:G:H8	1.60	0.66
15:N:20:ARG:NH2	16:O:72:ARG:HH11	1.92	0.66
19:R:15:HIS:HE1	19:R:78:ALA:HB1	1.60	0.66
21:T:67:VAL:HG22	21:T:68:VAL:HG13	1.76	0.66
1:X:627:A:H2'	1:X:628:A:C8	2.30	0.66
14:M:32:THR:O	14:M:51:GLU:HA	1.94	0.66
1:X:649:G:H1	1:X:660:G:H1	1.43	0.66
1:X:1791:C:OP2	3:A:183:ARG:NH1	2.29	0.66
1:X:650:U:H2'	1:X:651:C:C6	2.30	0.66
1:X:2729:A:OP1	7:E:6:LYS:NZ	2.27	0.66
1:X:339:U:H3	1:X:343:A:H2	1.44	0.65
1:X:1225:G:H1'	1:X:1250:A:N6	2.11	0.65
3:A:36:ALA:HA	3:A:61:LEU:HD22	1.77	0.65
3:A:252:LYS:NZ	3:A:253:PRO:HD3	2.12	0.65
15:N:83:LEU:HD12	15:N:113:SER:HB2	1.78	0.65
2:Y:94:G:H5"	20:S:74:ARG:HH22	1.60	0.65
5:C:4:ILE:H	5:C:4:ILE:HD12	1.60	0.65
1:X:513:A:OP2	17:P:19:LYS:NZ	2.26	0.65
1:X:627:A:H2'	1:X:628:A:H8	1.61	0.65
1:X:812:G:H3'	1:X:813:A:H2'	1.78	0.65
1:X:1081:A:N7	1:X:1107:A:O2'	2.21	0.65
1:X:1310:C:H2'	1:X:1311:C:H6	1.60	0.65
19:R:12:ASP:OD1	19:R:42:ARG:HG2	1.95	0.65
1:X:2189:A:H3'	1:X:2190:A:H5"	1.78	0.65
5:C:2:ALA:N	5:C:14:THR:HB	2.12	0.65



A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	$distance ({ m \AA})$	overlap (Å)
5:C:3:GLN:NE2	5:C:116:LYS:O	2.29	0.65
20:S:3:LEU:HD11	20:S:34:LEU:HA	1.78	0.65
1:X:693:A:H2'	1:X:694:G:C8	2.31	0.65
8:G:79:PHE:CE1	8:G:147:ARG:HG2	2.31	0.65
1:X:249:A:H1'	1:X:381:C:H1'	1.78	0.65
1:X:1225:G:H1'	1:X:1250:A:H61	1.61	0.65
1:X:1816:G:H2'	1:X:1817:U:H6	1.62	0.65
5:C:144:GLY:HA3	5:C:166:TRP:CE2	2.31	0.65
11:J:15:ARG:HE	11:J:73:LYS:HZ1	1.43	0.65
16:O:13:ARG:HG2	16:O:14:VAL:HG23	1.79	0.65
4:B:176:ARG:HE	14:M:16:ILE:HG22	1.61	0.65
1:X:649:G:N2	1:X:660:G:H22	1.94	0.65
5:C:176:ASN:ND2	5:C:178:TYR:H	1.95	0.65
1:X:2020:G:H2'	1:X:2021:G:C8	2.32	0.64
4:B:132:LYS:HA	4:B:134:TRP:HD1	1.62	0.64
5:C:75:PRO:HG3	5:C:83:ALA:HB2	1.78	0.64
1:X:1070:G:H5"	1:X:1071:U:H2'	1.78	0.64
1:X:2290:A:N1	6:D:42:SER:OG	2.25	0.64
14:M:99:VAL:HG21	14:M:104:LEU:HD21	1.78	0.64
1:X:759:C:O2'	1:X:760:U:OP2	2.15	0.64
1:X:946:U:H2'	1:X:947:C:H6	1.63	0.64
1:X:2640:G:H2'	1:X:2641:A:C8	2.33	0.64
3:A:79:VAL:HG21	3:A:111:LEU:HD21	1.79	0.64
8:G:69:ASP:O	8:G:71:THR:N	2.30	0.64
10:I:122:VAL:O	10:I:126:SER:N	2.27	0.64
1:X:2043:A:H1'	1:X:2481:G:C1'	2.27	0.64
1:X:2811:G:H2'	1:X:2812:A:C8	2.32	0.64
1:X:512:A:H4'	17:P:15:LYS:HB3	1.79	0.64
1:X:1503:G:H2'	1:X:1504:G:C8	2.32	0.64
1:X:2322:U:O2'	1:X:2323:U:OP1	2.15	0.64
2:Y:51:G:OP2	13:L:99:ARG:NH1	2.29	0.64
4:B:37:LYS:NZ	4:B:80:GLU:OE2	2.25	0.64
13:L:68:ALA:HB1	13:L:102:ALA:HB3	1.80	0.64
1:X:1373:G:H22	1:X:2192:U:H3	1.45	0.64
1:X:105:G:H21	1:X:357:A:H61	1.45	0.64
1:X:1061:A:N6	1:X:2731:G:O6	2.28	0.64
1:X:2543:A:OP1	1:X:2627:G:O2'	2.15	0.64
4:B:114:GLN:OE1	4:B:118:LYS:HD3	1.97	0.64
8:G:62:ILE:HD11	8:G:80:VAL:HG22	1.80	0.64
8:G:104:THR:CG2	8:G:109:GLY:HA3	2.28	0.64
1:X:501:G:OP1	32:X:3246:MPD:H11	1.97	0.64



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:X:2225:G:H2'	1:X:2226:A:C8	2.32	0.64
1:X:2311:U:H4'	1:X:2315:A:H62	1.63	0.64
8:G:98:LYS:O	8:G:116:ARG:N	2.29	0.64
15:N:66:ASN:HB3	15:N:76:TYR:CB	2.24	0.64
15:N:95:LEU:HA	15:N:98:ILE:HD13	1.78	0.64
2:Y:30:C:H2'	2:Y:31:A:H8	1.63	0.64
7:E:107:ILE:O	7:E:152:ARG:NH1	2.29	0.64
11:J:12:LYS:O	11:J:13:GLN:HG2	1.97	0.64
8:G:114:THR:HG22	8:G:119:LEU:HD22	1.80	0.63
13:L:11:LEU:HA	13:L:14:ARG:NE	2.13	0.63
1:X:38:G:H21	5:C:42:THR:HG21	1.63	0.63
5:C:118:VAL:CG2	5:C:120:VAL:H	2.10	0.63
13:L:9:ARG:O	13:L:11:LEU:N	2.31	0.63
6:D:4:LEU:HD13	6:D:101:GLU:HB2	1.80	0.63
16:O:5:ILE:O	16:O:7:THR:N	2.31	0.63
1:X:2245:A:H4'	1:X:2246:A:N3	2.13	0.63
1:X:1770:U:H5	1:X:1775:A:N7	1.97	0.63
1:X:135:U:H2'	1:X:136:A:C8	2.33	0.63
1:X:455:A:N7	5:C:39:ARG:HD2	2.14	0.63
6:D:35:VAL:HG22	6:D:90:THR:HG22	1.81	0.63
7:E:18:ASN:O	7:E:24:PHE:HB2	1.99	0.63
1:X:795:A:C2	3:A:226:MET:HG2	2.34	0.63
2:Y:32:C:H1'	2:Y:59:A:N6	2.12	0.63
6:D:119:PRO:HB3	6:D:177:PHE:HD2	1.64	0.63
7:E:56:SER:HB3	7:E:61:HIS:ND1	2.14	0.63
11:J:44:LYS:HD3	11:J:47:GLN:NE2	2.13	0.63
13:L:8:ARG:HG3	13:L:9:ARG:H	1.63	0.63
13:L:26:ARG:NH1	13:L:87:VAL:O	2.30	0.63
1:X:2222:U:H2'	1:X:2223:U:C6	2.34	0.63
1:X:2226:A:H2'	1:X:2227:C:H6	1.64	0.63
3:A:252:LYS:H	3:A:253:PRO:CD	2.12	0.63
1:X:136:A:H2'	1:X:137:A:C8	2.33	0.62
1:X:267:C:H2'	1:X:268:G:H8	1.62	0.62
1:X:1437:A:H2'	1:X:1438:G:C8	2.33	0.62
1:X:1963:G:O2'	1:X:1965:U:OP2	2.13	0.62
1:X:2175:A:H2'	1:X:2176:U:C6	2.34	0.62
1:X:2246:A:H5"	1:X:2247:A:H5"	1.81	0.62
28:3:52:LYS:NZ	28:3:56:ALA:HB2	2.13	0.62
1:X:1675:C:OP1	4:B:134:TRP:NE1	2.32	0.62
2:Y:50:U:H2'	2:Y:51:G:C8	2.34	0.62
3:A:38:PRO:HB3	3:A:60:ARG:O	2.00	0.62



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:X:2324:G:H21	1:X:2360:C:H3'	1.64	0.62
1:X:2621:G:H5'	8:G:106:TYR:CD2	2.33	0.62
10:I:81:GLN:O	10:I:81:GLN:HG2	1.98	0.62
1:X:79:G:H2'	1:X:80:A:H8	1.63	0.62
1:X:172:A:H61	1:X:175:C:H3'	1.64	0.62
2:Y:68:A:H61	2:Y:110:U:H2'	1.65	0.62
1:X:946:U:H2'	1:X:947:C:C6	2.33	0.62
1:X:1839:A:H8	1:X:1839:A:OP2	1.83	0.62
6:D:5:LYS:O	6:D:8:TYR:HB3	2.00	0.62
1:X:1785:A:H2'	1:X:1786:C:C6	2.34	0.62
1:X:2261:G:H21	1:X:2369:U:H3	1.46	0.62
1:X:2556:A:O2'	25:Z:3:LYS:HA	2.00	0.62
1:X:2807:U:H4'	1:X:2808:U:H5"	1.81	0.62
9:H:76:ARG:O	9:H:94:ASN:HA	2.00	0.62
1:X:494:A:O2'	19:R:68:GLY:N	2.32	0.62
1:X:590:C:H2'	1:X:591:G:H8	1.65	0.62
1:X:628:A:OP1	5:C:100:ARG:HG3	2.00	0.62
1:X:2279:G:H2'	1:X:2280:A:C8	2.34	0.62
1:X:2394:G:H4'	10:I:58:ALA:O	1.99	0.62
7:E:94:PHE:HA	7:E:107:ILE:HG22	1.82	0.62
8:G:85:ALA:HB3	8:G:152:ALA:HA	1.82	0.62
1:X:1465:G:H2'	1:X:1466:C:C6	2.34	0.61
1:X:1562:G:H5'	1:X:1563:U:H5'	1.83	0.61
1:X:1698:C:O2	31:X:3243:SPD:H32	1.99	0.61
1:X:2:G:H2'	1:X:3:U:C6	2.34	0.61
1:X:2728:A:H2'	1:X:2729:A:C8	2.35	0.61
8:G:51:LEU:HB2	8:G:88:VAL:HG21	1.81	0.61
1:X:1097:A:OP1	1:X:1115:C:O2'	2.13	0.61
4:B:92:ASN:HD21	4:B:182:ILE:HB	1.64	0.61
6:D:135:GLN:HG3	6:D:151:GLY:HA2	1.82	0.61
19:R:53:VAL:HG22	19:R:54:ILE:H	1.64	0.61
4:B:176:ARG:NE	14:M:16:ILE:HG22	2.15	0.61
1:X:1024:G:H2'	1:X:1025:A:C8	2.35	0.61
5:C:71:ASP:OD1	5:C:72:ARG:N	2.33	0.61
1:X:318:G:H21	1:X:341:A:N6	1.97	0.61
1:X:542:A:OP1	1:X:570:G:N2	2.30	0.61
1:X:1057:A:H5'	1:X:1058:G:OP2	2.00	0.61
1:X:2795:A:H4'	12:K:3:HIS:HD1	1.64	0.61
4:B:50:GLY:HA3	4:B:75:THR:HG21	1.81	0.61
11:J:49:GLU:OE2	11:J:52:ARG:NH1	2.34	0.61
11:J:64:LYS:HD2	11:J:108:ALA:O	2.00	0.61



A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
19:R:77:HIS:C	19:R:79:SER:H	2.04	0.61
1:X:136:A:H2'	1:X:137:A:H8	1.66	0.61
1:X:2047:C:H2'	1:X:2048:C:C6	2.36	0.61
3:A:143:HIS:ND1	3:A:194:GLY:O	2.22	0.61
9:H:125:LYS:H	9:H:125:LYS:CD	2.07	0.61
1:X:617:U:H5	1:X:632:A:N7	1.99	0.61
1:X:1030:U:H3	1:X:1153:A:N6	1.99	0.61
1:X:1673:C:H2'	1:X:1674:C:H6	1.66	0.61
2:Y:7:C:O2'	2:Y:29:C:O2	2.14	0.61
4:B:111:LYS:HG2	12:K:1:MET:HE1	1.83	0.61
16:O:10:LYS:H	16:O:10:LYS:HD2	1.65	0.61
1:X:1439:G:H2'	1:X:1440:G:C8	2.36	0.60
1:X:2477:C:H5'	1:X:2477:C:H6	1.66	0.60
5:C:181:LEU:HD11	10:I:1:MET:HB3	1.83	0.60
19:R:82:ALA:HB1	19:R:83:LEU:HD12	1.82	0.60
1:X:304:A:OP1	1:X:304:A:H4'	2.01	0.60
1:X:310:A:N3	1:X:330:C:O2'	2.33	0.60
10:I:55:ARG:H	10:I:55:ARG:NE	1.98	0.60
20:S:7:PRO:HD2	20:S:33:ALA:H	1.65	0.60
1:X:70:A:H5"	1:X:71:A:H2'	1.83	0.60
1:X:408:U:H2'	1:X:409:G:C8	2.35	0.60
1:X:1283:C:H5"	1:X:1284:G:H5'	1.83	0.60
2:Y:30:C:OP1	13:L:37:HIS:HB2	2.01	0.60
15:N:58:ARG:O	15:N:61:TRP:HB2	2.02	0.60
15:N:91:ASN:O	15:N:93:LYS:N	2.34	0.60
1:X:1219:C:H2'	1:X:1220:G:O4'	2.01	0.60
3:A:238:GLY:O	3:A:239:ARG:HG3	2.02	0.60
28:3:30:ARG:HG3	28:3:31:HIS:H	1.65	0.60
1:X:1311:C:H5"	1:X:1312:G:OP2	2.01	0.60
1:X:2867:G:OP2	1:X:2867:G:H8	1.85	0.60
19:R:83:LEU:HD12	19:R:83:LEU:H	1.66	0.60
1:X:5:A:H2'	1:X:6:A:H8	1.66	0.60
1:X:1223:G:H4'	1:X:1224:A:H5"	1.84	0.60
1:X:1882:G:N2	1:X:1885:C:H41	1.97	0.60
1:X:2623:A:H62	31:X:3242:SPD:H41	1.67	0.60
1:X:1082:G:H5'	1:X:1083:C:H5	1.66	0.60
1:X:1264:C:H5"	15:N:13:ARG:HH22	1.66	0.60
1:X:1270:C:P	5:C:69:HIS:HE2	2.23	0.60
1:X:2372:A:H5"	10:I:55:ARG:HB3	1.84	0.60
10:I:53:ARG:HD3	28:3:12:ARG:HH21	1.67	0.60
1:X:567:G:H5"	8:G:140:GLN:HG2	1.84	0.60



Atom 1	A + 0	Interatomic	Clash
Atom-1	Atom-2	$distance ({ m \AA})$	overlap (Å)
1:X:2378:G:HO2'	26:1:20:PHE:HE1	1.49	0.60
1:X:2692:A:H5"	1:X:2693:U:OP2	2.02	0.60
26:1:21:TYR:HD2	26:1:50:PHE:HZ	1.48	0.60
1:X:478:G:OP1	27:2:33:ARG:NE	2.32	0.60
1:X:1443:G:H2'	1:X:1444:C:C6	2.37	0.60
10:I:58:ALA:HA	28:3:11:LYS:HD2	1.84	0.60
11:J:20:GLY:C	11:J:99:LYS:HE2	2.23	0.60
13:L:64:LYS:H	13:L:64:LYS:HD2	1.65	0.60
16:O:68:LYS:HE3	16:O:70:TYR:CE1	2.37	0.60
20:S:75:LYS:HG3	20:S:76:ARG:H	1.67	0.60
1:X:2873:G:H2'	1:X:2874:A:C8	2.36	0.60
1:X:265:U:O2'	1:X:266:U:H6	1.85	0.59
1:X:2522:G:H2'	1:X:2523:G:C8	2.36	0.59
8:G:141:GLY:O	8:G:145:HIS:ND1	2.32	0.59
1:X:1212:U:H2'	1:X:1213:U:C6	2.36	0.59
1:X:1985:G:OP1	12:K:17:ARG:NH2	2.35	0.59
1:X:572:G:N3	15:N:37:GLN:NE2	2.50	0.59
1:X:1037:U:H2'	1:X:1037:U:O2	2.00	0.59
1:X:1366:A:H2'	1:X:1367:A:C8	2.36	0.59
1:X:2282:G:H1'	6:D:129:ASN:HD21	1.67	0.59
1:X:2434:G:H2'	1:X:2435:C:C6	2.37	0.59
6:D:9:ASN:HA	6:D:12:VAL:HG22	1.85	0.59
6:D:91:LEU:HD13	6:D:96:MET:HA	1.83	0.59
1:X:1148:G:H5"	1:X:1149:G:OP2	2.02	0.59
1:X:1465:G:H2'	1:X:1466:C:H6	1.66	0.59
1:X:2556:A:H5"	1:X:2557:G:H5'	1.84	0.59
2:Y:51:G:H2'	2:Y:52:G:H8	1.67	0.59
3:A:5:LYS:C	3:A:6:TYR:HD1	2.05	0.59
20:S:88:TYR:HA	20:S:127:PRO:HB3	1.83	0.59
1:X:567:G:P	8:G:140:GLN:NE2	2.75	0.59
1:X:602:C:H1'	28:3:2:PRO:O	2.02	0.59
1:X:2605:C:H2'	1:X:2606:G:H8	1.67	0.59
15:N:61:TRP:CE2	15:N:94:VAL:HG12	2.37	0.59
17:P:80:LEU:HD21	17:P:87:GLU:HB3	1.84	0.59
1:X:1503:G:H2'	1:X:1504:G:H8	1.65	0.59
4:B:48:GLN:NE2	4:B:78:LEU:HD13	2.18	0.59
7:E:22:GLY:HA2	7:E:43:VAL:HG11	1.83	0.59
13:L:108:ARG:CZ	13:L:111:GLY:HA3	2.33	0.59
15:N:22:LYS:O	15:N:24:PHE:N	2.31	0.59
1:X:699:G:N1	27:2:12:ARG:HD2	2.13	0.59
1:X:1284:G:H5"	31:X:3238:SPD:H82	1.85	0.59



Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
5:C:2:ALA:HA	5:C:13:ARG:O	2.03	0.59
9:H:73:VAL:HG21	9:H:123:PHE:CE2	2.37	0.59
1:X:517:A:H5"	1:X:518:A:H5'	1.84	0.59
1:X:1475:U:HO2'	1:X:1476:G:P	2.26	0.59
1:X:1989:C:OP1	31:X:3240:SPD:H32	2.02	0.59
9:H:23:ARG:HB3	9:H:52:VAL:HB	1.85	0.59
10:I:74:VAL:HG21	10:I:108:LEU:HD12	1.84	0.59
10:I:89:ASP:OD1	10:I:90:ARG:N	2.36	0.59
17:P:9:ARG:H	17:P:9:ARG:HD3	1.68	0.59
17:P:27:VAL:HG23	17:P:125:THR:HG22	1.84	0.59
18:Q:10:PRO:HD3	23:V:30:PHE:CD1	2.38	0.59
1:X:408:U:H2'	1:X:409:G:H8	1.67	0.58
4:B:131:SER:O	4:B:131:SER:OG	2.11	0.58
10:I:106:VAL:HG22	10:I:107:LYS:H	1.67	0.58
1:X:1100:G:N2	1:X:1113:C:H42	2.01	0.58
1:X:1798:G:H5"	1:X:1799:A:OP2	2.03	0.58
6:D:3:GLN:O	6:D:5:LYS:N	2.34	0.58
7:E:69:ARG:HH22	7:E:73:ALA:HB2	1.68	0.58
11:J:76:THR:HG21	11:J:88:LYS:HE3	1.85	0.58
14:M:2:GLN:HG2	14:M:3:THR:N	2.17	0.58
27:2:30:ILE:O	27:2:34:ARG:HG3	2.03	0.58
3:A:34:THR:C	3:A:36:ALA:H	2.06	0.58
5:C:72:ARG:HA	5:C:77:PHE:CD2	2.38	0.58
16:O:34:GLU:HB2	16:O:56:VAL:HB	1.86	0.58
16:O:57:GLN:N	16:O:97:GLY:HA3	2.18	0.58
22:U:11:LYS:HE3	22:U:60:VAL:HG21	1.85	0.58
1:X:717:G:H2'	1:X:739:G:H22	1.68	0.58
6:D:126:GLY:HA3	6:D:160:ALA:HB3	1.85	0.58
14:M:16:ILE:HD12	14:M:16:ILE:O	2.03	0.58
1:X:1079:G:H22	1:X:1106:A:C2'	2.15	0.58
1:X:2030:U:H2'	1:X:2031:A:H8	1.69	0.58
1:X:1270:C:H5'	5:C:69:HIS:CE1	2.38	0.58
19:R:85:ASP:HB3	19:R:86:PRO:HD3	1.85	0.58
1:X:24:G:H2'	1:X:25:U:H6	1.68	0.58
1:X:383:G:H4'	1:X:384:A:OP2	2.03	0.58
1:X:958:G:H2'	1:X:959:C:C6	2.39	0.58
1:X:2634:G:O2'	1:X:2643:G:O6	2.15	0.58
3:A:12:SER:O	3:A:14:ARG:N	2.35	0.58
3:A:210:GLY:HA2	3:A:213:ARG:HG2	1.86	0.58
3:A:210:GLY:HA2	3:A:213:ARG:H	1.67	0.58
6:D:170:LEU:HB2	6:D:175:LEU:HB2	1.85	0.58



A 4 1	• • • • •	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:X:760:U:O2	1:X:1997:A:H1'	2.04	0.58
1:X:1333:G:N2	1:X:1344:C:H41	2.01	0.58
1:X:2076:G:N1	1:X:2077:G:O6	2.36	0.58
25:Z:6:VAL:HG22	25:Z:7:PRO:HD2	1.85	0.58
1:X:276:A:H2'	1:X:277:G:C8	2.38	0.58
1:X:313:U:H2'	1:X:314:G:H8	1.69	0.58
1:X:942:U:O2'	24:W:22:ALA:HA	2.04	0.58
1:X:1710:U:O2'	3:A:14:ARG:NH1	2.37	0.58
1:X:1770:U:C5	1:X:1775:A:N7	2.71	0.58
2:Y:52:G:OP1	13:L:65:THR:OG1	2.19	0.58
14:M:41:GLU:HG3	14:M:46:ARG:NE	2.17	0.58
16:O:36:LYS:O	16:O:52:GLY:HA2	2.03	0.58
17:P:89:ARG:HE	17:P:131:LYS:HG3	1.68	0.58
1:X:455:A:H2	1:X:1258:G:N3	2.02	0.58
1:X:578:U:H5"	1:X:579:G:OP2	2.04	0.58
1:X:1468:A:H8	1:X:1468:A:OP2	1.87	0.58
1:X:2295:C:H5'	6:D:125:ARG:NH1	2.19	0.58
5:C:152:THR:HA	5:C:190:ALA:HB2	1.85	0.58
7:E:24:PHE:HE1	7:E:37:TYR:HE2	1.50	0.58
8:G:110:LEU:O	8:G:112:THR:OG1	2.17	0.58
10:I:91:ASP:OD1	10:I:92:THR:N	2.29	0.58
1:X:5:A:H2'	1:X:6:A:C8	2.39	0.57
1:X:503:G:H2'	1:X:504:G:O4'	2.03	0.57
1:X:564:U:H2'	1:X:565:A:C8	2.39	0.57
1:X:2728:A:H2'	1:X:2729:A:H8	1.69	0.57
9:H:110:VAL:HG23	9:H:129:LEU:HB2	1.86	0.57
20:S:125:PRO:HD2	20:S:157:GLY:O	2.03	0.57
1:X:485:G:C6	1:X:520:C:N4	2.72	0.57
1:X:597:U:H2'	1:X:598:U:C6	2.39	0.57
1:X:868:U:H2'	1:X:869:C:C6	2.39	0.57
1:X:1153:A:O2'	1:X:1154:A:O5'	2.18	0.57
2:Y:44:C:N3	6:D:90:THR:OG1	2.36	0.57
1:X:405:C:H2'	1:X:406:G:C8	2.38	0.57
1:X:1664:G:OP2	31:X:3238:SPD:H32	2.04	0.57
1:X:2769:C:H2'	1:X:2770:A:C8	2.38	0.57
4:B:184:VAL:HG11	4:B:188:ILE:HD11	1.85	0.57
6:D:15:ALA:O	6:D:19:GLN:HG2	2.04	0.57
19:R:26:SER:OG	19:R:27:GLY:N	2.36	0.57
28:3:2:PRO:O	28:3:3:LYS:HB2	2.03	0.57
1:X:717:G:C2'	1:X:739:G:H22	2.17	0.57
1:X:1171:A:H1'	16:O:7:THR:HG23	1.87	0.57


Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:X:2307:A:H2'	1:X:2308:A:C8	2.39	0.57
3:A:142:VAL:HG12	3:A:193:ILE:HA	1.87	0.57
8:G:85:ALA:HB1	8:G:127:ILE:HD12	1.85	0.57
11:J:134:LYS:HD2	11:J:135:ARG:HB3	1.86	0.57
18:Q:4:TYR:CE2	23:V:23:LYS:HB2	2.39	0.57
3:A:12:SER:OG	3:A:13:ARG:N	2.37	0.57
3:A:246:PRO:HD2	3:A:250:TRP:N	2.18	0.57
9:H:56:LYS:CD	9:H:57:ASP:HB2	2.32	0.57
22:U:19:ILE:HD11	22:U:40:ARG:HA	1.86	0.57
9:H:4:PRO:HA	9:H:21:CYS:HB3	1.85	0.57
18:Q:10:PRO:HA	18:Q:27:PHE:CB	2.32	0.57
1:X:824:U:H2'	10:I:21:ARG:HA	1.87	0.57
1:X:1675:C:OP1	4:B:134:TRP:CE2	2.58	0.57
1:X:243:G:N1	1:X:244:C:C5	2.72	0.57
1:X:1085:G:H2'	1:X:1086:C:C5	2.40	0.57
1:X:1466:C:H2'	1:X:1467:U:C1'	2.33	0.57
1:X:1674:C:H2'	1:X:1675:C:C6	2.39	0.57
1:X:2265:A:N3	1:X:2325:A:N6	2.52	0.57
17:P:8:PHE:CD2	17:P:14:ARG:HG3	2.39	0.57
28:3:8:LYS:O	28:3:8:LYS:HG2	2.05	0.57
1:X:1068:A:N6	1:X:1098:G:OP1	2.38	0.57
14:M:110:LEU:O	14:M:112:GLY:N	2.37	0.57
1:X:759:C:HO2'	1:X:760:U:P	2.28	0.57
5:C:46:ARG:HD3	5:C:51:VAL:HG12	1.87	0.57
9:H:18:GLU:HB3	9:H:57:ASP:HB3	1.86	0.57
18:Q:48:VAL:HG21	18:Q:82:LEU:HD13	1.86	0.57
1:X:71:A:O2'	1:X:72:A:OP1	2.19	0.56
1:X:1051:U:H2'	1:X:1052:C:H6	1.70	0.56
1:X:1806:G:H5"	1:X:1807:A:H2'	1.85	0.56
1:X:1954:A:C2	3:A:240:THR:HG22	2.39	0.56
13:L:26:ARG:HD3	13:L:86:GLN:HB3	1.87	0.56
17:P:89:ARG:HH11	17:P:131:LYS:HD2	1.70	0.56
1:X:591:G:H2'	1:X:592:G:C8	2.40	0.56
1:X:1443:G:H2'	1:X:1444:C:H6	1.70	0.56
2:Y:37:C:H2'	2:Y:38:C:O4'	2.05	0.56
8:G:104:THR:CG2	8:G:106:TYR:H	2.18	0.56
27:2:37:LYS:HE2	27:2:39:ARG:NH2	2.20	0.56
1:X:168:A:H2'	1:X:169:C:H6	1.66	0.56
1:X:1332:G:O2'	1:X:1333:G:H5'	2.05	0.56
1:X:1469:U:H5"	1:X:1470:G:N7	2.19	0.56
1:X:2193:C:H2'	1:X:2194:A:H8	1.69	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (A)	overlap (Å)
1:X:2605:C:H2'	1:X:2606:G:C8	2.41	0.56
1:X:2871:U:H2'	1:X:2872:U:C6	2.40	0.56
8:G:104:THR:HG23	8:G:106:TYR:H	1.70	0.56
20:S:103:ARG:HG3	20:S:107:GLU:HB3	1.86	0.56
1:X:256:C:H42	1:X:263:G:H22	1.50	0.56
1:X:1264:C:H5"	15:N:13:ARG:HH12	1.69	0.56
1:X:1816:G:H2'	1:X:1817:U:C6	2.40	0.56
1:X:2726:U:H2'	1:X:2727:G:H5'	1.88	0.56
2:Y:66:G:H2'	2:Y:67:C:O4'	2.05	0.56
7:E:105:MET:HB2	7:E:113:VAL:HG23	1.86	0.56
18:Q:29:VAL:HG11	18:Q:38:ILE:HD11	1.87	0.56
1:X:537:C:H1'	1:X:538:A:C5	2.40	0.56
1:X:1499:A:H2'	1:X:1500:U:C6	2.40	0.56
2:Y:6:C:H2'	2:Y:7:C:H6	1.69	0.56
2:Y:14:C:H5'	21:T:72:LYS:HE3	1.87	0.56
5:C:6:VAL:HG13	5:C:7:ILE:N	2.18	0.56
5:C:118:VAL:HG22	5:C:120:VAL:N	2.20	0.56
1:X:242:A:H1'	1:X:243:G:H1'	1.87	0.56
1:X:857:U:H2'	1:X:858:G:O4'	2.05	0.56
1:X:2866:A:H3'	1:X:2867:G:C8	2.41	0.56
4:B:33:ILE:HG21	4:B:36:ARG:NH2	2.21	0.56
5:C:48:ARG:HH11	5:C:74:VAL:HG12	1.70	0.56
13:L:76:ALA:HB1	13:L:111:GLY:HA2	1.87	0.56
15:N:61:TRP:NE1	15:N:94:VAL:HG12	2.20	0.56
18:Q:8:GLN:O	23:V:29:ARG:HD2	2.05	0.56
19:R:80:LYS:C	19:R:80:LYS:HD2	2.26	0.56
19:R:106:VAL:O	19:R:112:LYS:HA	2.05	0.56
20:S:7:PRO:HD2	20:S:32:PHE:HB2	1.88	0.56
1:X:24:G:H2'	1:X:25:U:C6	2.41	0.56
1:X:859:U:O2'	1:X:860:U:O5'	2.22	0.56
1:X:2467:A:O2'	1:X:2468:G:H5'	2.06	0.56
2:Y:29:C:O3'	13:L:37:HIS:ND1	2.38	0.56
22:U:65:ASN:HA	22:U:68:ARG:HD3	1.87	0.56
19:R:44:GLN:O	19:R:77:HIS:HA	2.05	0.56
1:X:256:C:H1'	1:X:257:G:H5'	1.86	0.56
1:X:1935:A:C4	9:H:22:ILE:HD11	2.40	0.56
1:X:2475:C:OP2	11:J:83:ARG:HG2	2.05	0.56
2:Y:30:C:H2'	2:Y:31:A:C8	2.41	0.56
7:E:20:GLN:O	7:E:22:GLY:N	2.38	0.56
24:W:2:LYS:HE3	24:W:33:GLU:OE2	2.05	0.56
9:H:10:VAL:HA	9:H:96:ALA:O	2.06	0.56



		Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
11:J:21:ASP:HB2	20:S:74:ARG:HD2	1.88	0.56
14:M:110:LEU:HB3	14:M:115:ALA:HB1	1.87	0.56
18:Q:35:LYS:O	18:Q:38:ILE:HG22	2.06	0.56
1:X:649:G:H1	1:X:660:G:H22	1.54	0.55
1:X:1271:C:O4'	5:C:78:VAL:HG11	2.06	0.55
1:X:2011:U:H2'	1:X:2012:A:C8	2.41	0.55
9:H:29:ILE:HD13	9:H:123:PHE:CD1	2.40	0.55
9:H:42:LYS:HE3	9:H:44:TYR:O	2.05	0.55
17:P:36:ARG:NH2	25:Z:20:ARG:HH12	2.05	0.55
21:T:56:ASP:OD1	21:T:58:THR:HG22	2.05	0.55
3:A:65:ILE:HG22	3:A:88:ARG:HH21	1.71	0.55
1:X:89:A:O3'	1:X:91:A:N6	2.39	0.55
1:X:597:U:O4	1:X:683:A:H1'	2.06	0.55
1:X:1264:C:H5"	15:N:13:ARG:NH2	2.22	0.55
1:X:2039:G:C2	1:X:2040:A:C8	2.95	0.55
1:X:2285:U:H5"	1:X:2286:G:N7	2.22	0.55
1:X:2312:A:H5'	1:X:2314:A:C8	2.40	0.55
1:X:2821:G:H2'	1:X:2822:U:C6	2.41	0.55
13:L:11:LEU:HA	13:L:14:ARG:HE	1.70	0.55
1:X:267:C:H2'	1:X:268:G:C8	2.42	0.55
1:X:1919:A:H61	1:X:1946:U:H3	1.51	0.55
1:X:2667:C:N4	1:X:2700:U:OP2	2.39	0.55
1:X:1218:C:O4'	10:I:4:HIS:NE2	2.39	0.55
1:X:1781:C:H2'	1:X:1782:A:C5	2.40	0.55
28:3:30:ARG:HG3	28:3:31:HIS:N	2.21	0.55
1:X:683:A:H5"	10:I:40:ARG:HG3	1.88	0.55
1:X:827:C:OP1	16:O:82:ARG:HA	2.07	0.55
1:X:1919:A:H2	1:X:1926:U:N3	2.01	0.55
1:X:2266:A:H62	1:X:2323:U:H3	1.54	0.55
1:X:2372:A:P	28:3:30:ARG:HB2	2.47	0.55
1:X:2431:C:H2'	1:X:2432:A:C8	2.41	0.55
5:C:22:VAL:HG23	5:C:106:MET:HB3	1.89	0.55
5:C:57:LYS:HD2	5:C:58:MET:N	2.22	0.55
6:D:44:LYS:H	6:D:44:LYS:HD2	1.71	0.55
13:L:47:ARG:O	13:L:49:GLN:N	2.37	0.55
14:M:3:THR:O	14:M:3:THR:OG1	2.21	0.55
18:Q:56:MET:CE	18:Q:77:LYS:HE3	2.36	0.55
1:X:255:A:H1'	1:X:256:C:H5'	1.88	0.55
4:B:135:HIS:CG	4:B:136:ARG:HG2	2.41	0.55
7:E:69:ARG:NH2	7:E:73:ALA:HB2	2.22	0.55
15:N:55:ARG:HA	15:N:58:ARG:HD2	1.88	0.55



A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
17:P:103:LEU:HB2	17:P:119:LYS:HB2	1.88	0.55
21:T:32:LYS:N	21:T:35:ASN:OD1	2.38	0.55
1:X:661:C:H2'	1:X:662:G:H8	1.69	0.55
1:X:2407:G:H5"	1:X:2408:G:OP1	2.06	0.55
9:H:88:THR:HB	14:M:80:VAL:HB	1.88	0.55
1:X:543:G:H5'	15:N:24:PHE:CE1	2.41	0.55
1:X:1086:C:O2'	1:X:1087:C:OP1	2.22	0.55
1:X:1322:G:H4'	27:2:7:PRO:HB2	1.88	0.55
1:X:1779:C:H2'	1:X:1780:A:C8	2.42	0.55
1:X:2418:A:C4'	1:X:2419:C:H5"	2.36	0.55
6:D:40:LEU:HD13	6:D:50:ILE:HA	1.89	0.55
17:P:89:ARG:HE	17:P:131:LYS:CG	2.20	0.55
1:X:922:A:H2'	1:X:923:A:C8	2.42	0.55
1:X:1586:A:H2'	1:X:1587:A:C8	2.42	0.55
1:X:1981:A:P	4:B:136:ARG:HH12	2.29	0.55
9:H:104:GLU:OE1	9:H:125:LYS:HG3	2.07	0.55
11:J:45:SER:HB3	11:J:71:PRO:HG3	1.89	0.55
16:O:40:VAL:HG13	16:O:43:GLU:HA	1.87	0.55
19:R:61:SER:N	19:R:64:ASN:O	2.36	0.55
1:X:70:A:C4'	1:X:71:A:H5"	2.34	0.54
1:X:394:U:H2'	1:X:395:G:C8	2.42	0.54
1:X:580:A:H4'	1:X:581:A:OP1	2.06	0.54
1:X:1707:A:H3'	1:X:1708:C:H6	1.72	0.54
1:X:1790:G:N2	3:A:155:LEU:HD23	2.21	0.54
1:X:2292:C:H5"	6:D:88:LYS:HD3	1.89	0.54
1:X:2402:U:O2'	1:X:2404:A:H2'	2.07	0.54
1:X:2800:C:H3'	1:X:2801:A:H8	1.72	0.54
8:G:168:THR:HB	8:G:169:GLN:OE1	2.07	0.54
1:X:83:A:C2	1:X:101:A:C5	2.94	0.54
1:X:90:G:H5'	1:X:91:A:OP2	2.07	0.54
1:X:995:A:H5"	1:X:996:C:H5	1.71	0.54
1:X:1670:G:H3'	12:K:2:ARG:HG2	1.89	0.54
1:X:2226:A:H2'	1:X:2227:C:C6	2.42	0.54
6:D:127:ASN:OD1	6:D:157:VAL:HA	2.07	0.54
13:L:29:LEU:HA	13:L:41:GLN:O	2.07	0.54
19:R:108:VAL:HG22	19:R:109:ALA:H	1.72	0.54
23:V:14:PHE:CD2	23:V:57:LYS:HD3	2.41	0.54
1:X:341:A:O2'	1:X:342:G:OP1	2.25	0.54
1:X:1098:G:N2	1:X:1114:A:H1'	2.22	0.54
1:X:2516:U:H2'	1:X:2517:C:C6	2.42	0.54
19:R:22:VAL:CG1	19:R:80:LYS:HD3	2.36	0.54



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:X:17:G:H2'	1:X:18:U:C6	2.43	0.54
1:X:686:C:OP1	5:C:48:ARG:HD2	2.08	0.54
1:X:1162:A:H4'	15:N:81:ASN:ND2	2.23	0.54
1:X:2659:C:H5'	4:B:189:PRO:HA	1.89	0.54
3:A:77:ALA:HB3	3:A:117:VAL:HB	1.89	0.54
5:C:120:VAL:HA	5:C:191:ALA:HB2	1.90	0.54
22:U:10:LYS:HG2	22:U:12:ASN:CB	2.36	0.54
1:X:2400:G:O6	28:3:32:GLN:NE2	2.41	0.54
2:Y:14:C:H4'	2:Y:17:A:H61	1.72	0.54
8:G:115:ALA:O	8:G:116:ARG:HG2	2.06	0.54
9:H:125:LYS:HD3	9:H:125:LYS:N	2.07	0.54
14:M:110:LEU:HD13	14:M:115:ALA:HB1	1.88	0.54
22:U:47:HIS:CG	22:U:48:LYS:H	2.24	0.54
1:X:339:U:H4'	19:R:77:HIS:CE1	2.42	0.54
1:X:830:C:O2'	1:X:852:U:H5"	2.07	0.54
1:X:1329:U:H2'	1:X:1330:G:H8	1.72	0.54
1:X:2399:C:H41	28:3:31:HIS:HB3	1.72	0.54
1:X:2788:C:H2'	1:X:2789:U:H6	1.72	0.54
6:D:40:LEU:HA	6:D:150:ARG:NH1	2.23	0.54
8:G:35:LYS:CD	8:G:37:ASP:H	2.14	0.54
15:N:12:ARG:HD2	15:N:15:LYS:NZ	2.22	0.54
20:S:147:ILE:HB	20:S:169:VAL:HG22	1.90	0.54
1:X:338:G:H2'	1:X:339:U:O4'	2.08	0.54
1:X:712:A:H2'	1:X:713:G:O4'	2.07	0.54
1:X:1510:A:H2'	1:X:1511:A:O4'	2.08	0.54
1:X:2220:A:H2'	1:X:2221:G:C8	2.42	0.54
11:J:30:PHE:HB3	11:J:66:TYR:CE2	2.42	0.54
16:O:19:VAL:HG13	16:O:90:PHE:CD2	2.42	0.54
1:X:314:G:H2'	1:X:315:G:H8	1.71	0.54
1:X:1051:U:H2'	1:X:1052:C:C6	2.42	0.54
1:X:1193:G:H2'	1:X:1194:U:C6	2.42	0.54
1:X:1268:U:C6	5:C:67:ALA:HA	2.43	0.54
1:X:1998:A:N3	25:Z:6:VAL:HG23	2.23	0.54
1:X:2006:G:H5'	1:X:2596:C:H4'	1.90	0.54
3:A:25:THR:HB	3:A:81:ALA:HB1	1.89	0.54
7:E:163:ARG:NH2	7:E:169:ILE:HG21	2.23	0.54
10:I:83:LEU:HA	10:I:86:THR:HG23	1.88	0.54
12:K:17:ARG:H	12:K:17:ARG:HD2	1.71	0.54
12:K:24:GLN:HB3	12:K:44:LEU:HD22	1.90	0.54
1:X:1999:U:O2'	25:Z:7:PRO:O	2.22	0.54
1:X:2691:C:H2'	1:X:2694:G:H5"	1.89	0.54



	Atom 0	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
13:L:33:ARG:HE	13:L:38:ILE:HG21	1.72	0.54
17:P:25:PHE:HD1	17:P:26:ALA:N	2.06	0.54
19:R:98:ILE:HG22	19:R:99:VAL:H	1.73	0.54
24:W:46:THR:HG22	24:W:47:VAL:HG13	1.88	0.54
1:X:691:C:H2'	1:X:692:C:H6	1.73	0.54
1:X:1076:U:H3	1:X:1085:G:N2	2.06	0.54
1:X:1582:A:OP1	3:A:211:ARG:NH2	2.40	0.54
2:Y:46:G:N2	2:Y:50:U:H1'	2.23	0.54
4:B:18:ASP:N	4:B:18:ASP:OD1	2.40	0.54
7:E:136:ILE:HG13	7:E:137:ASP:H	1.73	0.54
14:M:48:GLN:HG2	14:M:49:ALA:N	2.22	0.54
17:P:8:PHE:CE2	17:P:14:ARG:HG3	2.43	0.54
20:S:71:MET:HB2	20:S:78:PRO:HA	1.90	0.54
1:X:832:A:OP2	1:X:1201:G:N2	2.33	0.53
1:X:1030:U:OP1	1:X:1046:U:O2'	2.17	0.53
1:X:1333:G:N2	1:X:1344:C:N4	2.56	0.53
1:X:1787:U:H2'	1:X:1788:C:H6	1.72	0.53
1:X:2085:G:H2'	1:X:2086:U:C6	2.42	0.53
3:A:252:LYS:CD	3:A:253:PRO:HD3	2.29	0.53
24:W:1:MET:HB3	24:W:34:VAL:HG12	1.90	0.53
1:X:1812:U:H4'	1:X:1813:A:OP2	2.08	0.53
1:X:753:U:H2'	1:X:754:G:C8	2.43	0.53
1:X:1451:C:H2'	1:X:1452:U:C6	2.43	0.53
1:X:2402:U:O2'	1:X:2403:C:OP2	2.25	0.53
3:A:146:GLU:OE1	3:A:149:PRO:HA	2.09	0.53
6:D:16:LEU:HD21	6:D:28:VAL:HG21	1.89	0.53
11:J:19:THR:HG23	11:J:99:LYS:HD3	1.90	0.53
1:X:1925:C:H2'	1:X:1926:U:C5	2.43	0.53
1:X:1935:A:N3	9:H:22:ILE:HD11	2.23	0.53
1:X:2526:U:H2'	1:X:2527:G:H8	1.73	0.53
3:A:231:HIS:CD2	3:A:247:VAL:HA	2.43	0.53
1:X:224:G:H4'	1:X:399:G:C5	2.43	0.53
1:X:427:C:H2'	1:X:428:A:C8	2.43	0.53
1:X:991:A:N7	1:X:1146:G:H5"	2.23	0.53
1:X:1069:G:H2'	1:X:1070:G:C8	2.43	0.53
1:X:1674:C:H2'	1:X:1675:C:H6	1.73	0.53
1:X:1911:A:H5"	1:X:1912:G:OP2	2.08	0.53
1:X:2024:U:H2'	1:X:2025:A:C8	2.43	0.53
1:X:2291:U:C2'	6:D:37:ASN:HD21	2.22	0.53
1:X:2670:C:H5'	1:X:2847:G:H5"	1.90	0.53
2:Y:78:A:H2'	2:Y:79:U:O4'	2.09	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:C:49:ALA:O	5:C:51:VAL:N	2.41	0.53
6:D:111:ILE:HB	6:D:114:PHE:HB2	1.90	0.53
8:G:164:GLN:HG3	8:G:165:VAL:H	1.73	0.53
17:P:9:ARG:HE	17:P:13:GLN:CB	2.21	0.53
20:S:8:ARG:NE	20:S:8:ARG:HA	2.23	0.53
1:X:590:C:H2'	1:X:591:G:C8	2.42	0.53
1:X:654:A:N1	1:X:2348:A:O2'	2.37	0.53
1:X:1164:C:H2'	1:X:1165:G:C8	2.44	0.53
1:X:1573:G:H3'	1:X:1574:A:H5"	1.91	0.53
1:X:1993:G:H5"	17:P:63:SER:HB2	1.90	0.53
1:X:2273:C:OP1	13:L:11:LEU:HD21	2.08	0.53
3:A:252:LYS:HZ2	3:A:253:PRO:HD3	1.72	0.53
13:L:33:ARG:NH1	13:L:100:VAL:HA	2.23	0.53
1:X:504:G:H4'	17:P:27:VAL:HG13	1.89	0.53
1:X:652:C:H42	1:X:657:A:N6	2.03	0.53
1:X:1753:A:H2'	31:X:3243:SPD:N1	2.23	0.53
1:X:2448:A:N6	1:X:2460:G:H1'	2.24	0.53
4:B:2:LYS:HA	4:B:84:PHE:CD1	2.44	0.53
1:X:78:C:H2'	1:X:79:G:H8	1.74	0.53
1:X:399:G:H5'	1:X:401:G:H22	1.74	0.53
1:X:2448:A:H61	1:X:2460:G:H1'	1.73	0.53
4:B:119:ARG:HG2	4:B:120:TRP:NE1	2.24	0.53
8:G:164:GLN:NE2	8:G:165:VAL:HG22	2.24	0.53
19:R:24:VAL:O	19:R:31:GLY:N	2.41	0.53
20:S:17:SER:O	20:S:35:ASP:HA	2.08	0.53
20:S:40:ASP:OD2	20:S:44:ARG:NH2	2.41	0.53
21:T:77:ARG:C	21:T:78:PHE:HD1	2.11	0.53
1:X:1279:G:O2'	1:X:1995:G:O6	2.22	0.53
1:X:1787:U:H2'	1:X:1788:C:C6	2.44	0.53
1:X:1845:A:H2'	1:X:1846:A:C8	2.44	0.53
1:X:2551:A:H5"	1:X:2553:G:H4'	1.90	0.53
1:X:2559:U:H5"	1:X:2560:G:N2	2.24	0.53
6:D:117:ILE:HG13	6:D:118:ASN:N	2.24	0.53
10:I:56:LEU:HA	28:3:12:ARG:HA	1.91	0.53
13:L:14:ARG:O	13:L:18:ARG:HB2	2.09	0.53
1:X:692:C:H2'	1:X:693:A:H8	1.74	0.53
1:X:1429:A:N3	1:X:1603:A:H1'	2.25	0.53
1:X:1843:U:H3	1:X:1874:G:H1	1.57	0.53
1:X:1991:C:H2'	1:X:1992:G:H8	1.72	0.53
1:X:2393:G:N3	10:I:59:ARG:NH1	2.57	0.53
3:A:251:GLY:H	3:A:255:LYS:CE	2.21	0.53



A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
8:G:32:TYR:O	15:N:64:ARG:NH1	2.39	0.53
1:X:562:G:H2'	1:X:563:U:O4'	2.08	0.52
1:X:787:A:H2	1:X:800:U:HO2'	1.55	0.52
1:X:1079:G:N2	1:X:1106:A:H2'	2.22	0.52
1:X:1264:C:H5"	15:N:13:ARG:NH1	2.24	0.52
1:X:1823:G:H2'	1:X:1824:C:C6	2.44	0.52
9:H:81:ILE:CD1	9:H:117:GLU:HG3	2.37	0.52
16:O:16:GLU:H	16:O:95:ILE:HB	1.74	0.52
16:O:57:GLN:H	16:O:97:GLY:HA3	1.72	0.52
17:P:25:PHE:CD1	17:P:25:PHE:C	2.82	0.52
19:R:95:ARG:HB3	19:R:104:VAL:HB	1.91	0.52
1:X:1645:U:H2'	1:X:1646:G:C8	2.44	0.52
13:L:9:ARG:C	13:L:11:LEU:H	2.13	0.52
1:X:401:G:OP1	22:U:34:THR:OG1	2.28	0.52
1:X:480:G:O6	27:2:37:LYS:HE3	2.09	0.52
1:X:542:A:N6	1:X:2003:A:H1'	2.24	0.52
1:X:1062:G:H2'	1:X:1063:C:C5	2.44	0.52
1:X:2855:C:O2'	12:K:93:GLY:HA3	2.10	0.52
2:Y:80:A:H2'	2:Y:81:C:O4'	2.09	0.52
16:O:20:ILE:HG22	16:O:91:THR:O	2.09	0.52
1:X:257:G:H2'	1:X:258:C:C6	2.45	0.52
1:X:1284:G:C5'	31:X:3238:SPD:H82	2.40	0.52
1:X:1801:C:H41	22:U:48:LYS:HB2	1.73	0.52
1:X:1888:C:H5'	1:X:1889:G:O5'	2.08	0.52
5:C:2:ALA:HA	5:C:13:ARG:C	2.29	0.52
1:X:227:G:H5'	28:3:8:LYS:NZ	2.24	0.52
1:X:1104:G:H2'	1:X:1105:U:H5	1.73	0.52
1:X:1673:C:H2'	1:X:1674:C:C6	2.43	0.52
1:X:1997:A:H2'	1:X:1998:A:C8	2.44	0.52
1:X:2557:G:O2'	1:X:2558:C:H5'	2.10	0.52
1:X:2690:A:OP2	31:X:3239:SPD:N1	2.42	0.52
1:X:2725:C:H2'	1:X:2726:U:C6	2.45	0.52
2:Y:122:U:H5"	2:Y:123:U:OP2	2.08	0.52
4:B:143:GLN:N	4:B:143:GLN:OE1	2.43	0.52
7:E:37:TYR:HE2	7:E:72:VAL:HG12	1.75	0.52
10:I:76:LYS:HE2	10:I:90:ARG:NH2	2.24	0.52
13:L:21:THR:HG23	13:L:45:ASP:HB3	1.91	0.52
14:M:54:VAL:HG22	14:M:68:VAL:HG12	1.91	0.52
1:X:546:A:H2'	1:X:547:U:C6	2.45	0.52
1:X:670:U:H2'	1:X:671:A:C8	2.44	0.52
1:X:2764:U:H4'	4:B:42:ASP:OD1	2.09	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
4:B:49:ILE:HD11	4:B:90:SER:HB3	1.91	0.52
5:C:89:ARG:HG3	5:C:91:TYR:HE1	1.73	0.52
25:Z:45:ILE:HG22	25:Z:52:TYR:HB2	1.91	0.52
1:X:1288:A:H2'	1:X:1289:A:O4'	2.09	0.52
1:X:2030:U:H2'	1:X:2031:A:C8	2.45	0.52
1:X:2245:A:H4'	1:X:2246:A:C2	2.45	0.52
1:X:2269:G:H2'	1:X:2270:U:O4'	2.10	0.52
5:C:148:VAL:O	5:C:167:VAL:HA	2.10	0.52
14:M:102:ALA:O	14:M:103:LYS:HE2	2.10	0.52
28:3:14:ILE:HA	28:3:23:MET:O	2.10	0.52
1:X:575:U:H5"	10:I:28:LYS:HD2	1.90	0.52
1:X:810:U:P	5:C:56:ARG:HD3	2.49	0.52
1:X:1082:G:H3'	1:X:1083:C:H6	1.74	0.52
4:B:48:GLN:HE21	4:B:78:LEU:HD13	1.74	0.52
15:N:90:LEU:HD23	15:N:90:LEU:O	2.09	0.52
25:Z:36:CYS:SG	25:Z:48:ASN:HB2	2.50	0.52
1:X:2:G:H2'	1:X:3:U:H6	1.75	0.52
1:X:79:G:H2'	1:X:80:A:C8	2.44	0.52
1:X:242:A:N3	1:X:243:G:C8	2.78	0.52
1:X:836:G:H2'	1:X:837:U:H6	1.75	0.52
1:X:1827:G:H1'	1:X:1914:U:C2	2.45	0.52
1:X:2440:C:H2'	1:X:2441:U:C6	2.45	0.52
1:X:2709:C:H2'	1:X:2710:C:C6	2.44	0.52
5:C:146:GLU:OE1	5:C:185:ARG:HD2	2.09	0.52
19:R:85:ASP:O	19:R:87:GLU:N	2.42	0.52
1:X:63:A:O2'	18:Q:70:GLY:HA2	2.10	0.52
1:X:790:A:O2'	3:A:48:ARG:NH2	2.39	0.52
1:X:2441:U:H2'	1:X:2442:C:C6	2.44	0.52
1:X:2594:U:C6	25:Z:7:PRO:HA	2.45	0.52
8:G:100:TYR:OH	8:G:126:VAL:HG13	2.10	0.52
9:H:11:ALA:O	9:H:110:VAL:HA	2.10	0.52
10:I:100:ARG:HA	10:I:117:ALA:O	2.10	0.52
1:X:39:C:O2	5:C:40:ARG:NH2	2.44	0.51
1:X:600:G:O2'	1:X:601:A:H5'	2.10	0.51
1:X:711:C:O2'	1:X:747:A:N6	2.43	0.51
1:X:1171:A:H2'	1:X:1172:U:C6	2.45	0.51
1:X:1270:C:H4'	5:C:77:PHE:HE1	1.71	0.51
1:X:1800:A:H4'	1:X:1801:C:OP1	2.10	0.51
1:X:1845:A:H2'	1:X:1846:A:H8	1.75	0.51
1:X:2200:G:O2'	3:A:149:PRO:HG2	2.10	0.51
4:B:93:VAL:HG23	4:B:94:ASP:N	2.25	0.51



	Atom 0	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
6:D:15:ALA:O	6:D:19:GLN:NE2	2.43	0.51
18:Q:20:MET:HG2	18:Q:92:ALA:HB1	1.91	0.51
2:Y:68:A:N6	2:Y:110:U:H2'	2.23	0.51
3:A:165:VAL:HG12	3:A:175:VAL:HG12	1.92	0.51
19:R:58:VAL:HG12	19:R:60:PRO:O	2.10	0.51
27:2:17:GLY:O	27:2:21:ARG:HG2	2.10	0.51
28:3:23:MET:HA	28:3:48:PHE:HB2	1.91	0.51
1:X:39:C:H2'	1:X:40:U:C6	2.46	0.51
1:X:1031:C:O4'	1:X:1032:A:C2	2.63	0.51
1:X:1398:G:O2'	1:X:1399:C:O5'	2.28	0.51
1:X:1865:C:H3'	1:X:1866:G:H8	1.75	0.51
1:X:2526:U:H2'	1:X:2527:G:C8	2.46	0.51
5:C:27:LEU:O	5:C:31:VAL:HG23	2.10	0.51
14:M:29:PRO:HB3	14:M:54:VAL:O	2.10	0.51
19:R:108:VAL:HG13	19:R:109:ALA:N	2.25	0.51
28:3:5:LYS:CE	28:3:62:LEU:HB3	2.32	0.51
1:X:1441:A:H4'	1:X:1442:C:O5'	2.10	0.51
8:G:115:ALA:C	8:G:116:ARG:HG2	2.31	0.51
24:W:5:LEU:HA	24:W:51:LEU:HD23	1.92	0.51
1:X:689:A:H8	1:X:2052:G:N2	2.02	0.51
1:X:1504:G:H5"	1:X:1505:U:OP2	2.11	0.51
1:X:2212:U:H2'	1:X:2213:G:C8	2.46	0.51
1:X:2595:C:H2'	1:X:2596:C:H6	1.76	0.51
14:M:104:LEU:HA	14:M:106:TYR:CE1	2.46	0.51
28:3:30:ARG:CG	28:3:31:HIS:H	2.20	0.51
1:X:123:A:H5"	27:2:19:ARG:HG2	1.92	0.51
1:X:554:U:H5"	1:X:556:A:C2	2.45	0.51
1:X:2542:U:H5'	9:H:37:GLY:HA2	1.92	0.51
7:E:18:ASN:OD1	7:E:19:ALA:N	2.43	0.51
1:X:1486:A:H2'	1:X:1487:C:C6	2.46	0.51
1:X:1989:C:OP1	31:X:3240:SPD:N6	2.41	0.51
1:X:2325:A:HO2'	1:X:2326:C:P	2.34	0.51
4:B:14:ILE:HG13	14:M:20:HIS:NE2	2.26	0.51
4:B:188:ILE:HG23	4:B:189:PRO:HD2	1.93	0.51
16:O:28:GLU:O	16:O:30:GLY:N	2.44	0.51
18:Q:60:GLY:HA3	18:Q:73:ASN:N	2.21	0.51
26:1:14:SER:HB2	26:1:22:TYR:O	2.11	0.51
1:X:1030:U:O4	1:X:1031:C:N4	2.44	0.51
1:X:1270:C:O2'	5:C:78:VAL:HG12	2.11	0.51
1:X:2855:C:C2'	12:K:93:GLY:HA3	2.41	0.51
4:B:96:PHE:CE1	4:B:102:ILE:HG21	2.46	0.51



		Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
9:H:91:PHE:N	9:H:91:PHE:CD1	2.78	0.51
11:J:27:TYR:CG	11:J:28:VAL:N	2.78	0.51
17:P:9:ARG:HH11	17:P:13:GLN:HA	1.76	0.51
19:R:100:ASP:HB3	19:R:102:LYS:HD2	1.92	0.51
1:X:863:C:H42	1:X:940:G:H1	1.59	0.51
1:X:876:A:H2'	1:X:877:G:C8	2.46	0.51
1:X:1937:G:O2'	1:X:1939:U:O4	2.19	0.51
7:E:24:PHE:HE1	7:E:37:TYR:CE2	2.27	0.51
9:H:3:MET:HB2	9:H:4:PRO:HD2	1.93	0.51
20:S:54:ILE:HG13	20:S:62:PHE:HE1	1.75	0.51
1:X:1349:A:H2'	1:X:1350:G:C8	2.46	0.51
1:X:1705:U:O2	1:X:1717:A:H5'	2.11	0.51
1:X:2020:G:H2'	1:X:2021:G:H8	1.74	0.51
6:D:3:GLN:O	6:D:4:LEU:HD23	2.11	0.51
9:H:13:ASN:OD1	9:H:108:THR:N	2.43	0.51
18:Q:63:LYS:O	18:Q:70:GLY:HA3	2.10	0.51
1:X:487:G:H4'	1:X:512:A:N1	2.27	0.50
1:X:938:G:O2'	1:X:940:G:N7	2.33	0.50
1:X:1060:C:N4	1:X:1061:A:H62	2.09	0.50
1:X:1584:G:OP2	3:A:63:ARG:NH2	2.44	0.50
1:X:1954:A:O2'	3:A:239:ARG:HB3	2.11	0.50
1:X:2467:A:C2'	1:X:2468:G:H5'	2.41	0.50
7:E:22:GLY:O	7:E:37:TYR:HB2	2.11	0.50
9:H:29:ILE:HD13	9:H:123:PHE:CE1	2.45	0.50
16:O:70:TYR:HD2	16:O:83:ARG:HE	1.55	0.50
1:X:797:A:N7	3:A:229:VAL:HG21	2.27	0.50
1:X:957:G:H2'	1:X:958:G:C8	2.41	0.50
1:X:1422:C:H2'	1:X:1423:A:H8	1.76	0.50
1:X:1514:C:HO2'	1:X:1592:U:HO2'	1.58	0.50
1:X:2869:U:H2'	1:X:2870:C:C6	2.46	0.50
2:Y:17:A:H1'	2:Y:112:A:C8	2.47	0.50
5:C:191:ALA:O	5:C:195:ILE:HG12	2.11	0.50
10:I:118:VAL:HG12	10:I:119:THR:N	2.26	0.50
1:X:308:C:OP2	31:X:3244:SPD:N10	2.38	0.50
1:X:1690:U:H2'	1:X:1691:G:H5"	1.92	0.50
2:Y:6:C:H2'	2:Y:7:C:C6	2.46	0.50
4:B:14:ILE:HG13	14:M:20:HIS:CD2	2.45	0.50
4:B:105:THR:CG2	4:B:197:VAL:HB	2.40	0.50
13:L:33:ARG:NH2	13:L:68:ALA:HA	2.26	0.50
15:N:55:ARG:O	15:N:58:ARG:HB2	2.10	0.50
17:P:97:VAL:HG22	17:P:124:ILE:HG23	1.93	0.50



A 4 1		Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
22:U:47:HIS:CD2	22:U:48:LYS:H	2.30	0.50
1:X:330:C:H2'	1:X:331:U:O4'	2.11	0.50
1:X:543:G:C5	1:X:544:U:C4	2.99	0.50
1:X:649:G:H1	1:X:660:G:N2	2.08	0.50
2:Y:27:A:H2'	2:Y:27:A:N3	2.27	0.50
2:Y:39:C:H5'	2:Y:40:C:OP2	2.11	0.50
8:G:140:GLN:O	8:G:144:MET:HG3	2.11	0.50
16:O:40:VAL:CG1	16:O:43:GLU:HA	2.41	0.50
25:Z:16:ARG:HG3	25:Z:17:ASP:N	2.26	0.50
1:X:227:G:H5'	28:3:8:LYS:HZ2	1.77	0.50
1:X:393:U:H4'	22:U:19:ILE:O	2.11	0.50
1:X:1063:C:H2'	1:X:1064:C:C6	2.46	0.50
1:X:1436:G:N1	1:X:1593:C:O2	2.44	0.50
1:X:2372:A:OP1	28:3:30:ARG:HB2	2.12	0.50
2:Y:12:C:N3	2:Y:113:G:N1	2.39	0.50
17:P:107:ILE:HG13	17:P:107:ILE:O	2.11	0.50
1:X:1428:G:H22	1:X:1602:G:H5'	1.77	0.50
1:X:1563:U:H2'	1:X:1564:U:C6	2.46	0.50
1:X:2077:G:C6	1:X:2078:G:C2	2.99	0.50
1:X:2629:U:H2'	1:X:2630:C:H6	1.77	0.50
1:X:2796:A:H2'	1:X:2797:G:H8	1.77	0.50
2:Y:31:A:H2'	2:Y:32:C:C6	2.46	0.50
3:A:261:ARG:HG3	3:A:262:LYS:O	2.12	0.50
4:B:133:LYS:HB3	4:B:137:ARG:HH21	1.77	0.50
5:C:30:VAL:HG11	5:C:177:VAL:HG21	1.92	0.50
11:J:44:LYS:HB2	11:J:47:GLN:HG3	1.94	0.50
1:X:317:U:O2'	1:X:1224:A:N7	2.45	0.50
1:X:428:A:H2'	1:X:429:C:C6	2.47	0.50
1:X:847:C:C2	1:X:848:A:C8	2.99	0.50
1:X:2008:C:OP1	4:B:149:ARG:NH1	2.44	0.50
1:X:2292:C:H2'	1:X:2293:G:C8	2.47	0.50
1:X:2402:U:HO2'	1:X:2403:C:P	2.33	0.50
1:X:2546:G:H2'	1:X:2547:C:H6	1.77	0.50
10:I:101:ARG:C	10:I:118:VAL:HG13	2.32	0.50
1:X:306:G:H2'	1:X:307:C:H6	1.76	0.50
1:X:318:G:N2	1:X:320:A:H3'	2.27	0.50
1:X:393:U:H2'	1:X:394:U:C6	2.47	0.50
1:X:537:C:H1'	1:X:538:A:C6	2.47	0.50
1:X:732:G:H2'	1:X:733:G:H8	1.77	0.50
1:X:1050:G:H8	1:X:1050:G:O5'	1.95	0.50
1:X:2677:U:H2'	1:X:2678:C:C6	2.47	0.50



A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	$distance ({ m \AA})$	overlap (Å)
19:R:52:ASN:CG	19:R:73:GLU:HA	2.31	0.50
1:X:492:G:H1'	1:X:516:G:N2	2.27	0.50
1:X:1349:A:H2'	1:X:1350:G:H8	1.77	0.50
1:X:1656:U:H2'	1:X:1657:A:H5"	1.93	0.50
1:X:1870:U:H2'	1:X:1871:G:H5"	1.94	0.50
1:X:1989:C:O5'	1:X:1989:C:H6	1.95	0.50
1:X:2796:A:OP2	12:K:3:HIS:HE1	1.95	0.50
7:E:21:ASP:O	7:E:39:THR:HG22	2.12	0.50
20:S:63:PRO:HG2	20:S:88:TYR:HE2	1.77	0.50
20:S:113:VAL:HG22	20:S:171:VAL:HG22	1.93	0.50
1:X:231:G:O6	28:3:4:MET:HG3	2.12	0.49
1:X:265:U:O2'	1:X:266:U:O5'	2.30	0.49
1:X:1179:A:H2'	1:X:1180:A:C8	2.47	0.49
1:X:1816:G:O2'	3:A:252:LYS:HG3	2.12	0.49
5:C:56:ARG:HG2	5:C:57:LYS:N	2.14	0.49
11:J:27:TYR:CE2	11:J:137:VAL:O	2.65	0.49
25:Z:51:TYR:CE1	25:Z:55:ARG:HG2	2.34	0.49
1:X:1991:C:H2'	1:X:1992:G:C8	2.47	0.49
1:X:2241:U:H5	21:T:16:SER:HB3	1.77	0.49
8:G:97:ASP:O	8:G:99:VAL:HG23	2.11	0.49
13:L:28:ARG:HG3	13:L:90:ASP:HB2	1.94	0.49
20:S:3:LEU:CD1	20:S:34:LEU:HA	2.41	0.49
24:W:49:HIS:CD2	24:W:49:HIS:H	2.30	0.49
1:X:398:C:O2'	1:X:399:G:OP2	2.22	0.49
1:X:877:G:H2'	1:X:878:C:C6	2.47	0.49
1:X:1072:U:H4'	1:X:1081:A:O2'	2.12	0.49
1:X:1377:G:C5	22:U:6:TYR:N	2.79	0.49
1:X:1484:G:H2'	1:X:1485:U:C6	2.47	0.49
1:X:1504:G:H21	3:A:99:ASP:HA	1.77	0.49
1:X:1939:U:H1'	1:X:2531:U:OP1	2.13	0.49
1:X:2569:A:H2'	1:X:2570:C:C6	2.47	0.49
5:C:7:ILE:CG1	5:C:122:GLY:HA2	2.42	0.49
14:M:110:LEU:HB3	14:M:115:ALA:CB	2.41	0.49
17:P:9:ARG:NH1	17:P:13:GLN:HA	2.26	0.49
1:X:654:A:H2'	1:X:655:A:C5'	2.40	0.49
1:X:810:U:OP1	5:C:56:ARG:HD3	2.13	0.49
2:Y:58:G:H21	2:Y:60:A:H61	1.60	0.49
3:A:211:ARG:HD2	3:A:214:TRP:CE3	2.46	0.49
20:S:72:ASP:HB3	20:S:75:LYS:HB3	1.94	0.49
28:3:50:LEU:HD12	28:3:51:ALA:N	2.28	0.49
1:X:240:U:H2'	1:X:241:C:O4'	2.12	0.49



	A 4 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:X:339:U:H4'	19:R:77:HIS:ND1	2.27	0.49
1:X:1267:A:H5"	1:X:1268:U:H5"	1.94	0.49
1:X:1562:G:H8	1:X:1562:G:OP2	1.95	0.49
1:X:1581:C:H2'	3:A:21:PHE:CE2	2.48	0.49
1:X:1688:U:HO2'	1:X:1690:U:H5	1.60	0.49
1:X:1762:C:H2'	1:X:1763:G:C8	2.47	0.49
1:X:1827:G:H1	1:X:1888:C:H42	1.59	0.49
1:X:2011:U:H2'	1:X:2012:A:H8	1.78	0.49
3:A:210:GLY:HA2	3:A:213:ARG:CG	2.43	0.49
8:G:93:LYS:HB2	8:G:97:ASP:HB2	1.95	0.49
9:H:56:LYS:HD3	9:H:56:LYS:C	2.32	0.49
1:X:51:A:H2'	1:X:52:A:C8	2.48	0.49
1:X:618:A:H2'	1:X:619:A:H8	1.74	0.49
1:X:1034:U:H2'	1:X:1035:G:H5'	1.94	0.49
1:X:1607:A:H2'	1:X:1608:U:C6	2.48	0.49
1:X:1882:G:O2'	1:X:1883:A:H5"	2.11	0.49
1:X:1988:A:H5"	31:X:3240:SPD:C7	2.43	0.49
1:X:1989:C:O5'	1:X:1989:C:C6	2.66	0.49
1:X:2218:G:H5'	3:A:249:PRO:HG3	1.94	0.49
1:X:2604:G:H2'	1:X:2605:C:C6	2.47	0.49
5:C:56:ARG:CG	5:C:57:LYS:N	2.75	0.49
7:E:27:LYS:HA	7:E:31:GLY:HA3	1.94	0.49
1:X:636:G:H5"	1:X:637:G:OP2	2.12	0.49
1:X:2795:A:H4'	12:K:3:HIS:ND1	2.27	0.49
1:X:2796:A:H2'	1:X:2797:G:C8	2.48	0.49
2:Y:22:U:H2'	2:Y:23:G:C8	2.47	0.49
3:A:181:GLU:HG3	3:A:271:VAL:HB	1.93	0.49
5:C:176:ASN:ND2	5:C:178:TYR:HB3	2.27	0.49
7:E:83:TYR:CE2	7:E:138:LYS:HB2	2.48	0.49
15:N:66:ASN:O	15:N:70:ARG:HG3	2.12	0.49
18:Q:71:GLN:HG3	18:Q:72:ARG:O	2.12	0.49
22:U:43:ARG:HG2	22:U:44:ALA:H	1.78	0.49
1:X:198:A:H61	1:X:441:A:H62	1.61	0.49
1:X:531:G:H2'	1:X:532:A:H8	1.78	0.49
1:X:1050:G:H1'	1:X:1128:G:H22	1.78	0.49
1:X:1100:G:H22	1:X:1113:C:H42	1.60	0.49
1:X:1310:C:H2'	1:X:1311:C:C6	2.45	0.49
1:X:2561:G:H5'	1:X:2561:G:C8	2.48	0.49
3:A:16:MET:HE3	3:A:211:ARG:HD3	1.95	0.49
3:A:163:VAL:HG13	3:A:175:VAL:HB	1.95	0.49
4:B:27:LEU:HD22	4:B:51:TYR:OH	2.11	0.49



A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
6:D:132:ILE:HB	6:D:152:MET:O	2.13	0.49
7:E:17:VAL:HG21	7:E:50:LEU:HD11	1.94	0.49
1:X:249:A:H8	1:X:278:G:H21	1.56	0.49
1:X:1192:A:H5'	1:X:1193:G:OP2	2.13	0.49
1:X:1332:G:C2	1:X:1333:G:C2	3.00	0.49
1:X:1357:U:H4'	1:X:1397:A:C6	2.48	0.49
1:X:1429:A:C2	1:X:1603:A:H1'	2.47	0.49
1:X:1510:A:H8	1:X:1511:A:C8	2.31	0.49
2:Y:58:G:H4'	2:Y:59:A:O5'	2.13	0.49
7:E:98:LEU:HD12	7:E:102:ALA:O	2.12	0.49
12:K:52:ILE:HD11	12:K:94:TYR:CD2	2.47	0.49
13:L:70:ALA:HA	13:L:73:LYS:HE2	1.94	0.49
20:S:71:MET:CB	20:S:78:PRO:HA	2.42	0.49
1:X:1043:A:H2	1:X:1133:G:H1	1.60	0.49
1:X:1255:A:H2'	1:X:1256:C:H6	1.76	0.49
1:X:1712:G:C8	3:A:8:PRO:HB2	2.48	0.49
1:X:1948:C:H5"	1:X:1949:A:H2'	1.94	0.49
1:X:2362:G:H2'	1:X:2363:G:C8	2.48	0.49
1:X:2594:U:C2	25:Z:7:PRO:HA	2.48	0.49
1:X:2672:U:H2'	1:X:2673:G:C8	2.45	0.49
4:B:87:ASP:N	4:B:87:ASP:OD1	2.45	0.49
5:C:46:ARG:CD	5:C:51:VAL:HG12	2.43	0.49
9:H:80:ALA:HA	9:H:90:ARG:HG2	1.94	0.49
12:K:100:VAL:HG23	12:K:101:GLY:N	2.28	0.49
14:M:29:PRO:CG	14:M:99:VAL:HG11	2.43	0.49
15:N:94:VAL:HG23	15:N:94:VAL:O	2.13	0.49
16:O:35:LEU:HD23	16:O:35:LEU:H	1.77	0.49
20:S:154:LEU:HD11	20:S:160:LEU:HB2	1.95	0.49
1:X:219:G:O2'	1:X:220:U:P	2.71	0.48
1:X:439:C:H2'	1:X:440:U:O4'	2.13	0.48
1:X:1520:G:H2'	1:X:1521:U:O4'	2.13	0.48
3:A:65:ILE:CG2	3:A:88:ARG:HH21	2.25	0.48
5:C:6:VAL:HG22	5:C:7:ILE:HG12	1.94	0.48
5:C:41:GLY:HA3	5:C:89:ARG:O	2.13	0.48
18:Q:56:MET:HE3	18:Q:77:LYS:HE3	1.95	0.48
1:X:839:U:H5"	1:X:2408:G:OP2	2.12	0.48
1:X:2073:A:C6	1:X:2209:G:C6	3.01	0.48
1:X:2705:A:O2'	1:X:2706:U:C6	2.66	0.48
9:H:116:ARG:NE	14:M:38:LYS:HD2	2.28	0.48
11:J:64:LYS:HE3	11:J:110:VAL:HG22	1.94	0.48
14:M:44:ARG:NH2	14:M:46:ARG:HH21	2.11	0.48



		Interatomic	Clash
Atom-1	Atom-2	$distance ({ m \AA})$	overlap (Å)
20:S:69:VAL:HG13	20:S:81:VAL:HG22	1.94	0.48
26:1:9:ILE:HG22	26:1:28:ARG:HA	1.94	0.48
1:X:30:G:C6	1:X:31:C:C4	3.01	0.48
1:X:1753:A:H3'	31:X:3243:SPD:H21	1.94	0.48
1:X:2344:G:H4'	21:T:60:PHE:CZ	2.49	0.48
1:X:2369:U:O5'	1:X:2369:U:H6	1.97	0.48
1:X:2398:U:O4	28:3:31:HIS:ND1	2.46	0.48
16:O:70:TYR:HE2	16:O:83:ARG:HH11	1.57	0.48
1:X:63:A:C4	18:Q:65:VAL:HG21	2.48	0.48
1:X:417:C:H4'	1:X:418:C:O5'	2.13	0.48
1:X:1134:C:H2'	1:X:1135:C:C6	2.48	0.48
1:X:1370:U:H3'	1:X:1371:G:C8	2.49	0.48
1:X:2424:G:O2'	1:X:2425:G:H5'	2.13	0.48
1:X:2738:A:C6	7:E:67:LEU:HD11	2.49	0.48
4:B:2:LYS:HE2	4:B:95:ILE:HB	1.94	0.48
5:C:13:ARG:NE	5:C:13:ARG:HA	2.28	0.48
10:I:86:THR:HA	10:I:89:ASP:CG	2.34	0.48
15:N:66:ASN:HD22	15:N:70:ARG:HH21	1.61	0.48
18:Q:29:VAL:HG21	18:Q:38:ILE:HD12	1.95	0.48
19:R:93:ARG:HG3	19:R:94:VAL:N	2.29	0.48
20:S:49:THR:OG1	20:S:132:GLN:HA	2.13	0.48
1:X:247:A:N1	1:X:382:U:H4'	2.28	0.48
1:X:500:G:O5'	1:X:500:G:H8	1.96	0.48
1:X:772:G:O2'	1:X:773:G:H5'	2.13	0.48
1:X:1425:G:H2'	1:X:1426:U:C6	2.48	0.48
1:X:2074:U:H1'	22:U:48:LYS:HE2	1.96	0.48
1:X:2663:U:C2	1:X:2664:G:C8	3.01	0.48
2:Y:50:U:O3'	13:L:97:HIS:NE2	2.47	0.48
2:Y:54:U:H2'	2:Y:55:C:O4'	2.13	0.48
7:E:42:THR:OG1	7:E:53:GLU:O	2.28	0.48
8:G:44:VAL:CG1	8:G:54:LEU:HD11	2.41	0.48
8:G:63:ARG:HA	8:G:63:ARG:HD2	1.62	0.48
11:J:105:PHE:HA	11:J:106:GLU:OE1	2.14	0.48
18:Q:12:ILE:HD12	18:Q:12:ILE:O	2.12	0.48
20:S:63:PRO:HG2	20:S:88:TYR:CE2	2.48	0.48
22:U:28:GLY:HA3	22:U:34:THR:HA	1.94	0.48
26:1:21:TYR:CD2	26:1:50:PHE:HZ	2.30	0.48
1:X:531:G:H2'	1:X:532:A:C8	2.49	0.48
1:X:626:A:H5'	5:C:38:ARG:HH12	1.79	0.48
1:X:751:G:H2'	1:X:752:G:C8	2.49	0.48
1:X:1029:C:H2'	1:X:1030:U:C6	2.49	0.48



		Interatomic	Clash
Atom-1	Atom-2	$distance ({ m \AA})$	overlap (Å)
1:X:1104:G:H2'	1:X:1105:U:C5	2.48	0.48
1:X:1608:U:H2'	1:X:1609:G:C8	2.49	0.48
5:C:149:LEU:HD23	5:C:180:ILE:HG22	1.94	0.48
9:H:83:ARG:HH12	9:H:134:LEU:HD21	1.77	0.48
11:J:78:LYS:HG2	11:J:79:PRO:HD2	1.95	0.48
12:K:92:GLY:HA2	12:K:94:TYR:CE2	2.49	0.48
22:U:9:GLY:C	22:U:10:LYS:HD3	2.34	0.48
22:U:27:ASP:HB3	22:U:32:ARG:CB	2.44	0.48
28:3:52:LYS:HZ2	28:3:56:ALA:HB2	1.77	0.48
1:X:936:A:H2'	1:X:937:C:C6	2.48	0.48
1:X:1665:C:OP1	31:X:3238:SPD:C5	2.61	0.48
5:C:164:VAL:CG1	5:C:167:VAL:HG22	2.44	0.48
10:I:53:ARG:HD3	28:3:12:ARG:NH2	2.28	0.48
17:P:58:ARG:HE	25:Z:39:LYS:CE	2.27	0.48
18:Q:27:PHE:CE2	18:Q:42:ILE:HD12	2.48	0.48
28:3:47:GLY:O	28:3:48:PHE:HB3	2.13	0.48
1:X:615:C:O2	1:X:670:U:O2'	2.32	0.48
1:X:1422:C:H2'	1:X:1423:A:C8	2.49	0.48
1:X:2029:G:H5'	25:Z:19:ARG:HG2	1.96	0.48
1:X:2284:U:N3	1:X:2285:U:O4	2.47	0.48
1:X:2299:A:H4'	1:X:2300:G:C4	2.48	0.48
1:X:2498:U:C5	1:X:2520:A:C6	3.02	0.48
2:Y:14:C:H3'	2:Y:14:C:H6	1.78	0.48
3:A:41:GLY:O	3:A:43:ARG:N	2.44	0.48
3:A:52:ARG:O	3:A:53:PHE:HB2	2.14	0.48
5:C:48:ARG:NH1	5:C:74:VAL:HG12	2.28	0.48
8:G:94:LYS:HE2	8:G:117:GLU:HG2	1.96	0.48
15:N:78:THR:HB	15:N:117:ARG:CZ	2.43	0.48
28:3:36:LYS:HG2	28:3:37:SER:N	2.25	0.48
1:X:310:A:H8	1:X:310:A:OP2	1.97	0.48
1:X:356:A:H2	1:X:357:A:H62	1.57	0.48
1:X:500:G:H2'	1:X:501:G:O4'	2.12	0.48
1:X:537:C:O2'	1:X:538:A:P	2.72	0.48
1:X:540:G:O6	1:X:2006:G:OP1	2.32	0.48
1:X:2237:C:H5"	1:X:2237:C:H6	1.78	0.48
1:X:79:G:H1'	1:X:356:A:H2	1.79	0.48
1:X:538:A:C2	1:X:2025:A:C6	3.02	0.48
1:X:1581:C:H2'	3:A:21:PHE:HE2	1.79	0.48
1:X:1670:G:C5'	12:K:2:ARG:HD2	2.42	0.48
1:X:2311:U:C4'	1:X:2315:A:H62	2.26	0.48
1:X:2368:G:H5"	1:X:2369:U:H5'	1.96	0.48



		Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:X:2441:U:H2'	1:X:2442:C:H6	1.78	0.48
1:X:2446:C:H2'	1:X:2447:G:O4'	2.14	0.48
1:X:2533:U:H2'	1:X:2534:U:C5	2.48	0.48
22:U:48:LYS:HD2	22:U:49:LYS:N	2.29	0.48
1:X:109:A:H5"	23:V:62:ARG:NH2	2.29	0.47
1:X:1750:A:H4'	1:X:2695:C:O4'	2.14	0.47
1:X:2513:A:C2	1:X:2514:G:H1'	2.48	0.47
3:A:239:ARG:O	3:A:240:THR:HG23	2.14	0.47
4:B:93:VAL:CG2	4:B:94:ASP:N	2.77	0.47
14:M:55:ILE:O	14:M:103:LYS:O	2.32	0.47
20:S:1:MET:N	20:S:52:PHE:HE2	2.12	0.47
1:X:384:A:O2'	1:X:386:U:O4'	2.31	0.47
1:X:545:C:H2'	1:X:546:A:H8	1.78	0.47
1:X:1085:G:H2'	1:X:1086:C:H5	1.79	0.47
1:X:1681:A:N1	1:X:2706:U:C6	2.82	0.47
1:X:2278:A:H2'	1:X:2279:G:C8	2.48	0.47
1:X:2399:C:P	28:3:34:THR:H	2.37	0.47
1:X:2675:U:H2'	1:X:2676:G:C8	2.50	0.47
6:D:6:THR:O	6:D:10:ASP:N	2.40	0.47
9:H:116:ARG:NH1	14:M:41:GLU:OE2	2.46	0.47
9:H:117:GLU:H	9:H:117:GLU:HG2	1.41	0.47
1:X:67:G:H2'	1:X:68:C:C6	2.49	0.47
1:X:780:U:O2'	1:X:781:G:H5'	2.15	0.47
1:X:1212:U:H2'	1:X:1213:U:H6	1.79	0.47
1:X:1332:G:C6	1:X:1333:G:N1	2.83	0.47
1:X:1608:U:H2'	1:X:1609:G:H8	1.78	0.47
1:X:2721:A:H2'	1:X:2722:C:O4'	2.14	0.47
1:X:2760:G:N1	8:G:128:GLU:OE2	2.47	0.47
1:X:2819:G:H2'	1:X:2820:C:C6	2.49	0.47
9:H:81:ILE:HD11	9:H:117:GLU:CG	2.43	0.47
1:X:599:A:O2'	1:X:600:G:H5'	2.13	0.47
1:X:834:A:H5'	1:X:835:U:C6	2.49	0.47
1:X:1329:U:H2'	1:X:1330:G:C8	2.49	0.47
1:X:1412:C:H2'	1:X:1413:U:H6	1.80	0.47
1:X:1469:U:H5"	1:X:1470:G:C8	2.48	0.47
1:X:2474:G:OP1	11:J:83:ARG:HG3	2.14	0.47
3:A:70:ARG:HA	3:A:190:TYR:HE2	1.80	0.47
4:B:32:PRO:HD2	4:B:50:GLY:O	2.15	0.47
6:D:13:ARG:HA	6:D:16:LEU:HD23	1.97	0.47
11:J:33:TYR:O	11:J:106:GLU:HA	2.14	0.47
12:K:84:ALA:N	12:K:85:PRO:HD2	2.30	0.47



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	$distance ({ m \AA})$	overlap (Å)
15:N:10:ARG:O	15:N:14:HIS:HD2	1.97	0.47
16:O:65:ARG:HG2	16:O:87:ARG:HG2	1.95	0.47
1:X:1193:G:H2'	1:X:1194:U:H6	1.80	0.47
1:X:1278:A:H61	1:X:1996:A:H5"	1.78	0.47
1:X:1468:A:H8	1:X:1468:A:C5'	2.22	0.47
1:X:2186:G:H2'	1:X:2187:A:H8	1.78	0.47
1:X:2188:A:H5"	1:X:2189:A:OP2	2.15	0.47
1:X:2270:U:H2'	1:X:2271:C:C6	2.50	0.47
2:Y:25:G:H2'	2:Y:26:G:N7	2.28	0.47
7:E:17:VAL:HG22	7:E:26:VAL:HG22	1.96	0.47
11:J:134:LYS:HD2	11:J:135:ARG:N	2.30	0.47
20:S:146:HIS:HB3	20:S:170:SER:OG	2.14	0.47
24:W:36:ASP:HA	24:W:41:ARG:NH2	2.29	0.47
1:X:525:A:C8	1:X:526:C:C6	3.03	0.47
1:X:2277:A:H1'	1:X:2300:G:N2	2.29	0.47
1:X:2394:G:H2'	1:X:2395:C:C6	2.50	0.47
1:X:2477:C:O2'	1:X:2478:C:H5'	2.15	0.47
6:D:13:ARG:O	6:D:16:LEU:HB2	2.14	0.47
6:D:53:ALA:HA	6:D:56:GLU:HG2	1.95	0.47
1:X:78:C:H2'	1:X:79:G:C8	2.50	0.47
1:X:203:G:H2'	1:X:204:A:C8	2.49	0.47
1:X:487:G:H22	1:X:490:A:C5'	2.26	0.47
1:X:683:A:OP1	10:I:40:ARG:NE	2.48	0.47
1:X:1070:G:H5"	1:X:1071:U:C2'	2.44	0.47
1:X:1073:G:N2	1:X:1074:G:N7	2.60	0.47
1:X:1255:A:H2'	1:X:1256:C:C6	2.50	0.47
1:X:1801:C:N4	22:U:48:LYS:HB2	2.30	0.47
1:X:2187:A:H5'	3:A:151:LYS:CB	2.44	0.47
1:X:2217:G:H2'	1:X:2217:G:N3	2.30	0.47
1:X:2677:U:H2'	1:X:2678:C:H6	1.79	0.47
1:X:2698:G:H4'	14:M:103:LYS:HG3	1.96	0.47
5:C:182:ARG:HE	5:C:183:HIS:CE1	2.33	0.47
6:D:54:ALA:HB1	6:D:65:PRO:HG2	1.96	0.47
8:G:35:LYS:C	8:G:35:LYS:HD2	2.35	0.47
8:G:51:LEU:HB2	8:G:88:VAL:CG2	2.43	0.47
10:I:58:ALA:HB2	28:3:11:LYS:HB3	1.96	0.47
12:K:56:LYS:NZ	12:K:88:ALA:HA	2.30	0.47
14:M:44:ARG:HH21	14:M:46:ARG:HH21	1.63	0.47
23:V:49:GLU:O	23:V:53:LEU:HB2	2.13	0.47
1:X:23:G:C2	1:X:24:G:C8	3.03	0.47
1:X:312:G:C6	1:X:328:A:C6	3.03	0.47



<u> </u>	h	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:X:404:A:H2'	1:X:404:A:N3	2.29	0.47
1:X:540:G:N2	1:X:2005:U:OP1	2.47	0.47
1:X:640:C:C4'	1:X:660:G:H21	2.26	0.47
1:X:691:C:H2'	1:X:692:C:C6	2.50	0.47
1:X:742:G:OP2	3:A:13:ARG:NH2	2.48	0.47
1:X:834:A:H5'	1:X:835:U:H6	1.77	0.47
1:X:1602:G:H5"	1:X:1603:A:OP2	2.14	0.47
1:X:1920:A:O2'	1:X:1921:A:H5'	2.15	0.47
2:Y:23:G:H2'	2:Y:24:U:H6	1.80	0.47
3:A:4:LYS:HB2	3:A:18:THR:CG2	2.42	0.47
4:B:61:LYS:N	4:B:62:PRO:HD2	2.30	0.47
6:D:81:GLN:HG3	6:D:82:GLY:N	2.29	0.47
8:G:54:LEU:HD12	8:G:54:LEU:HA	1.69	0.47
8:G:132:PHE:CE2	8:G:145:HIS:HD2	2.32	0.47
10:I:52:GLY:O	10:I:53:ARG:NH1	2.48	0.47
11:J:66:TYR:HB2	11:J:106:GLU:CG	2.45	0.47
13:L:56:SER:HB2	13:L:71:VAL:HG11	1.97	0.47
14:M:44:ARG:HH21	14:M:46:ARG:NH2	2.13	0.47
15:N:52:ASN:O	15:N:55:ARG:HG2	2.15	0.47
16:O:15:SER:HA	16:O:95:ILE:HB	1.97	0.47
27:2:41:GLN:O	27:2:43:THR:N	2.47	0.47
1:X:870:C:H4'	21:T:23:VAL:HG21	1.96	0.47
1:X:1068:A:H2'	1:X:1068:A:N3	2.30	0.47
1:X:1142:G:O3'	8:G:110:LEU:HD22	2.15	0.47
1:X:1573:G:O5'	1:X:1574:A:H5"	2.14	0.47
1:X:1865:C:H3'	1:X:1866:G:C8	2.49	0.47
1:X:2196:U:H5'	1:X:2197:U:OP2	2.15	0.47
1:X:2324:G:N3	1:X:2360:C:H2'	2.29	0.47
1:X:2433:G:C4	1:X:2434:G:C8	3.03	0.47
1:X:2546:G:H2'	1:X:2547:C:C6	2.49	0.47
2:Y:52:G:C2	2:Y:53:G:C8	3.03	0.47
9:H:70:VAL:HG13	9:H:98:ILE:HG23	1.96	0.47
1:X:824:U:C4	10:I:21:ARG:NH2	2.83	0.47
1:X:1430:G:O2'	1:X:1431:U:O5'	2.33	0.47
1:X:2310:G:N2	1:X:2364:C:C4	2.83	0.47
1:X:2371:A:H2	1:X:2403:C:H42	1.61	0.47
2:Y:23:G:H2'	2:Y:24:U:C6	2.50	0.47
3:A:34:THR:C	3:A:36:ALA:N	2.68	0.47
4:B:105:THR:HG22	4:B:197:VAL:HB	1.96	0.47
6:D:56:GLU:O	6:D:60:ILE:HG12	2.15	0.47
9:H:22:ILE:HD13	9:H:22:ILE:HG21	1.63	0.47



A 4 1		Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
9:H:89:ILE:CD1	9:H:134:LEU:HD22	2.45	0.47
15:N:10:ARG:HG2	15:N:14:HIS:HD2	1.79	0.47
15:N:88:ILE:CB	16:O:49:GLU:HB2	2.45	0.47
18:Q:64:ARG:HD3	18:Q:67:ARG:CA	2.44	0.47
1:X:686:C:OP1	5:C:48:ARG:CD	2.63	0.46
1:X:751:G:O2'	1:X:752:G:OP1	2.30	0.46
1:X:1715:A:C8	1:X:1717:A:O4'	2.68	0.46
1:X:2395:C:OP1	10:I:57:ILE:HG22	2.15	0.46
5:C:154:ASP:HB2	5:C:157:THR:OG1	2.15	0.46
9:H:91:PHE:N	9:H:91:PHE:HD1	2.13	0.46
1:X:879:A:H2'	1:X:879:A:N3	2.30	0.46
1:X:1788:C:O2'	3:A:257:LEU:HD12	2.14	0.46
1:X:2696:A:O2'	1:X:2697:G:H5'	2.16	0.46
1:X:2705:A:O2'	1:X:2706:U:P	2.73	0.46
2:Y:51:G:H2'	2:Y:52:G:C8	2.48	0.46
13:L:9:ARG:C	13:L:11:LEU:N	2.67	0.46
1:X:129:A:H2'	1:X:130:C:C6	2.50	0.46
1:X:1776:A:C8	1:X:1778:U:C5	3.03	0.46
1:X:2262:C:C6	1:X:2368:G:H2'	2.50	0.46
1:X:2630:C:H2'	1:X:2631:C:H6	1.80	0.46
4:B:146:THR:H	4:B:147:PRO:HD2	1.80	0.46
7:E:32:GLU:O	7:E:34:THR:HG23	2.16	0.46
19:R:16:PHE:HZ	19:R:46:VAL:HG22	1.81	0.46
1:X:1810:U:H2'	3:A:154:GLN:O	2.16	0.46
1:X:2042:A:O3'	5:C:63:GLY:HA2	2.15	0.46
1:X:2274:C:H2'	1:X:2275:U:H5'	1.97	0.46
2:Y:36:A:H4'	2:Y:37:C:OP1	2.16	0.46
4:B:136:ARG:HD3	4:B:136:ARG:HA	1.77	0.46
5:C:148:VAL:CG2	5:C:167:VAL:HG12	2.45	0.46
7:E:97:LYS:HG3	7:E:98:LEU:N	2.22	0.46
12:K:10:LEU:HD23	12:K:10:LEU:HA	1.69	0.46
14:M:13:LEU:HA	14:M:13:LEU:HD13	1.63	0.46
17:P:45:ILE:HD11	17:P:57:LEU:CG	2.45	0.46
17:P:59:PHE:HD2	25:Z:30:LEU:HD11	1.80	0.46
20:S:1:MET:H3	20:S:52:PHE:HE2	1.61	0.46
22:U:10:LYS:HD2	22:U:63:SER:HB3	1.97	0.46
22:U:10:LYS:HG3	22:U:66:ALA:HB2	1.98	0.46
1:X:125:A:H5"	1:X:126:C:C6	2.50	0.46
1:X:143:A:H2'	1:X:144:U:C6	2.51	0.46
1:X:242:A:N3	1:X:243:G:H8	2.13	0.46
1:X:2065:A:P	22:U:20:ARG:HH12	2.38	0.46



	Atom 0	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:C:39:ARG:CZ	5:C:91:TYR:CE2	2.99	0.46
5:C:53:LYS:O	5:C:54:THR:HG23	2.15	0.46
6:D:158:THR:HG21	6:D:169:LEU:HD22	1.98	0.46
7:E:89:LEU:HD23	7:E:107:ILE:HG21	1.96	0.46
10:I:66:ASN:O	10:I:100:ARG:N	2.43	0.46
11:J:27:TYR:HE2	11:J:137:VAL:O	1.98	0.46
1:X:597:U:H5"	10:I:16:ARG:NH1	2.31	0.46
1:X:797:A:H5"	3:A:227:ASN:ND2	2.31	0.46
1:X:1005:U:O2	16:O:6:GLN:NE2	2.47	0.46
1:X:1352:G:OP2	18:Q:77:LYS:NZ	2.49	0.46
1:X:1484:G:H2'	1:X:1485:U:H6	1.79	0.46
1:X:1594:U:H2'	1:X:1595:A:H8	1.80	0.46
1:X:1655:C:H4'	1:X:2689:C:O2	2.15	0.46
1:X:1790:G:H4'	1:X:1791:C:O5'	2.16	0.46
1:X:1925:C:H2'	1:X:1926:U:H5	1.81	0.46
1:X:2261:G:H5"	1:X:2262:C:O4'	2.14	0.46
1:X:2295:C:H2'	1:X:2296:U:H6	1.80	0.46
1:X:2422:C:O2'	1:X:2423:G:H5'	2.16	0.46
5:C:142:LEU:HD22	5:C:148:VAL:HG11	1.97	0.46
9:H:14:SER:O	9:H:16:ALA:N	2.49	0.46
10:I:53:ARG:HA	10:I:53:ARG:NE	2.30	0.46
11:J:64:LYS:O	11:J:107:VAL:HA	2.16	0.46
13:L:64:LYS:HD2	13:L:64:LYS:N	2.28	0.46
22:U:47:HIS:CG	22:U:48:LYS:N	2.84	0.46
1:X:205:A:H2'	1:X:206:U:H5'	1.97	0.46
1:X:260:U:H5'	1:X:261:G:OP2	2.15	0.46
1:X:1398:G:HO2'	1:X:1399:C:H6	1.61	0.46
1:X:1673:C:C2	1:X:1674:C:C5	3.04	0.46
1:X:1778:U:H2'	1:X:1779:C:H6	1.81	0.46
1:X:2270:U:H2'	1:X:2271:C:H6	1.80	0.46
1:X:2362:G:H2'	1:X:2363:G:H8	1.80	0.46
1:X:2403:C:H2'	1:X:2408:G:O2'	2.15	0.46
1:X:2495:G:O2'	1:X:2496:C:H5'	2.16	0.46
8:G:68:PRO:HB2	8:G:70:PHE:CD1	2.50	0.46
17:P:25:PHE:HD1	17:P:25:PHE:C	2.18	0.46
22:U:43:ARG:HG2	22:U:44:ALA:N	2.31	0.46
28:3:14:ILE:HD13	28:3:24:ALA:HB2	1.97	0.46
1:X:38:G:H2'	1:X:39:C:H6	1.75	0.46
1:X:814:G:C1'	5:C:48:ARG:HH21	2.27	0.46
1:X:836:G:H2'	1:X:837:U:C6	2.50	0.46
1:X:838:A:H2'	1:X:839:U:O4'	2.16	0.46



	t i c	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:X:1412:C:H2'	1:X:1413:U:C6	2.51	0.46
1:X:1834:G:H2'	1:X:1835:C:H6	1.81	0.46
1:X:2307:A:H2'	1:X:2308:A:H8	1.80	0.46
1:X:2528:G:C2	1:X:2529:G:N7	2.83	0.46
3:A:166:GLN:HB2	3:A:174:ILE:HB	1.96	0.46
7:E:27:LYS:HG2	7:E:32:GLU:H	1.80	0.46
17:P:59:PHE:CE2	25:Z:39:LYS:HG3	2.51	0.46
1:X:122:G:C2	27:2:19:ARG:NH2	2.84	0.46
1:X:133:C:C5	1:X:134:G:H1'	2.51	0.46
1:X:1739:G:H2'	1:X:1740:G:C8	2.51	0.46
1:X:2839:G:H2'	1:X:2840:U:C6	2.50	0.46
5:C:39:ARG:HD3	5:C:91:TYR:CD2	2.51	0.46
7:E:97:LYS:HD2	7:E:97:LYS:HA	1.78	0.46
9:H:88:THR:O	14:M:79:ARG:HG3	2.16	0.46
10:I:55:ARG:NH1	28:3:25:PHE:HB2	2.30	0.46
10:I:79:GLN:C	10:I:80:LEU:HD23	2.35	0.46
13:L:11:LEU:O	13:L:14:ARG:HG2	2.16	0.46
13:L:33:ARG:HG2	13:L:38:ILE:HD12	1.97	0.46
27:2:39:ARG:O	27:2:40:HIS:CB	2.64	0.46
28:3:24:ALA:H	28:3:48:PHE:HA	1.81	0.46
1:X:19:C:OP2	15:N:30:LYS:NZ	2.49	0.46
1:X:242:A:O3'	1:X:243:G:O4'	2.34	0.46
1:X:1056:U:OP1	1:X:1057:A:H5"	2.16	0.46
1:X:1326:U:H2'	1:X:1626:A:C2	2.51	0.46
1:X:1408:A:O2'	1:X:1409:U:O5'	2.32	0.46
1:X:1448:A:H61	1:X:1574:A:N6	2.10	0.46
4:B:2:LYS:HA	4:B:84:PHE:CE1	2.51	0.46
4:B:119:ARG:HG2	4:B:120:TRP:CD1	2.50	0.46
5:C:58:MET:O	5:C:59:TYR:HB3	2.17	0.46
7:E:86:ASN:HB2	7:E:165:VAL:CG1	2.46	0.46
7:E:107:ILE:O	7:E:107:ILE:HG13	2.16	0.46
14:M:66:PHE:HD1	14:M:83:PHE:CE1	2.33	0.46
1:X:548:G:H5'	8:G:33:ILE:HD11	1.98	0.45
1:X:796:A:H8	1:X:797:A:H4'	1.80	0.45
1:X:1488:G:H3'	1:X:1489:C:C5'	2.46	0.45
1:X:1982:C:H5"	1:X:2703:C:O2'	2.16	0.45
1:X:2500:C:H2'	1:X:2501:U:C6	2.51	0.45
4:B:135:HIS:ND1	4:B:136:ARG:HG2	2.31	0.45
7:E:86:ASN:HB2	7:E:165:VAL:HG12	1.97	0.45
17:P:103:LEU:H	17:P:103:LEU:HD12	1.81	0.45
1:X:1022:A:H2'	1:X:1024:G:H5"	1.97	0.45



		Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:X:1781:C:H2'	1:X:1782:A:N7	2.31	0.45
1:X:2086:U:H2'	1:X:2087:U:C5	2.51	0.45
2:Y:46:G:N3	2:Y:49:C:N4	2.64	0.45
7:E:136:ILE:HG13	7:E:137:ASP:N	2.30	0.45
9:H:34:LEU:HD12	9:H:101:ASN:HA	1.98	0.45
10:I:83:LEU:HD21	10:I:99:VAL:CG1	2.39	0.45
10:I:101:ARG:N	10:I:118:VAL:HG22	2.23	0.45
16:O:17:GLY:HA2	16:O:94:LYS:HA	1.97	0.45
19:R:25:LEU:HD12	19:R:25:LEU:O	2.17	0.45
20:S:7:PRO:HB3	20:S:11:LYS:CD	2.41	0.45
1:X:492:G:H1'	1:X:516:G:H22	1.81	0.45
1:X:540:G:C8	1:X:540:G:H3'	2.51	0.45
1:X:748:A:H3'	1:X:749:C:H6	1.82	0.45
1:X:1790:G:C2	3:A:155:LEU:HD23	2.50	0.45
1:X:1807:A:H4'	1:X:1808:C:OP1	2.16	0.45
1:X:1810:U:O4	3:A:154:GLN:HG3	2.15	0.45
1:X:2447:G:O2'	1:X:2448:A:C8	2.69	0.45
1:X:2639:A:H2'	1:X:2640:G:O4'	2.16	0.45
2:Y:12:C:H2'	2:Y:13:C:O4'	2.16	0.45
2:Y:29:C:O2'	13:L:37:HIS:HE1	1.99	0.45
5:C:39:ARG:CZ	5:C:91:TYR:HE2	2.29	0.45
6:D:19:GLN:HG3	6:D:20:PHE:N	2.27	0.45
9:H:83:ARG:HH12	9:H:134:LEU:CD2	2.30	0.45
24:W:25:LEU:HD22	24:W:30:ASP:CB	2.39	0.45
26:1:36:GLU:OE1	26:1:36:GLU:N	2.49	0.45
1:X:88:G:OP2	1:X:89:A:H3'	2.16	0.45
1:X:231:G:O2'	1:X:397:U:H5'	2.16	0.45
1:X:724:C:H3'	1:X:725:C:OP1	2.16	0.45
1:X:1085:G:C2	1:X:1086:C:N4	2.84	0.45
1:X:1165:G:H5"	1:X:1166:A:OP2	2.16	0.45
1:X:1336:G:H2'	1:X:1337:G:H5'	1.99	0.45
1:X:1385:C:H2'	1:X:1386:A:O4'	2.17	0.45
1:X:2262:C:H2'	1:X:2263:C:O4'	2.16	0.45
1:X:2367:A:N7	1:X:2368:G:C6	2.84	0.45
2:Y:8:C:HO2'	13:L:39:TYR:HE2	1.64	0.45
5:C:125:ILE:HD12	5:C:125:ILE:O	2.17	0.45
8:G:124:GLU:O	8:G:128:GLU:HB2	2.17	0.45
10:I:19:VAL:CG1	10:I:30:ALA:HB1	2.47	0.45
11:J:40:PRO:HB3	11:J:99:LYS:HZ3	1.80	0.45
11:J:99:LYS:HE3	11:J:100:PRO:HD2	1.99	0.45
20:S:49:THR:HG22	20:S:95:SER:O	2.16	0.45



		Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:X:2352:A:H2'	1:X:2353:G:C8	2.52	0.45
1:X:2492:G:N2	4:B:143:GLN:HE21	2.14	0.45
2:Y:120:G:C6	2:Y:121:G:N7	2.84	0.45
8:G:114:THR:HG22	8:G:119:LEU:CD2	2.47	0.45
14:M:113:LYS:O	14:M:116:ARG:HD2	2.16	0.45
16:O:5:ILE:C	16:O:7:THR:H	2.19	0.45
17:P:35:PRO:O	17:P:39:ARG:HG3	2.15	0.45
20:S:124:ALA:HA	20:S:158:CYS:SG	2.56	0.45
28:3:6:THR:HG22	28:3:59:LYS:HB3	1.98	0.45
1:X:399:G:H5'	1:X:401:G:N2	2.31	0.45
1:X:791:G:H5'	3:A:48:ARG:CZ	2.46	0.45
1:X:792:U:OP1	3:A:49:ILE:HG13	2.15	0.45
1:X:1161:U:H2'	1:X:1162:A:H8	1.81	0.45
1:X:1246:G:C5	1:X:1247:U:C5	3.05	0.45
1:X:1587:A:H2'	1:X:1588:A:C8	2.51	0.45
1:X:2855:C:H2'	12:K:93:GLY:HA3	1.99	0.45
2:Y:46:G:H21	2:Y:50:U:H1'	1.81	0.45
3:A:6:TYR:HB2	3:A:13:ARG:O	2.17	0.45
12:K:97:ILE:HG13	12:K:113:ILE:CD1	2.46	0.45
1:X:45:C:OP2	1:X:192:G:H2'	2.16	0.45
1:X:476:G:OP1	27:2:12:ARG:NH2	2.50	0.45
1:X:788:G:C5	1:X:807:A:C8	3.05	0.45
1:X:817:A:H5"	1:X:818:G:OP1	2.17	0.45
1:X:930:A:N3	2:Y:82:U:O2'	2.42	0.45
1:X:1433:A:O2'	1:X:1434:U:OP1	2.35	0.45
1:X:1474:A:H2'	1:X:1474:A:N3	2.32	0.45
1:X:2487:G:C2	1:X:2561:G:C6	3.04	0.45
1:X:2557:G:C2	1:X:2558:C:C5	3.05	0.45
1:X:2701:A:H2'	1:X:2702:G:O4'	2.16	0.45
2:Y:69:G:C8	2:Y:69:G:OP1	2.70	0.45
3:A:14:ARG:HG3	3:A:15:GLN:N	2.32	0.45
6:D:142:THR:HG22	6:D:144:ASP:H	1.81	0.45
6:D:166:ALA:O	6:D:169:LEU:HG	2.16	0.45
8:G:52:GLY:O	8:G:55:ALA:HB3	2.16	0.45
10:I:27:ASP:OD1	10:I:27:ASP:N	2.50	0.45
14:M:64:LYS:HE3	14:M:83:PHE:CE2	2.52	0.45
17:P:96:TYR:CE1	17:P:125:THR:OG1	2.68	0.45
22:U:14:VAL:HG12	22:U:15:VAL:N	2.27	0.45
1:X:858:G:O5'	1:X:858:G:H8	2.00	0.45
1:X:1116:U:H2'	1:X:1117:G:H8	1.81	0.45
1:X:1785:A:H2'	1:X:1786:C:H6	1.82	0.45



		Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:X:1810:U:O2'	1:X:1811:A:P	2.75	0.45
1:X:2306:A:H2'	1:X:2307:A:C8	2.52	0.45
1:X:2325:A:O2'	1:X:2326:C:P	2.74	0.45
1:X:2659:C:O2'	1:X:2660:C:H5'	2.17	0.45
3:A:146:GLU:HB2	3:A:189:CYS:HB3	1.99	0.45
9:H:24:VAL:HG12	9:H:42:LYS:HD3	1.99	0.45
9:H:83:ARG:NH1	9:H:117:GLU:OE2	2.50	0.45
9:H:112:GLY:O	9:H:131:PRO:HD2	2.17	0.45
11:J:134:LYS:HD2	11:J:135:ARG:CB	2.46	0.45
13:L:8:ARG:HG3	13:L:9:ARG:N	2.31	0.45
13:L:63:ASN:HB3	13:L:66:ASP:HB2	1.98	0.45
1:X:276:A:H2'	1:X:277:G:H8	1.80	0.45
1:X:343:A:C2	1:X:346:C:C4	3.05	0.45
1:X:554:U:H4'	1:X:555:U:OP2	2.16	0.45
1:X:1202:U:H5'	16:O:78:VAL:HG22	1.99	0.45
1:X:1229:C:H5"	15:N:11:ARG:NH2	2.32	0.45
1:X:1737:G:H2'	1:X:1738:U:C6	2.51	0.45
1:X:2043:A:H5'	5:C:62:LYS:HZ2	1.82	0.45
1:X:2273:C:H2'	1:X:2274:C:H6	1.82	0.45
1:X:2277:A:H3'	1:X:2278:A:H8	1.82	0.45
1:X:2492:G:H2'	1:X:2493:U:C6	2.52	0.45
1:X:2691:C:O2'	1:X:2693:U:H5'	2.16	0.45
3:A:6:TYR:OH	3:A:18:THR:HG21	2.17	0.45
3:A:72:LYS:HE2	3:A:97:TYR:HD2	1.81	0.45
5:C:28:HIS:CE1	10:I:8:PRO:HB3	2.52	0.45
9:H:83:ARG:HH22	9:H:134:LEU:HD13	1.81	0.45
18:Q:56:MET:HE3	18:Q:77:LYS:HG2	1.98	0.45
1:X:198:A:H61	1:X:441:A:N6	2.14	0.45
1:X:1123:G:H2'	1:X:1124:U:O4'	2.17	0.45
1:X:1485:U:H2'	1:X:1486:A:C8	2.52	0.45
1:X:1802:A:H2'	1:X:1803:G:O4'	2.17	0.45
1:X:2457:A:C8	1:X:2508:G:C5	3.05	0.45
1:X:2757:G:H5'	1:X:2758:A:H5'	1.99	0.45
3:A:246:PRO:HD2	3:A:250:TRP:H	1.81	0.45
17:P:11:LYS:HG3	17:P:14:ARG:HH12	1.81	0.45
19:R:108:VAL:HG13	19:R:109:ALA:H	1.81	0.45
21:T:23:VAL:HB	21:T:26:PHE:CE1	2.52	0.45
23:V:45:GLN:O	23:V:48:ARG:HB3	2.17	0.45
24:W:40:VAL:HG22	24:W:43:MET:HE3	1.99	0.45
28:3:37:SER:HB3	28:3:40:GLU:OE1	2.17	0.45
1:X:946:U:C2	1:X:947:C:C5	3.05	0.44



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:X:1053:G:H4'	1:X:1054:C:OP1	2.17	0.44
1:X:1985:G:OP2	12:K:9:LYS:HE3	2.17	0.44
1:X:2086:U:H2'	1:X:2087:U:C6	2.52	0.44
1:X:2669:C:OP2	12:K:17:ARG:NH1	2.50	0.44
1:X:2873:G:H2'	1:X:2874:A:H8	1.82	0.44
3:A:21:PHE:CD1	3:A:21:PHE:N	2.83	0.44
3:A:63:ARG:N	3:A:63:ARG:HD2	2.32	0.44
3:A:146:GLU:HG2	3:A:152:GLY:CA	2.48	0.44
8:G:116:ARG:CZ	8:G:118:ALA:HB2	2.47	0.44
10:I:28:LYS:HG2	10:I:29:THR:N	2.32	0.44
11:J:117:GLU:OE2	11:J:120:ARG:NH2	2.50	0.44
14:M:58:ASN:O	14:M:64:LYS:HA	2.17	0.44
17:P:96:TYR:HD1	17:P:96:TYR:O	1.99	0.44
26:1:42:PRO:HB2	26:1:43:VAL:H	1.58	0.44
1:X:736:G:H2'	1:X:737:C:O4'	2.18	0.44
1:X:1998:A:C2	25:Z:6:VAL:HG23	2.53	0.44
1:X:2277:A:H2	1:X:2300:G:H2'	1.82	0.44
1:X:2387:U:H2'	1:X:2388:G:H8	1.81	0.44
1:X:2399:C:N4	28:3:31:HIS:HB3	2.32	0.44
1:X:2598:C:O2'	1:X:2599:U:H5'	2.17	0.44
3:A:72:LYS:O	3:A:75:VAL:HG22	2.17	0.44
3:A:203:ASN:OD1	3:A:203:ASN:N	2.38	0.44
4:B:5:LEU:HD21	4:B:79:ARG:CG	2.47	0.44
8:G:70:PHE:C	15:N:64:ARG:HH11	2.17	0.44
19:R:85:ASP:C	19:R:87:GLU:H	2.20	0.44
1:X:48:A:H4'	1:X:49:U:O5'	2.17	0.44
1:X:88:G:C8	1:X:89:A:H2'	2.53	0.44
1:X:163:A:H2'	1:X:164:G:C8	2.52	0.44
1:X:312:G:C4	1:X:313:U:C5	3.06	0.44
1:X:1129:A:H2'	1:X:1130:U:O4'	2.16	0.44
1:X:1800:A:O2'	1:X:1801:C:H5'	2.18	0.44
1:X:1918:G:H1'	1:X:1947:G:N2	2.33	0.44
1:X:2522:G:H2'	1:X:2523:G:H8	1.82	0.44
1:X:2679:G:H2'	1:X:2680:U:C6	2.52	0.44
1:X:2790:C:H2'	1:X:2791:C:H6	1.82	0.44
1:X:2869:U:H2'	1:X:2870:C:H6	1.80	0.44
6:D:123:ASP:OD2	6:D:127:ASN:HB3	2.18	0.44
10:I:19:VAL:HG11	10:I:30:ALA:HB1	1.98	0.44
27:2:5:TYR:CE2	27:2:7:PRO:HG3	2.53	0.44
1:X:339:U:N3	1:X:343:A:H2	2.11	0.44
1:X:568:G:H2'	1:X:569:C:O4'	2.18	0.44



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	$distance ({ m \AA})$	overlap (Å)
1:X:742:G:H5'	1:X:743:A:H5"	1.98	0.44
1:X:1162:A:H2'	1:X:1163:C:C6	2.52	0.44
1:X:1469:U:H5'	1:X:1470:G:P	2.57	0.44
1:X:1656:U:C2'	1:X:1657:A:H5"	2.47	0.44
1:X:1755:G:C6	1:X:1972:G:C2	3.05	0.44
1:X:2811:G:H2'	1:X:2812:A:H8	1.78	0.44
5:C:120:VAL:HG22	5:C:121:ASP:OD1	2.17	0.44
17:P:45:ILE:HD11	17:P:57:LEU:HG	1.99	0.44
19:R:54:ILE:HB	19:R:71:GLN:OE1	2.18	0.44
20:S:107:GLU:HG2	20:S:113:VAL:HG23	1.99	0.44
24:W:49:HIS:ND1	24:W:50:LEU:HD12	2.31	0.44
1:X:39:C:H2'	1:X:40:U:H6	1.82	0.44
1:X:249:A:H1'	1:X:381:C:C1'	2.45	0.44
1:X:314:G:H2'	1:X:315:G:C8	2.51	0.44
1:X:528:G:H2'	1:X:529:U:C6	2.53	0.44
1:X:682:G:H2'	1:X:682:G:N3	2.31	0.44
1:X:2270:U:O2'	1:X:2353:G:N3	2.46	0.44
1:X:2370:G:N2	1:X:2408:G:H1'	2.32	0.44
1:X:2410:U:O2	1:X:2412:A:C8	2.70	0.44
2:Y:3:A:C6	2:Y:4:C:N4	2.86	0.44
3:A:67:PHE:HB3	3:A:153:ALA:CB	2.47	0.44
3:A:139:GLY:H	3:A:165:VAL:HG23	1.83	0.44
3:A:181:GLU:HB2	3:A:271:VAL:HG23	1.99	0.44
8:G:43:VAL:HG12	8:G:81:VAL:HB	2.00	0.44
9:H:20:MET:HG2	9:H:21:CYS:N	2.32	0.44
12:K:87:TYR:OH	12:K:115:LEU:HB3	2.17	0.44
15:N:17:VAL:HG21	15:N:32:TYR:HE1	1.83	0.44
1:X:121:G:H2'	1:X:122:G:O4'	2.17	0.44
1:X:175:C:H2'	1:X:176:A:H5"	2.00	0.44
1:X:1016:C:H1'	1:X:1023:U:H3	1.83	0.44
1:X:1210:C:C2	1:X:1211:G:C8	3.06	0.44
1:X:1698:C:H42	31:X:3243:SPD:H101	1.65	0.44
1:X:1727:C:H2'	1:X:1728:A:C8	2.52	0.44
2:Y:25:G:H5"	2:Y:26:G:OP1	2.17	0.44
2:Y:50:U:H2'	2:Y:51:G:H8	1.78	0.44
2:Y:53:G:N3	2:Y:53:G:H2'	2.33	0.44
6:D:62:LEU:HD23	6:D:62:LEU:O	2.18	0.44
8:G:90:LEU:HD23	8:G:91:THR:N	2.33	0.44
14:M:90:GLN:HG2	14:M:91:VAL:N	2.25	0.44
20:S:3:LEU:HD23	20:S:54:ILE:HB	1.99	0.44
22:U:50:ALA:HB3	22:U:62:LEU:HB2	2.00	0.44



		Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:X:1268:U:C5	5:C:67:ALA:HA	2.52	0.44
1:X:1645:U:H2'	1:X:1646:G:H8	1.81	0.44
1:X:1705:U:H1'	1:X:1718:A:C6	2.53	0.44
1:X:2083:G:H2'	1:X:2083:G:N3	2.33	0.44
1:X:2329:C:H2'	1:X:2330:G:O4'	2.18	0.44
1:X:2336:G:N2	1:X:2339:A:OP2	2.50	0.44
2:Y:9:G:H5"	13:L:32:TYR:CE1	2.53	0.44
2:Y:77:G:H2'	2:Y:78:A:O4'	2.17	0.44
3:A:96:HIS:CE1	3:A:102:LYS:HE2	2.52	0.44
5:C:176:ASN:HD21	5:C:178:TYR:HB3	1.83	0.44
5:C:189:ASP:HB3	5:C:190:ALA:H	1.68	0.44
6:D:13:ARG:HB3	6:D:14:PRO:HD3	1.99	0.44
7:E:12:PRO:HG3	7:E:80:SER:CB	2.47	0.44
8:G:41:TRP:O	8:G:42:VAL:HG13	2.17	0.44
14:M:14:ARG:NH2	14:M:18:GLN:HB3	2.33	0.44
18:Q:25:TYR:CE1	18:Q:88:ILE:HG12	2.52	0.44
19:R:99:VAL:C	19:R:101:GLY:H	2.20	0.44
28:3:56:ALA:O	28:3:59:LYS:HB2	2.17	0.44
1:X:32:C:H2'	1:X:33:C:C6	2.52	0.44
1:X:263:G:N2	1:X:264:U:O4	2.47	0.44
1:X:800:U:H5"	1:X:801:A:H5'	2.00	0.44
1:X:840:U:H4'	1:X:841:G:C2	2.53	0.44
1:X:1034:U:H5	1:X:1035:G:C4	2.34	0.44
1:X:1335:A:N1	1:X:1346:C:O2'	2.39	0.44
1:X:1439:G:O5'	1:X:1439:G:H8	2.01	0.44
1:X:2067:U:H2'	1:X:2068:C:C6	2.53	0.44
1:X:2078:G:H2'	1:X:2079:A:N9	2.33	0.44
2:Y:71:G:C4	2:Y:72:C:C5	3.06	0.44
4:B:56:GLU:HA	4:B:59:VAL:HG23	2.00	0.44
6:D:72:LYS:HA	6:D:81:GLN:HB3	2.00	0.44
12:K:10:LEU:HD11	12:K:43:GLU:HG2	1.99	0.44
15:N:95:LEU:HA	15:N:98:ILE:CD1	2.47	0.44
20:S:30:VAL:HG12	20:S:31:SER:N	2.33	0.44
20:S:105:GLN:HA	20:S:108:VAL:HG12	1.99	0.44
28:3:62:LEU:HA	28:3:63:PRO:HD3	1.63	0.44
1:X:7:G:H2'	1:X:8:A:H8	1.83	0.44
1:X:704:G:H2'	1:X:705:C:H6	1.82	0.44
1:X:1066:G:H2'	1:X:1067:G:O4'	2.18	0.44
1:X:1451:C:H2'	1:X:1452:U:H6	1.83	0.44
1:X:1485:U:H2'	1:X:1486:A:H8	1.82	0.44
1:X:1681:A:C6	1:X:2706:U:C5	3.05	0.44



		Interatomic	Clash
Atom-1	Atom-2	$distance ({ m \AA})$	overlap (Å)
1:X:1774:A:H5'	1:X:2587:G:H4'	2.00	0.44
1:X:1982:C:H4'	1:X:2703:C:O2	2.18	0.44
1:X:2191:A:H5"	1:X:2192:U:C5	2.40	0.44
1:X:2312:A:H4'	1:X:2313:G:O5'	2.18	0.44
1:X:2440:C:H2'	1:X:2441:U:H6	1.82	0.44
3:A:5:LYS:C	3:A:6:TYR:CD1	2.89	0.44
3:A:212:SER:HB2	3:A:217:ARG:HG3	1.99	0.44
5:C:126:ALA:H	5:C:132:ASN:HD22	1.65	0.44
5:C:159:ARG:HG3	5:C:162:ARG:HH22	1.83	0.44
6:D:43:SER:HG	6:D:150:ARG:HH22	1.63	0.44
6:D:127:ASN:HA	6:D:158:THR:HG22	2.00	0.44
9:H:119:ARG:NH1	14:M:40:ARG:O	2.50	0.44
15:N:53:LYS:HA	15:N:53:LYS:HD3	1.62	0.44
21:T:19:LYS:O	21:T:21:LEU:N	2.41	0.44
25:Z:40:LYS:HG2	25:Z:41:LEU:N	2.32	0.44
1:X:576:A:H4'	1:X:821:A:OP1	2.18	0.43
1:X:688:A:H4'	5:C:61:GLN:OE1	2.17	0.43
1:X:755:C:H2'	1:X:756:C:C6	2.53	0.43
1:X:917:U:H2'	1:X:918:A:H5'	2.00	0.43
1:X:1137:A:H4'	1:X:1138:A:C5'	2.47	0.43
1:X:1270:C:H4'	5:C:77:PHE:HD1	1.79	0.43
1:X:1433:A:C8	1:X:1595:A:N6	2.86	0.43
1:X:1679:U:H2'	1:X:1680:U:O4'	2.18	0.43
1:X:1805:G:N3	3:A:50:THR:HG21	2.32	0.43
1:X:2262:C:C2	1:X:2368:G:C2	3.06	0.43
1:X:2291:U:H5'	6:D:85:VAL:HG21	1.99	0.43
1:X:2299:A:H5'	1:X:2300:G:C8	2.53	0.43
1:X:2511:G:C4	1:X:2512:A:C8	3.05	0.43
3:A:131:LEU:HD23	3:A:131:LEU:HA	1.81	0.43
3:A:245:VAL:CA	3:A:252:LYS:HZ1	2.30	0.43
5:C:121:ASP:OD1	5:C:121:ASP:N	2.51	0.43
6:D:57:LEU:HD22	6:D:89:VAL:HG21	2.00	0.43
8:G:75:ILE:HG13	8:G:75:ILE:O	2.18	0.43
15:N:43:ALA:O	15:N:44:THR:C	2.55	0.43
16:O:70:TYR:CE2	16:O:83:ARG:NH1	2.81	0.43
17:P:29:LYS:HA	17:P:123:HIS:ND1	2.32	0.43
1:X:259:U:HO2'	1:X:260:U:P	2.39	0.43
1:X:623:G:C2	1:X:624:A:H1'	2.53	0.43
1:X:746:G:H2'	1:X:747:A:H5"	1.99	0.43
1:X:1354:A:H8	1:X:1354:A:O5'	2.00	0.43
1:X:1469:U:H5'	1:X:1470:G:OP2	2.18	0.43



	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:X:1563:U:H2'	1:X:1564:U:H6	1.82	0.43
1:X:1751:A:H2'	1:X:1752:U:C6	2.54	0.43
1:X:2628:C:H2'	1:X:2629:U:H6	1.83	0.43
3:A:12:SER:C	3:A:14:ARG:H	2.21	0.43
6:D:44:LYS:HG2	6:D:44:LYS:O	2.18	0.43
11:J:40:PRO:HB3	11:J:99:LYS:NZ	2.33	0.43
17:P:59:PHE:CE2	25:Z:39:LYS:CG	3.01	0.43
1:X:883:A:H2'	1:X:884:C:O4'	2.17	0.43
1:X:1281:A:H2'	1:X:1282:A:O4'	2.18	0.43
1:X:2193:C:C2	1:X:2194:A:C8	3.05	0.43
2:Y:3:A:OP1	2:Y:3:A:H3'	2.17	0.43
2:Y:36:A:C2	2:Y:46:G:C6	3.05	0.43
2:Y:42:U:C5	2:Y:44:C:H5'	2.54	0.43
4:B:12:THR:OG1	14:M:17:GLU:OE1	2.31	0.43
4:B:93:VAL:CG1	4:B:177:ALA:HB1	2.48	0.43
4:B:132:LYS:O	4:B:133:LYS:HG2	2.18	0.43
11:J:27:TYR:CZ	11:J:28:VAL:HG22	2.53	0.43
12:K:52:ILE:HG21	12:K:52:ILE:HD13	1.78	0.43
28:3:10:ALA:HB2	28:3:64:ARG:HD3	2.00	0.43
28:3:10:ALA:CB	28:3:64:ARG:HD3	2.48	0.43
1:X:169:C:O2	1:X:815:A:O2'	2.29	0.43
1:X:392:G:C6	1:X:409:G:C6	3.06	0.43
1:X:717:G:O2'	1:X:739:G:N2	2.51	0.43
1:X:1084:A:C5	1:X:1085:G:H1'	2.53	0.43
1:X:1391:A:O2'	1:X:1393:G:N7	2.45	0.43
1:X:1922:U:OP1	1:X:2583:U:O2'	2.34	0.43
1:X:2379:G:H1'	26:1:20:PHE:CZ	2.53	0.43
1:X:2464:G:OP1	11:J:47:GLN:NE2	2.48	0.43
1:X:2495:G:C6	1:X:2548:G:C2	3.06	0.43
1:X:2770:A:H4'	1:X:2771:C:H5'	2.01	0.43
1:X:2793:G:O2'	1:X:2794:G:H5'	2.17	0.43
31:X:3239:SPD:H21	12:K:15:SER:HB3	2.00	0.43
5:C:72:ARG:HA	5:C:77:PHE:HE2	1.79	0.43
9:H:72:ALA:HA	9:H:98:ILE:HA	1.99	0.43
14:M:104:LEU:HD23	14:M:106:TYR:HE1	1.84	0.43
16:O:38:LEU:HD22	16:O:47:PHE:HB3	2.00	0.43
26:1:9:ILE:HG22	26:1:28:ARG:CB	2.48	0.43
1:X:7:G:H2'	1:X:8:A:C8	2.53	0.43
1:X:243:G:N1	1:X:244:C:C6	2.87	0.43
1:X:504:G:H4'	17:P:27:VAL:CG1	2.48	0.43
1:X:1288:A:OP2	1:X:1663:C:N4	2.51	0.43



	Atom D	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:X:1310:C:C2	1:X:1311:C:C5	3.07	0.43
1:X:1978:U:H3'	1:X:1979:C:H2'	1.99	0.43
1:X:2737:A:C2'	1:X:2738:A:H5"	2.43	0.43
4:B:59:VAL:HG12	4:B:64:GLN:HG3	2.01	0.43
4:B:161:GLY:O	4:B:162:MET:HB3	2.18	0.43
10:I:83:LEU:HD12	10:I:86:THR:HG21	2.00	0.43
11:J:6:LYS:HB3	11:J:7:ARG:H	1.64	0.43
13:L:33:ARG:NH1	13:L:99:ARG:O	2.52	0.43
14:M:90:GLN:CG	14:M:91:VAL:H	2.27	0.43
14:M:110:LEU:HD23	14:M:110:LEU:HA	1.77	0.43
19:R:25:LEU:O	19:R:26:SER:HB3	2.18	0.43
19:R:108:VAL:HG22	19:R:109:ALA:N	2.33	0.43
20:S:121:GLN:O	20:S:161:ALA:HB3	2.19	0.43
20:S:129:ARG:O	20:S:129:ARG:HG3	2.17	0.43
25:Z:30:LEU:HA	25:Z:30:LEU:HD23	1.68	0.43
1:X:34:U:N3	19:R:4:PRO:HG3	2.34	0.43
1:X:876:A:H2'	1:X:877:G:H8	1.83	0.43
1:X:1367:A:H2'	1:X:1368:G:O4'	2.19	0.43
1:X:1753:A:H3'	31:X:3243:SPD:C4	2.49	0.43
1:X:1805:G:H21	3:A:50:THR:HG22	1.83	0.43
1:X:2079:A:H5'	1:X:2080:U:OP2	2.19	0.43
1:X:2280:A:H2'	1:X:2281:C:C6	2.53	0.43
1:X:2705:A:O2'	1:X:2706:U:H2'	2.18	0.43
6:D:34:ILE:HB	6:D:91:LEU:HD11	2.00	0.43
7:E:165:VAL:HG23	7:E:166:GLY:N	2.25	0.43
8:G:132:PHE:CD2	8:G:145:HIS:HD2	2.36	0.43
9:H:2:ILE:HD13	9:H:2:ILE:HA	1.86	0.43
13:L:9:ARG:O	13:L:9:ARG:HD2	2.18	0.43
16:O:3:ALA:O	16:O:11:GLN:HB2	2.17	0.43
22:U:42:GLN:OE1	22:U:42:GLN:N	2.51	0.43
26:1:39:LYS:HA	26:1:48:VAL:O	2.18	0.43
1:X:175:C:H6	1:X:175:C:O5'	2.02	0.43
1:X:338:G:N2	1:X:347:C:C2	2.86	0.43
1:X:647:G:O2'	1:X:649:G:O2'	2.27	0.43
1:X:758:G:H2'	1:X:759:C:H5'	2.00	0.43
1:X:848:A:C4	1:X:849:G:C8	3.07	0.43
1:X:886:A:O2'	11:J:66:TYR:HE1	2.01	0.43
1:X:956:A:C4	1:X:2427:A:C2	3.07	0.43
1:X:1670:G:H8	1:X:1670:G:OP2	2.02	0.43
1:X:2220:A:H2'	1:X:2221:G:H8	1.82	0.43
2:Y:35:C:H2'	2:Y:36:A:C8	2.54	0.43



A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
3:A:77:ALA:HB2	3:A:97:TYR:CE1	2.54	0.43
3:A:226:MET:SD	3:A:231:HIS:HB2	2.59	0.43
15:N:14:HIS:ND1	15:N:32:TYR:CG	2.80	0.43
16:O:10:LYS:HD2	16:O:10:LYS:N	2.31	0.43
26:1:10:VAL:HG12	26:1:11:LYS:O	2.18	0.43
28:3:38:GLY:HA2	28:3:41:ILE:HG22	2.01	0.43
1:X:338:G:H1'	19:R:10:HIS:NE2	2.34	0.43
1:X:518:A:H5"	1:X:518:A:N3	2.34	0.43
1:X:814:G:OP1	5:C:50:GLN:HB2	2.18	0.43
1:X:1225:G:H2'	1:X:1249:G:H22	1.84	0.43
1:X:1431:U:H3'	1:X:1432:G:O4'	2.19	0.43
1:X:1445:A:H2'	1:X:1446:U:O4'	2.18	0.43
1:X:2043:A:HO2'	1:X:2044:G:P	2.42	0.43
1:X:2509:A:N7	7:E:172:LYS:NZ	2.65	0.43
1:X:2596:C:H2'	1:X:2597:G:H8	1.83	0.43
1:X:2737:A:N6	7:E:67:LEU:HD12	2.33	0.43
3:A:10:THR:HB	3:A:11:PRO:HD2	2.01	0.43
4:B:14:ILE:HG23	4:B:21:ILE:HG13	2.00	0.43
4:B:179:GLU:CB	4:B:181:LEU:HD23	2.49	0.43
8:G:164:GLN:CG	8:G:165:VAL:H	2.31	0.43
17:P:59:PHE:HE2	25:Z:39:LYS:HG3	1.83	0.43
20:S:3:LEU:HD13	20:S:3:LEU:HA	1.67	0.43
1:X:318:G:H22	1:X:321:A:P	2.42	0.43
1:X:725:C:N4	1:X:733:G:O6	2.52	0.43
1:X:1117:G:N2	1:X:1118:G:O6	2.52	0.43
1:X:1935:A:N3	1:X:2539:C:O2'	2.42	0.43
1:X:2043:A:H1'	1:X:2481:G:O4'	2.18	0.43
1:X:2279:G:C2	1:X:2280:A:C5	3.07	0.43
1:X:2315:A:C2	1:X:2364:C:H1'	2.54	0.43
1:X:2569:A:H2'	1:X:2570:C:H6	1.82	0.43
8:G:167:LYS:HG2	8:G:168:THR:H	1.83	0.43
9:H:7:ARG:HG2	9:H:18:GLU:OE2	2.19	0.43
13:L:9:ARG:C	13:L:9:ARG:HD2	2.39	0.43
15:N:6:THR:HG21	15:N:10:ARG:NH2	2.34	0.43
20:S:43:PHE:CE1	20:S:66:VAL:HG11	2.54	0.43
21:T:53:MET:HA	21:T:59:LEU:HA	2.00	0.43
24:W:34:VAL:HG22	24:W:40:VAL:HG11	2.00	0.43
1:X:540:G:C8	1:X:540:G:C3'	3.02	0.43
1:X:754:G:H2'	1:X:755:C:H6	1.82	0.43
1:X:1536:G:H2'	1:X:1537:U:C6	2.53	0.43
1:X:1855:G:H5'	1:X:1856:U:OP2	2.19	0.43



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (A)	overlap (Å)
1:X:2055:G:H2'	1:X:2056:C:H6	1.83	0.43
1:X:2290:A:H1'	6:D:77:PHE:HZ	1.84	0.43
1:X:2323:U:HO2'	1:X:2324:G:H3'	1.84	0.43
1:X:2433:G:C5	1:X:2434:G:N7	2.87	0.43
6:D:123:ASP:HB2	6:D:125:ARG:O	2.19	0.43
9:H:85:ASP:CG	9:H:87:SER:H	2.15	0.43
9:H:89:ILE:HD12	9:H:134:LEU:HD22	2.00	0.43
11:J:13:GLN:HG3	11:J:14:PHE:CD2	2.54	0.43
13:L:8:ARG:HE	13:L:9:ARG:H	1.66	0.43
16:O:80:TYR:CE1	16:O:82:ARG:NH1	2.87	0.43
17:P:56:LEU:HD23	17:P:56:LEU:HA	1.84	0.43
18:Q:33:ALA:O	18:Q:76:LYS:NZ	2.49	0.43
21:T:67:VAL:CG2	21:T:68:VAL:HG13	2.47	0.43
1:X:591:G:C6	1:X:592:G:C6	3.07	0.42
1:X:682:G:N3	1:X:682:G:C2'	2.81	0.42
1:X:1810:U:O2'	1:X:1811:A:OP2	2.33	0.42
10:I:57:ILE:HG12	28:3:25:PHE:CE2	2.53	0.42
14:M:22:ARG:HD3	14:M:24:LEU:HD12	2.00	0.42
1:X:986:A:H1'	1:X:1001:A:C2	2.54	0.42
1:X:1332:G:C2	1:X:1333:G:N2	2.87	0.42
1:X:2772:U:H2'	1:X:2773:G:C8	2.54	0.42
1:X:2845:C:H2'	1:X:2846:G:H5'	2.01	0.42
5:C:176:ASN:HD22	5:C:177:VAL:N	2.16	0.42
9:H:108:THR:O	9:H:109:ARG:HG3	2.19	0.42
10:I:49:PHE:CG	10:I:50:GLU:N	2.86	0.42
19:R:22:VAL:HG12	19:R:23:ILE:N	2.35	0.42
24:W:14:GLY:HA2	24:W:17:VAL:HG12	2.01	0.42
1:X:692:C:H2'	1:X:693:A:C8	2.54	0.42
1:X:2087:U:H2'	1:X:2088:U:O4'	2.19	0.42
1:X:2700:U:O2	1:X:2700:U:H2'	2.20	0.42
4:B:20:ALA:HB2	9:H:85:ASP:O	2.19	0.42
7:E:27:LYS:HA	7:E:31:GLY:CA	2.50	0.42
19:R:94:VAL:CB	19:R:107:ALA:HB3	2.50	0.42
20:S:124:ALA:O	20:S:126:GLY:N	2.47	0.42
1:X:588:G:O2'	1:X:2002:A:OP1	2.24	0.42
1:X:1473:U:O2	1:X:1473:U:O4'	2.37	0.42
1:X:1669:A:N6	12:K:11:ASN:OD1	2.52	0.42
1:X:1727:C:H2'	1:X:1728:A:H8	1.84	0.42
1:X:2218:G:H5'	3:A:249:PRO:CG	2.49	0.42
1:X:2277:A:C2	1:X:2300:G:H2'	2.54	0.42
1:X:2355:A:H2'	1:X:2356:A:O4'	2.20	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:X:2367:A:C8	1:X:2368:G:C5	3.08	0.42
1:X:2379:G:H1'	26:1:20:PHE:CE2	2.54	0.42
2:Y:53:G:OP2	13:L:64:LYS:HD3	2.19	0.42
8:G:132:PHE:CG	8:G:145:HIS:CD2	3.07	0.42
9:H:4:PRO:O	9:H:5:GLN:HB2	2.19	0.42
11:J:15:ARG:CD	11:J:73:LYS:HG3	2.45	0.42
11:J:86:LYS:HB3	11:J:87:GLY:H	1.56	0.42
12:K:89:GLU:HG3	12:K:90:ARG:N	2.31	0.42
1:X:491:A:N3	1:X:491:A:H2'	2.34	0.42
1:X:831:G:O2'	1:X:832:A:O4'	2.29	0.42
1:X:1030:U:H3	1:X:1153:A:H61	1.65	0.42
1:X:1478:U:H2'	1:X:1479:G:C8	2.55	0.42
1:X:1711:C:H4'	1:X:1712:G:O5'	2.20	0.42
1:X:1770:U:C5	1:X:1774:A:C8	3.07	0.42
1:X:2073:A:N6	1:X:2209:G:O6	2.52	0.42
1:X:2773:G:N2	1:X:2779:A:C2	2.85	0.42
1:X:2782:G:H2'	1:X:2783:U:O5'	2.19	0.42
1:X:2788:C:H2'	1:X:2789:U:C6	2.53	0.42
4:B:134:TRP:O	4:B:135:HIS:HB3	2.20	0.42
5:C:3:GLN:HE22	5:C:117:LEU:CA	2.32	0.42
5:C:17:LEU:HD23	5:C:17:LEU:HA	1.85	0.42
8:G:94:LYS:HG2	8:G:95:LEU:HD12	2.00	0.42
9:H:116:ARG:H	9:H:134:LEU:CD2	2.28	0.42
15:N:99:ALA:HB2	15:N:106:PHE:CE1	2.55	0.42
19:R:57:ASN:OD1	19:R:58:VAL:HG23	2.20	0.42
22:U:54:ASN:HB2	22:U:78:ILE:O	2.19	0.42
1:X:67:G:H2'	1:X:68:C:H6	1.82	0.42
1:X:333:A:H5'	1:X:351:A:H1'	2.02	0.42
1:X:389:G:H2'	1:X:390:U:C6	2.54	0.42
1:X:1134:C:H2'	1:X:1135:C:H6	1.85	0.42
1:X:1264:C:C5'	15:N:13:ARG:HH12	2.33	0.42
1:X:2390:A:H2'	1:X:2391:A:H8	1.85	0.42
1:X:2408:G:H5'	1:X:2409:A:P	2.60	0.42
1:X:2691:C:HO2'	1:X:2692:A:P	2.40	0.42
1:X:2746:G:H2'	1:X:2746:G:N3	2.34	0.42
1:X:2814:G:O2'	12:K:49:GLU:HG2	2.20	0.42
1:X:2819:G:H2'	1:X:2820:C:H6	1.84	0.42
4:B:146:THR:N	4:B:147:PRO:HD2	2.34	0.42
12:K:52:ILE:HD11	12:K:94:TYR:CD1	2.53	0.42
18:Q:27:PHE:CZ	18:Q:42:ILE:HD12	2.54	0.42
26:1:35:LEU:O	26:1:36:GLU:HB3	2.19	0.42



A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:X:172:A:N6	1:X:175:C:H3'	2.33	0.42
1:X:757:U:H2'	1:X:758:G:O4'	2.19	0.42
1:X:991:A:C6	1:X:992:A:C6	3.08	0.42
1:X:1518:C:H2'	1:X:1519:G:C8	2.55	0.42
1:X:1672:A:H3'	1:X:1673:C:C5	2.55	0.42
1:X:1675:C:OP1	4:B:134:TRP:CD1	2.72	0.42
1:X:1796:A:N3	3:A:50:THR:HG23	2.34	0.42
1:X:1935:A:C6	1:X:1936:A:N1	2.87	0.42
1:X:2057:U:H2'	1:X:2058:U:C6	2.54	0.42
1:X:2080:U:H2'	1:X:2081:U:C6	2.54	0.42
3:A:246:PRO:HD3	3:A:250:TRP:O	2.18	0.42
7:E:55:PRO:HG2	7:E:61:HIS:ND1	2.35	0.42
13:L:67:THR:O	13:L:71:VAL:HG22	2.19	0.42
15:N:66:ASN:HD22	15:N:70:ARG:NH2	2.17	0.42
20:S:43:PHE:HE1	20:S:66:VAL:HG11	1.84	0.42
20:S:75:LYS:HG3	20:S:76:ARG:N	2.35	0.42
1:X:648:A:C5'	10:I:103:ASN:HB2	2.49	0.42
1:X:870:C:O2'	1:X:871:U:H5'	2.20	0.42
1:X:958:G:H2'	1:X:959:C:H6	1.83	0.42
1:X:1030:U:C4	1:X:1031:C:N4	2.87	0.42
1:X:1332:G:C2	1:X:1347:C:C2	3.08	0.42
1:X:2330:G:O2'	1:X:2331:A:H5'	2.20	0.42
1:X:2373:C:H2'	1:X:2374:C:C6	2.54	0.42
1:X:2482:A:H4'	1:X:2483:U:OP1	2.20	0.42
1:X:2790:C:H2'	1:X:2791:C:C6	2.55	0.42
6:D:34:ILE:HB	6:D:91:LEU:CD1	2.50	0.42
8:G:70:PHE:HA	15:N:64:ARG:HE	1.84	0.42
17:P:59:PHE:CD2	25:Z:30:LEU:HD21	2.55	0.42
23:V:41:HIS:HA	23:V:44:ARG:HD3	2.02	0.42
1:X:219:G:N2	1:X:231:G:H2'	2.35	0.42
1:X:659:G:H3'	1:X:660:G:H8	1.84	0.42
1:X:1264:C:H5"	15:N:13:ARG:CZ	2.50	0.42
1:X:1699:A:H61	1:X:1723:U:H3	1.68	0.42
1:X:2234:G:H2'	1:X:2235:G:O4'	2.19	0.42
1:X:2393:G:N2	10:I:59:ARG:HH11	2.14	0.42
1:X:2608:A:C6	1:X:2869:U:C2	3.08	0.42
1:X:2692:A:OP2	31:X:3239:SPD:H22	2.20	0.42
1:X:2705:A:C2'	1:X:2706:U:H2'	2.49	0.42
2:Y:35:C:H2'	2:Y:36:A:H8	1.85	0.42
3:A:231:HIS:NE2	3:A:247:VAL:HA	2.35	0.42
5:C:6:VAL:HG12	5:C:120:VAL:HG12	2.02	0.42


	A + 0	Interatomic	Clash	
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)	
5:C:59:TYR:CG	5:C:60:GLY:N	2.87	0.42	
5:C:120:VAL:HG13	5:C:121:ASP:O	2.20	0.42	
7:E:69:ARG:O	7:E:72:VAL:HG22	2.19	0.42	
14:M:25:PRO:O	14:M:27:PHE:CD1	2.73	0.42	
15:N:57:PHE:HD1	15:N:61:TRP:CZ3	2.37	0.42	
22:U:51:ILE:HG13	22:U:59:THR:OG1	2.20	0.42	
1:X:31:C:O2'	1:X:32:C:H5'	2.19	0.42	
1:X:227:G:C6	1:X:228:A:C6	3.08	0.42	
1:X:306:G:H2'	1:X:307:C:C6	2.54	0.42	
1:X:573:C:H2'	1:X:574:C:O4'	2.19	0.42	
1:X:782:U:H5"	1:X:783:G:OP2	2.20	0.42	
8:G:135:LEU:HD23	8:G:135:LEU:HA	1.74	0.42	
16:O:55:THR:OG1	16:O:98:ILE:HD12	2.20	0.42	
16:O:71:ILE:HD13	16:O:71:ILE:HA	1.71	0.42	
20:S:146:HIS:HB3	20:S:170:SER:CB	2.49	0.42	
1:X:545:C:H2'	1:X:546:A:C8	2.55	0.41	
1:X:1399:C:H2'	1:X:1400:A:H8	1.85	0.41	
1:X:1428:G:N2	1:X:1601:U:H4'	2.34	0.41	
1:X:1475:U:O2'	1:X:1476:G:P	2.75	0.41	
1:X:2278:A:H2'	1:X:2279:G:H8	1.85	0.41	
1:X:2293:G:H2'	1:X:2294:U:C6	2.55	0.41	
1:X:2651:U:H2'	1:X:2652:G:O5'	2.20	0.41	
1:X:2729:A:C6	1:X:2730:A:N1	2.88	0.41	
3:A:215:LEU:HD23	3:A:215:LEU:HA	1.74	0.41	
4:B:133:LYS:HB3	4:B:137:ARG:HD3	2.02	0.41	
5:C:17:LEU:HD13	5:C:109:ALA:HA	2.02	0.41	
7:E:129:THR:O	7:E:129:THR:HG22	2.20	0.41	
9:H:83:ARG:HH22	9:H:134:LEU:CD1	2.32	0.41	
20:S:27:GLU:HG3	20:S:28:ASN:N	2.29	0.41	
20:S:91:PRO:HB3	20:S:125:PRO:HA	2.02	0.41	
26:1:10:VAL:HG12	26:1:11:LYS:N	2.35	0.41	
28:3:52:LYS:O	28:3:52:LYS:HD2	2.20	0.41	
1:X:656:U:O2'	1:X:657:A:OP2	2.30	0.41	
1:X:748:A:H5'	1:X:749:C:OP2	2.21	0.41	
1:X:787:A:H2	1:X:800:U:O2'	2.02	0.41	
1:X:1153:A:C8	1:X:1153:A:H5"	2.55	0.41	
1:X:1270:C:OP1	5:C:69:HIS:NE2	2.40	0.41	
1:X:1373:G:N2	1:X:2192:U:H3	2.14	0.41	
1:X:1505:U:H1'	1:X:1506:C:C5	2.55	0.41	
1:X:1539:U:H2'	1:X:1540:C:C6	2.55	0.41	
3:A:19:ALA:HB3	3:A:21:PHE:HE1	1.85	0.41	



A 4 1	A 4 5 775 0	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
3:A:106:LEU:O	3:A:108:PRO:HD3	2.20	0.41	
11:J:51:CYS:HA	11:J:54:VAL:HG12	2.02	0.41	
18:Q:17:TYR:O	18:Q:20:MET:HB3	2.20	0.41	
23:V:17:GLU:HB3	23:V:53:LEU:HD11	2.02	0.41	
1:X:37:C:H2'	1:X:38:G:C8	2.56	0.41	
1:X:425:A:H3'	1:X:426:C:H6	1.85	0.41	
1:X:487:G:H22	1:X:490:A:H5"	1.84	0.41	
1:X:1762:C:H2'	1:X:1763:G:H8	1.83	0.41	
1:X:2551:A:OP2	4:B:146:THR:HG22	2.21	0.41	
1:X:2641:A:H2'	1:X:2642:G:O4'	2.21	0.41	
1:X:2701:A:H1'	1:X:2848:A:O2'	2.20	0.41	
1:X:2705:A:C4	1:X:2707:G:C8	3.07	0.41	
2:Y:62:C:C2	2:Y:63:A:C8	3.08	0.41	
5:C:128:ALA:HB2	5:C:156:ASN:OD1	2.20	0.41	
6:D:127:ASN:HD21	6:D:157:VAL:HG13	1.85	0.41	
7:E:22:GLY:HA2	7:E:43:VAL:CG1	2.50	0.41	
13:L:16:LYS:NZ	13:L:90:ASP:OD2	2.53	0.41	
17:P:95:ALA:O	17:P:96:TYR:HB3	2.20	0.41	
20:S:25:ASN:HB3	20:S:85:MET:HB2	2.02	0.41	
26:1:6:PRO:C	26:1:7:ARG:HD2	2.41	0.41	
28:3:50:LEU:HD12	28:3:51:ALA:H	1.86	0.41	
1:X:129:A:H2'	1:X:130:C:H6	1.86	0.41	
1:X:158:A:H2'	1:X:159:A:C8	2.56	0.41	
1:X:530:G:H2'	1:X:531:G:H8	1.85	0.41	
1:X:596:C:N4	10:I:30:ALA:HB2	2.36	0.41	
1:X:761:G:C8	1:X:763:A:C8	3.08	0.41	
1:X:1076:U:H2'	1:X:1077:U:C2	2.55	0.41	
1:X:1137:A:H4'	1:X:1138:A:H5"	2.01	0.41	
1:X:1201:G:H5"	16:O:80:TYR:CE1	2.55	0.41	
1:X:1261:G:P	5:C:86:PRO:HG3	2.61	0.41	
1:X:2328:G:OP2	28:3:42:ARG:HD3	2.21	0.41	
4:B:9:ILE:HG22	14:M:13:LEU:CD2	2.50	0.41	
14:M:57:ILE:O	14:M:57:ILE:HG13	2.20	0.41	
18:Q:7:LEU:HD11	18:Q:42:ILE:HD13	2.02	0.41	
19:R:102:LYS:HD3	19:R:103:LYS:H	1.86	0.41	
23:V:40:PRO:O	23:V:43:VAL:HB	2.21	0.41	
24:W:36:ASP:HA	24:W:41:ARG:CZ	2.50	0.41	
28:3:11:LYS:HA	28:3:11:LYS:HD3	1.79	0.41	
1:X:1160:C:H2'	1:X:1161:U:O4'	2.21	0.41	
1:X:1278:A:N6	1:X:1996:A:H5"	2.36	0.41	
1:X:1517:C:H2'	1:X:1518:C:O4'	2.20	0.41	



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:X:1545:G:H2'	1:X:1546:C:C6	2.56	0.41	
1:X:1693:A:H2	1:X:1976:U:H5'	1.82	0.41	
1:X:2268:G:N3	1:X:2268:G:H2'	2.36	0.41	
1:X:2596:C:C2	1:X:2597:G:C8	3.08	0.41	
3:A:132:PRO:HD3	3:A:190:TYR:CE1	2.56	0.41	
4:B:188:ILE:CG2	4:B:189:PRO:HD2	2.50	0.41	
6:D:162:THR:CG2	6:D:164:GLU:HG2	2.50	0.41	
8:G:35:LYS:H	8:G:35:LYS:HG3	1.66	0.41	
12:K:20:LEU:O	12:K:23:ALA:N	2.53	0.41	
12:K:99:ARG:HD3	25:Z:43:HIS:O	2.21	0.41	
15:N:61:TRP:O	15:N:65:ILE:HG13	2.21	0.41	
20:S:39:PHE:CZ	20:S:81:VAL:HG21	2.56	0.41	
20:S:69:VAL:HG22	20:S:81:VAL:HG13	2.03	0.41	
1:X:199:A:C6	1:X:201:G:C2	3.09	0.41	
1:X:1142:G:O4'	8:G:110:LEU:HB2	2.20	0.41	
1:X:1271:C:H2'	1:X:1272:G:O4'	2.20	0.41	
1:X:1392:U:C6	1:X:1392:U:OP1	2.73	0.41	
1:X:1411:C:C2	1:X:1412:C:C5	3.09	0.41	
1:X:1699:A:H2'	1:X:1700:C:C6	2.55	0.41	
1:X:1749:G:H4'	1:X:1750:A:OP2	2.20	0.41	
1:X:1856:U:H2'	1:X:1857:G:O4'	2.21	0.41	
1:X:1979:C:H4'	1:X:1980:A:OP1	2.20	0.41	
1:X:2625:U:H2'	1:X:2626:U:O4'	2.21	0.41	
1:X:2734:U:H2'	1:X:2736:U:OP1	2.20	0.41	
4:B:93:VAL:HG12	4:B:177:ALA:HB1	2.01	0.41	
6:D:102:LYS:HE2	6:D:106:ILE:HD11	2.01	0.41	
12:K:27:ALA:O	12:K:31:GLU:HG2	2.21	0.41	
12:K:65:LEU:O	12:K:68:GLN:HG2	2.20	0.41	
17:P:31:VAL:O	17:P:122:SER:N	2.53	0.41	
22:U:48:LYS:O	22:U:62:LEU:O	2.39	0.41	
1:X:139:A:H2'	1:X:140:G:H8	1.85	0.41	
1:X:143:A:H2'	1:X:144:U:O4'	2.21	0.41	
1:X:475:U:C2	1:X:801:A:C6	3.09	0.41	
1:X:787:A:C2	1:X:800:U:O2'	2.73	0.41	
1:X:846:A:H2'	1:X:847:C:C6	2.56	0.41	
1:X:1197:U:O3'	24:W:26:ARG:NH2	2.54	0.41	
1:X:1342:U:H5"	1:X:1343:C:H5	1.84	0.41	
1:X:1489:C:H5"	1:X:1490:U:OP2	2.21	0.41	
1:X:1735:G:H2'	1:X:1736:C:C6	2.56	0.41	
1:X:1777:A:H1'	1:X:1921:A:N6	2.35	0.41	
1:X:2371:A:C4	1:X:2408:G:C6	3.08	0.41	



Atom 1	Atom 1 Atom 2		Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:X:2670:C:C5'	1:X:2847:G:H5"	2.51	0.41
3:A:6:TYR:HD1	3:A:6:TYR:N	2.19	0.41
3:A:142:VAL:O	3:A:163:VAL:N	2.54	0.41
5:C:78:VAL:O	5:C:78:VAL:HG13	2.20	0.41
12:K:49:GLU:HG3	12:K:94:TYR:HD2	1.85	0.41
19:R:87:GLU:O	19:R:88:THR:HB	2.21	0.41
20:S:20:ALA:O	20:S:80:HIS:HA	2.20	0.41
20:S:126:GLY:HA2	20:S:127:PRO:HD2	1.93	0.41
21:T:68:VAL:N	21:T:80:SER:O	2.48	0.41
1:X:116:A:N3	1:X:155:G:H1'	2.36	0.41
1:X:699:G:H4'	1:X:700:C:OP2	2.21	0.41
1:X:805:G:C8	1:X:2419:C:O2	2.74	0.41
1:X:1027:C:H5'	1:X:1028:G:OP2	2.21	0.41
1:X:1428:G:C2	1:X:1601:U:H4'	2.56	0.41
1:X:1454:U:H2'	1:X:1455:C:C6	2.56	0.41
1:X:1544:A:C4	1:X:1560:A:C6	3.09	0.41
10:I:83:LEU:HA	10:I:86:THR:CG2	2.50	0.41
15:N:115:ASN:C	15:N:115:ASN:HD22	2.23	0.41
16:O:11:GLN:N	16:O:11:GLN:OE1	2.53	0.41
20:S:39:PHE:O	20:S:43:PHE:N	2.47	0.41
1:X:215:G:C6	1:X:237:G:C6	3.09	0.41
1:X:457:C:O2'	1:X:458:G:H5'	2.21	0.41
1:X:530:G:H2'	1:X:531:G:C8	2.56	0.41
1:X:571:U:C2	1:X:581:A:C8	3.09	0.41
1:X:689:A:C2	1:X:815:A:N6	2.87	0.41
1:X:781:G:H2'	1:X:782:U:H6	1.86	0.41
1:X:793:G:N2	1:X:796:A:H62	2.08	0.41
1:X:849:G:H2'	1:X:850:C:C6	2.56	0.41
1:X:1117:G:N2	1:X:1118:G:N7	2.62	0.41
1:X:1191:G:C5	1:X:1192:A:C8	3.08	0.41
1:X:1225:G:HO2'	1:X:1226:A:P	2.43	0.41
1:X:1265:G:O2'	1:X:1266:G:C8	2.73	0.41
1:X:1609:G:H2'	1:X:1610:A:O4'	2.21	0.41
1:X:1790:G:C8	3:A:181:GLU:OE1	2.74	0.41
1:X:1872:A:O2'	1:X:2070:G:H5'	2.21	0.41
1:X:1998:A:C4	25:Z:6:VAL:HG23	2.55	0.41
1:X:2175:A:H2'	1:X:2176:U:H6	1.80	0.41
1:X:2208:U:H2'	1:X:2209:G:H8	1.85	0.41
1:X:2259:G:O2'	1:X:2367:A:N1	2.44	0.41
1:X:2273:C:H5"	13:L:11:LEU:HD11	2.03	0.41
1:X:2378:G:H2'	26:1:20:PHE:HE1	1.85	0.41



Atom 1 Atom 2		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:X:2493:U:H2'	1:X:2494:C:C6	2.56	0.41
1:X:2507:U:H2'	1:X:2509:A:H5"	2.02	0.41
1:X:2543:A:C2	1:X:2626:U:H4'	2.55	0.41
1:X:2661:G:C2'	1:X:2662:C:H5'	2.51	0.41
2:Y:39:C:O2	2:Y:39:C:H2'	2.20	0.41
3:A:70:ARG:NH2	3:A:146:GLU:OE1	2.53	0.41
4:B:32:PRO:O	4:B:49:ILE:HG13	2.20	0.41
4:B:56:GLU:HA	4:B:59:VAL:CG2	2.51	0.41
4:B:60:ASN:HB3	4:B:62:PRO:CD	2.43	0.41
7:E:83:TYR:HB2	7:E:135:GLY:O	2.21	0.41
7:E:83:TYR:HD1	7:E:83:TYR:HA	1.82	0.41
8:G:128:GLU:HG2	8:G:132:PHE:CE2	2.56	0.41
8:G:132:PHE:CD2	8:G:145:HIS:CD2	3.09	0.41
10:I:82:ASP:O	10:I:85:ASP:HB2	2.21	0.41
11:J:8:THR:HG22	11:J:70:PHE:CE2	2.55	0.41
11:J:99:LYS:HD2	11:J:99:LYS:HA	1.76	0.41
12:K:54:THR:O	12:K:62:SER:HB3	2.21	0.41
20:S:23:ALA:HB2	20:S:83:PHE:HB2	2.02	0.41
28:3:16:ILE:HD13	28:3:63:PRO:HG3	2.01	0.41
1:X:27:G:N2	1:X:522:G:H1'	2.36	0.41
1:X:1050:G:H21	1:X:1127:C:N4	2.18	0.41
1:X:1050:G:N3	1:X:1128:G:N1	2.69	0.41
1:X:1769:U:H3'	1:X:1775:A:N6	2.36	0.41
1:X:1834:G:H2'	1:X:1835:C:C6	2.56	0.41
1:X:2044:G:C2	1:X:2046:C:C4	3.09	0.41
1:X:2222:U:H2'	1:X:2223:U:H6	1.81	0.41
1:X:2599:U:O4'	4:B:156:MET:HG3	2.21	0.41
1:X:2621:G:H5'	8:G:106:TYR:CE2	2.56	0.41
3:A:67:PHE:HB3	3:A:153:ALA:HB2	2.02	0.41
4:B:179:GLU:HB2	4:B:181:LEU:HD23	2.02	0.41
6:D:68:THR:OG1	6:D:86:GLY:O	2.35	0.41
8:G:37:ASP:OD1	8:G:38:GLU:N	2.54	0.41
8:G:151:TYR:HH	8:G:158:HIS:CE1	2.39	0.41
8:G:164:GLN:HE21	8:G:165:VAL:HG22	1.85	0.41
15:N:39:LEU:HD23	15:N:39:LEU:HA	1.72	0.41
19:R:14:LEU:HA	19:R:14:LEU:HD23	1.83	0.41
20:S:62:PHE:HA	20:S:63:PRO:HD3	1.94	0.41
22:U:49:LYS:HA	22:U:61:TRP:CE3	2.56	0.41
23:V:18:ILE:HG13	23:V:53:LEU:HD22	2.02	0.41
25:Z:35:GLN:HB3	25:Z:51:TYR:CD2	2.56	0.41
1:X:5:A:C6	1:X:2873:G:C6	3.09	0.40



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:X:64:C:H1'	18:Q:68:PHE:HD2	1.85	0.40	
1:X:689:A:C2	1:X:690:A:C8	3.09	0.40	
1:X:1495:G:C2	1:X:1530:U:O2	2.73	0.40	
1:X:1609:G:H2'	1:X:1610:A:C8	2.55	0.40	
1:X:2295:C:H5'	6:D:125:ARG:HH12	1.82	0.40	
1:X:2315:A:N3	1:X:2364:C:H1'	2.36	0.40	
1:X:2799:C:H2'	1:X:2800:C:O4'	2.20	0.40	
2:Y:50:U:C2	2:Y:51:G:N7	2.89	0.40	
10:I:63:ARG:O	10:I:63:ARG:NH1	2.49	0.40	
11:J:36:ILE:HG13	11:J:102:ARG:O	2.21	0.40	
11:J:66:TYR:HD2	11:J:106:GLU:HG2	1.85	0.40	
14:M:38:LYS:HE3	14:M:79:ARG:HH22	1.85	0.40	
21:T:21:LEU:HD21	21:T:41:ARG:NH2	2.36	0.40	
24:W:12:ARG:HH11	24:W:12:ARG:HG3	1.86	0.40	
25:Z:52:TYR:O	25:Z:53:ASP:CG	2.59	0.40	
1:X:23:G:C6	1:X:528:G:C6	3.10	0.40	
1:X:94:C:H2'	1:X:95:G:O4'	2.21	0.40	
1:X:353:G:H2'	1:X:354:C:H6	1.86	0.40	
1:X:1050:G:H21	1:X:1127:C:H42	1.69	0.40	
1:X:1994:U:H2'	1:X:1995:G:H5'	2.03	0.40	
1:X:2073:A:C6	1:X:2209:G:O6	2.74	0.40	
1:X:2784:A:C6	1:X:2866:A:C8	3.09	0.40	
3:A:210:GLY:CA	3:A:213:ARG:H	2.33	0.40	
7:E:124:ALA:HB3	7:E:132:ASP:HB3	2.02	0.40	
7:E:127:GLU:HB3	7:E:130:ARG:HB2	2.04	0.40	
7:E:163:ARG:CZ	7:E:169:ILE:HG21	2.52	0.40	
16:O:70:TYR:HE2	16:O:83:ARG:NH1	2.17	0.40	
18:Q:35:LYS:HA	18:Q:38:ILE:HG22	2.03	0.40	
1:X:12:U:H6	1:X:12:U:H2'	1.66	0.40	
1:X:470:U:OP1	27:2:39:ARG:O	2.39	0.40	
1:X:529:U:C2	1:X:530:G:C8	3.09	0.40	
1:X:540:G:H3'	1:X:540:G:H8	1.86	0.40	
1:X:1217:U:O2	10:I:4:HIS:HD2	2.05	0.40	
1:X:1314:A:H2	1:X:1642:G:H21	1.68	0.40	
1:X:1332:G:C5	1:X:1333:G:C6	3.10	0.40	
1:X:1659:G:N7	32:X:3248:MPD:HM3	2.36	0.40	
1:X:1724:C:N3	1:X:1747:G:C6	2.89	0.40	
1:X:1883:A:H1'	1:X:1953:A:H2'	2.04	0.40	
1:X:2043:A:H3'	5:C:62:LYS:NZ	2.37	0.40	
1:X:2373:C:OP1	28:3:30:ARG:NH1	2.53	0.40	
1:X:2845:C:C2'	1:X:2846:G:H5'	2.51	0.40	



Atom 1 Atom 2		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:B:31:CYS:HB3	4:B:49:ILE:CG1	2.44	0.40
7:E:38:ASN:HB3	7:E:40:GLU:CD	2.41	0.40
11:J:21:ASP:OD1	11:J:22:ALA:N	2.55	0.40
20:S:54:ILE:HG13	20:S:62:PHE:CE1	2.55	0.40
27:2:27:GLY:HA2	27:2:30:ILE:HD12	2.02	0.40
1:X:555:U:H2'	1:X:1234:C:H5"	2.03	0.40
1:X:644:A:N7	1:X:645:G:H1'	2.37	0.40
1:X:741:G:C4	1:X:743:A:C8	3.09	0.40
1:X:839:U:H5"	1:X:2408:G:P	2.61	0.40
1:X:1301:U:O2'	1:X:1664:G:N2	2.55	0.40
1:X:1652:G:C6	1:X:1653:C:C4	3.09	0.40
1:X:1787:U:H4'	3:A:254:THR:OG1	2.21	0.40
1:X:2594:U:N1	25:Z:7:PRO:HA	2.35	0.40
1:X:2751:C:O2'	4:B:203:LYS:NZ	2.49	0.40
1:X:2824:C:H4'	1:X:2825:A:H5'	2.03	0.40
4:B:135:HIS:CE1	4:B:136:ARG:HG2	2.57	0.40
4:B:195:LEU:HB2	14:M:3:THR:CG2	2.51	0.40
6:D:40:LEU:HD23	6:D:150:ARG:HD2	2.03	0.40
8:G:33:ILE:HA	8:G:34:PRO:HD3	1.88	0.40
8:G:119:LEU:CD1	8:G:122:HIS:NE2	2.84	0.40
8:G:134:MET:HB2	8:G:134:MET:HE2	1.73	0.40
19:R:47:VAL:HG22	19:R:75:ALA:HB2	2.02	0.40
23:V:32:ALA:HA	23:V:37:LEU:HB2	2.03	0.40
28:3:5:LYS:HE3	28:3:61:MET:SD	2.61	0.40
1:X:528:G:H2'	1:X:529:U:H6	1.86	0.40
1:X:582:G:H5'	1:X:584:A:N7	2.36	0.40
1:X:969:U:C4	11:J:17:ARG:HB2	2.56	0.40
1:X:1171:A:H1'	16:O:7:THR:CG2	2.52	0.40
1:X:1175:A:C2	1:X:1176:U:C2	3.10	0.40
1:X:1286:U:OP2	31:X:3238:SPD:H92	2.22	0.40
1:X:1463:A:H2'	1:X:1464:A:C8	2.56	0.40
1:X:1752:U:H3	1:X:1753:A:N6	2.19	0.40
1:X:1912:G:O2'	1:X:1913:G:H5'	2.22	0.40
1:X:2198:U:OP2	1:X:2199:C:H5"	2.21	0.40
1:X:2358:C:H2'	1:X:2359:U:C6	2.56	0.40
2:Y:51:G:H5'	13:L:97:HIS:HE1	1.87	0.40
2:Y:90:C:H2'	2:Y:91:A:O4'	2.22	0.40
5:C:5:ASN:HA	5:C:118:VAL:HG23	2.03	0.40
6:D:31:ILE:HD11	6:D:34:ILE:HD11	2.04	0.40
6:D:68:THR:N	6:D:86:GLY:O	2.35	0.40
11:J:8:THR:HG22	11:J:70:PHE:HE2	1.86	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:56:MET:HE1	18:Q:77:LYS:HE3	2.00	0.40
18:Q:88:ILE:HD13	18:Q:91:LEU:HD23	2.02	0.40
20:S:63:PRO:HB2	20:S:86:VAL:HB	2.03	0.40
20:S:103:ARG:HG3	20:S:107:GLU:CB	2.52	0.40
20:S:104:SER:OG	20:S:105:GLN:N	2.55	0.40
21:T:33:ALA:N	21:T:64:ASP:OD1	2.54	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
3	А	270/274~(98%)	221 (82%)	30 (11%)	19 (7%)	1	7
4	В	204/206~(99%)	$180 \ (88\%)$	$18 \ (9\%)$	6 (3%)	4	27
5	С	194/205~(95%)	152 (78%)	29~(15%)	13 (7%)	1	8
6	D	175/177~(99%)	140 (80%)	29~(17%)	6 (3%)	3	23
7	Ε	169/171~(99%)	144 (85%)	18 (11%)	7 (4%)	3	19
8	G	140/143~(98%)	111 (79%)	18 (13%)	11 (8%)	1	5
9	Н	132/134~(98%)	120 (91%)	9 (7%)	3 (2%)	6	33
10	Ι	135/137~(98%)	109 (81%)	18 (13%)	8 (6%)	1	12
11	J	133/136~(98%)	102 (77%)	22~(16%)	9 (7%)	1	8
12	К	113/116~(97%)	101 (89%)	8 (7%)	4 (4%)	3	23
13	L	102/104~(98%)	80 (78%)	17 (17%)	5 (5%)	2	16
14	М	116/166~(70%)	100 (86%)	9 (8%)	7 (6%)	1	11
15	Ν	115/117~(98%)	101 (88%)	11 (10%)	3 (3%)	5	30
16	О	96/98~(98%)	75 (78%)	16 (17%)	5 (5%)	2	14
17	Р	127/134~(95%)	119 (94%)	8 (6%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perc	$\mathbf{entiles}$
18	Q	90/93~(97%)	80 (89%)	8 (9%)	2 (2%)	6	34
19	R	108/110~(98%)	73~(68%)	19 (18%)	16 (15%)	0	1
20	S	173/175~(99%)	136 (79%)	28 (16%)	9 (5%)	2	14
21	Т	72/91~(79%)	61 (85%)	8 (11%)	3 (4%)	3	19
22	U	72/74~(97%)	51 (71%)	17 (24%)	4 (6%)	2	13
23	V	52/61~(85%)	48 (92%)	3 (6%)	1 (2%)	8	38
24	W	53/55~(96%)	47 (89%)	6 (11%)	0	100	100
25	Z	55/58~(95%)	44 (80%)	7(13%)	4 (7%)	1	7
26	1	47/49~(96%)	33~(70%)	8 (17%)	6 (13%)	0	1
27	2	44/47~(94%)	38~(86%)	4 (9%)	2 (4%)	2	17
28	3	61/63~(97%)	45 (74%)	11 (18%)	5 (8%)	1	5
All	All	3048/3194~(95%)	2511 (82%)	379 (12%)	158 (5%)	2	14

All (158) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	А	90	ALA
3	А	153	ALA
3	А	242	ALA
3	А	247	VAL
3	А	252	LYS
5	С	16	GLU
5	С	22	VAL
5	С	69	HIS
5	С	118	VAL
5	С	189	ASP
6	D	4	LEU
6	D	72	LYS
6	D	78	LYS
7	Е	21	ASP
8	G	35	LYS
8	G	96	ASP
9	Н	18	GLU
10	Ι	30	ALA
10	Ι	34	HIS
10	Ι	105	PRO
11	J	13	GLN
11	J	86	LYS



Mol	Chain	Res	Type
11	J	136	GLU
12	K	100	VAL
13	L	10	LYS
14	М	28	ARG
14	М	29	PRO
14	М	96	ARG
15	N	92	ARG
16	0	14	VAL
19	R	26	SER
19	R	58	VAL
19	R	78	ALA
19	R	98	ILE
20	S	48	THR
20	S	127	PRO
21	Т	68	VAL
21	Т	69	PHE
22	U	10	LYS
22	U	45	ASN
26	1	23	THR
27	2	40	HIS
28	3	3	LYS
28	3	30	ARG
3	А	38	PRO
3	А	171	ASP
3	А	250	TRP
4	В	130	GLY
5	С	6	VAL
5	С	59	TYR
5	С	127	ASP
5	С	190	ALA
6	D	48	LYS
8	G	70	PHE
8	G	111	LYS
8	G	115	ALA
8	G	168	THR
10	Ι	28	LYS
10	Ι	39	SER
11	J	62	GLY
13	L	68	ALA
14	М	3	THR
14	M	30	GLY
14	М	111	ARG



Mol	Chain	Res	Type
15	N	8	ILE
16	0	6	GLN
16	0	48	GLY
19	R	89	GLY
20	S	30	VAL
22	U	12	ASN
25	Z	21	SER
25	Ζ	39	LYS
25	Z	53	ASP
26	1	20	PHE
26	1	21	TYR
26	1	42	PRO
28	3	13	ARG
28	3	14	ILE
3	A	35	GLU
3	A	39	LYS
3	A	80	ALA
4	В	144	ARG
5	С	116	LYS
5	C	128	ALA
6	D	47	SER
6	D	160	ALA
7	Е	7	GLN
7	Е	94	PHE
8	G	92	GLY
8	G	167	LYS
8	G	170	PRO
9	Н	61	ARG
10	Ι	35	LYS
10	Ι	43	ALA
11	J	11	ARG
11	J	12	LYS
11	J	60	ARG
11	J	93	TYR
12	К	4	GLY
13	L	21	THR
14	М	118	LYS
19	R	60	PRO
19	R	85	ASP
19	R	87	GLU
19	R	97	GLN
19	R	108	VAL



Mol	Chain	Res	Type
20	S	9	THR
20	S	13	LYS
20	S	47	SER
20	S	140	LYS
20	S	156	GLU
26	1	17	GLY
26	1	36	GLU
27	2	42	LEU
28	3	49	VAL
3	A	12	SER
3	A	53	PHE
3	A	156	ALA
3	A	254	THR
7	E	55	PRO
7	E E	164	PHE
. 7	E E	165	VAL
. 8	G	97	ASP
12	K	56	LYS
13	L	59	LEU
13	L	95	LYS
16	0	9	GLY
18	0	88	ILE
19	R.	65	PRO
19	R	82	ALA
22	U	30	VAL
25	Z	37	HIS
4	B	147	PRO
11	J	30	PHE
12	K	20	LEU
18	Q	83	ALA
19	R	51	VAL
21	T	47	ALA
3	A	144	ALA
3	A	240	THR
4	В	34	VAL
9	Н	22	ILE
10	Ι	108	LEU
16	0	8	GLY
19	R	90	LYS
23	V	43	VAL
8	G	163	PRO
20	S	157	GLY
			1



Mol	Chain	Res	Type
5	С	70	GLY
15	Ν	23	GLY
3	А	253	PRO
5	С	8	GLY
19	R	67	GLY
19	R	86	PRO
3	А	150	GLY
4	В	86	PRO
4	В	146	THR
7	Е	12	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	Perce	\mathbf{ntiles}
3	А	197/215~(92%)	195~(99%)	2(1%)	76	89
4	В	155/155~(100%)	153~(99%)	2(1%)	69	86
5	С	151/163~(93%)	144 (95%)	7(5%)	27	62
6	D	147/153~(96%)	144 (98%)	3(2%)	55	79
7	Е	136/136~(100%)	133~(98%)	3 (2%)	52	78
8	G	117/119~(98%)	114 (97%)	3(3%)	46	75
9	Н	103/103~(100%)	100 (97%)	3 (3%)	42	72
10	Ι	93/105~(89%)	89~(96%)	4 (4%)	29	63
11	J	104/110~(94%)	101 (97%)	3 (3%)	42	72
12	K	91/93~(98%)	83 (91%)	8 (9%)	10	36
13	L	69/74~(93%)	67 (97%)	2(3%)	42	72
14	М	97/134~(72%)	93~(96%)	4 (4%)	30	65
15	Ν	91/96~(95%)	89 (98%)	2 (2%)	52	78
16	Ο	71/78~(91%)	69 (97%)	2(3%)	43	73
17	Р	107/115~(93%)	102 (95%)	5 (5%)	26	61
18	Q	$7\overline{1/75}\ (95\%)$	71 (100%)	0	100	100



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
19	R	77/91~(85%)	73~(95%)	4(5%)	23	58
20	S	134/149~(90%)	132~(98%)	2 (2%)	65	84
21	Т	51/67~(76%)	49 (96%)	2 (4%)	32	66
22	U	45/59~(76%)	42 (93%)	3 (7%)	16	49
23	V	43/49~(88%)	42 (98%)	1 (2%)	50	77
24	W	48/48~(100%)	47 (98%)	1 (2%)	53	79
25	Z	50/51~(98%)	49 (98%)	1 (2%)	55	79
26	1	22/44~(50%)	20~(91%)	2(9%)	9	33
27	2	39/40~(98%)	38 (97%)	1 (3%)	46	75
28	3	42/50~(84%)	38 (90%)	4 (10%)	8	31
All	All	2351/2572~(91%)	2277 (97%)	74 (3%)	40	71

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
3	А	6	TYR
3	А	252	LYS
4	В	18	ASP
4	В	156	MET
5	С	59	TYR
5	С	91	TYR
5	С	100	ARG
5	С	120	VAL
5	С	166	TRP
5	С	176	ASN
5	С	182	ARG
6	D	4	LEU
6	D	44	LYS
6	D	71	LYS
7	Е	54	ARG
7	Е	69	ARG
7	Ε	106	ASN
8	G	35	LYS
8	G	104	THR
8	G	167	LYS
9	Н	81	ILE
9	Н	91	PHE
9	Н	125	LYS



10 I 4 HIS 10 I 55 ARG 10 I 63 ARG 10 I 105 PRO 11 J 17 ARG 11 J 21 ASP 11 J 93 TYR 12 K 2 ARG 12 K 17 ARG 12 K 35 GLN 12 K 102 THR 12 K 102 THR 12 K 102 THR 12 K 109 THR 13 L 9 ARG 14 M 5 ILE 14 M 14 ARG 15 N 115 ASN 16 O 6 GLN 17 P 9 ARG 17 P 125<	Mol	Chain	Res	Tvpe
10 I 55 ARG 10 I 63 ARG 10 I 105 PRO 11 J 17 ARG 11 J 21 ASP 11 J 93 TYR 12 K 2 ARG 12 K 35 GLN 12 K 35 GLN 12 K 99 ARG 12 K 102 THR 12 K 104 ARG 12 K 109 THR 13 L 9 ARG 14 M 5 ILE 14 M 14 ARG 14 M 12 ARG 15 N 61 TRP 15 N 115 ASN 16 O 6 GLN 17 P 9 </td <td>10</td> <td>T</td> <td>4</td> <td>HIS</td>	10	T	4	HIS
10 I 63 ARG 10 I 105 PRO 11 J 17 ARG 11 J 21 ASP 11 J 93 TYR 12 K 2 ARG 12 K 35 GLN 12 K 35 GLN 12 K 99 ARG 12 K 102 THR 12 K 102 THR 12 K 102 THR 12 K 109 THR 13 L 9 ARG 14 M 5 ILE 14 M 14 ARG 14 M 16 ARG 15 N 61 TRP 15 N 115 ASN 16 O 6 GLN 17 P 9<	10	I	55	ARG
10 I 105 PRO 11 J 17 ARG 11 J 21 ASP 11 J 93 TYR 12 K 2 ARG 12 K 17 ARG 12 K 35 GLN 12 K 35 GLN 12 K 99 ARG 12 K 102 THR 12 K 109 THR 12 K 109 THR 13 L 9 ARG 14 M 5 ILE 14 M 14 ARG 14 M 16 ARG 15 N 61 TRP 15 N 115 ASN 16 O 6 GLN 17 P 9 ARG 17 P 96 </td <td>10</td> <td>I</td> <td>63</td> <td>ARG</td>	10	I	63	ARG
10 1 100 1100 11 J 17 ARG 11 J 21 ASP 11 J 93 TYR 12 K 2 ARG 12 K 35 GLN 12 K 35 GLN 12 K 83 VAL 12 K 99 ARG 12 K 102 THR 12 K 102 THR 13 L 9 ARG 13 L 9 ARG 14 M 5 ILE 14 M 14 ARG 14 M 16 ARG 15 N 61 TRP 15 N 115 ASN 16 O 10 LYS 17 P 9 ARG 17 P 125<	10	I	105	PRO
11 J 21 ASP 11 J 93 TYR 12 K 2 ARG 12 K 17 ARG 12 K 35 GLN 12 K 35 GLN 12 K 83 VAL 12 K 99 ARG 12 K 102 THR 12 K 102 THR 12 K 102 THR 13 L 9 ARG 13 L 9 ARG 14 M 14 ARG 14 M 12 ARG 15 N 61 TRP 15 N 115 ASN 16 O 6 GLN 17 P 9 ARG 17 P 25 PHE 17 P 125 </td <td>11</td> <td>J</td> <td>17</td> <td>ARG</td>	11	J	17	ARG
11 J 93 TYR 12 K 2 ARG 12 K 17 ARG 12 K 35 GLN 12 K 83 VAL 12 K 99 ARG 12 K 99 ARG 12 K 102 THR 12 K 102 THR 12 K 109 THR 13 L 9 ARG 13 L 9 ARG 14 M 5 ILE 14 M 14 ARG 14 M 16 ARG 15 N 61 TRP 15 N 115 ASN 16 O 6 GLN 17 P 9 ARG 17 P 25 PHE 17 P 125 <td>11</td> <td>J</td> <td>21</td> <td>ASP</td>	11	J	21	ASP
11 0 05 144 12 K 2 ARG 12 K 17 ARG 12 K 35 GLN 12 K 83 VAL 12 K 99 ARG 12 K 102 THR 12 K 104 ARG 12 K 109 THR 13 L 9 ARG 13 L 64 LYS 14 M 14 ARG 14 M 16 ARG 15 N 61 TRP 15 N 115 ASN 16 O 6 GLN 17 P 9 ARG 17 P 95 PHE 17 P 100 LYS 17 P 96 TYR 17 P 125	11	J	93	TYB
12 R 12 RRG 12 K 17 ARG 12 K 35 GLN 12 K 99 ARG 12 K 102 THR 12 K 102 THR 12 K 104 ARG 12 K 109 THR 13 L 9 ARG 13 L 64 LYS 14 M 5 ILE 14 M 16 ARG 15 N 61 TRP 15 N 115 ASN 16 O 6 GLN 17 P 9 ARG 17 P 96 TYR 17 P 45 ILE 17 P 125 THR 19 R 30 LYS 19 R 10	12	K	$\frac{33}{2}$	ARG
12 R 35 GLN 12 K 35 GLN 12 K 83 VAL 12 K 99 ARG 12 K 102 THR 12 K 104 ARG 12 K 109 THR 13 L 9 ARG 13 L 64 LYS 14 M 5 ILE 14 M 12 ARG 14 M 16 ARG 15 N 61 TRP 15 N 115 ASN 16 O 6 GLN 16 O 10 LYS 17 P 9 ARG 17 P 25 PHE 17 P 125 THR 19 R 30 LYS 19 R 102	12	K	17	ARG
12 R 30 GLR 12 K 99 ARG 12 K 102 THR 12 K 104 ARG 12 K 109 THR 12 K 109 THR 13 L 9 ARG 13 L 64 LYS 14 M 5 ILE 14 M 22 ARG 14 M 16 ARG 15 N 61 TRP 15 N 115 ASN 16 O 6 GLN 17 P 9 ARG 17 P 25 PHE 17 P 25 PHE 17 P 125 THR 19 R 30 LYS 19 R 102 LYS 19 R 102 LYS 20 S 112 LEU 21	12	K	35	GLN
12 \mathbf{R} 90 \mathbf{ARG} 12 \mathbf{K} 102 \mathbf{THR} 12 \mathbf{K} 104 \mathbf{ARG} 12 \mathbf{K} 109 \mathbf{THR} 13 \mathbf{L} 9 \mathbf{ARG} 13 \mathbf{L} 9 \mathbf{ARG} 14 \mathbf{M} 5 \mathbf{ILE} 14 \mathbf{M} 22 \mathbf{ARG} 14 \mathbf{M} 22 \mathbf{ARG} 14 \mathbf{M} 12 \mathbf{ARG} 14 \mathbf{M} 14 \mathbf{ARG} 14 \mathbf{M} 16 \mathbf{ARG} 15 \mathbf{N} 61 \mathbf{TRP} 15 \mathbf{N} 115 \mathbf{ASN} 16 \mathbf{O} 6 \mathbf{GLN} 17 \mathbf{P} 25 \mathbf{PHE} 17 \mathbf{P} 96 \mathbf{TYR} 17 \mathbf{P} 30 \mathbf{LYS} 19 \mathbf{R} 30 \mathbf{LYS} 19 \mathbf{R} 102 LYS	12	K	83	VAL
12 K 102 THR 12 K 102 THR 12 K 109 THR 13 L 9 ARG 13 L 64 LYS 14 M 5 ILE 14 M 14 ARG 14 M 22 ARG 14 M 16 ARG 14 M 16 ARG 14 M 16 ARG 15 N 61 TRP 15 N 115 ASN 16 O 6 GLN 17 P 9 ARG 17 P 25 PHE 17 P 96 TYR 17 P 125 THR 19 R 30 LYS 19 R 102 LYS 20 S 9<	12	K	99	ARG
12 K 104 ARG 12 K 109 THR 13 L 9 ARG 13 L 64 LYS 14 M 5 ILE 14 M 14 ARG 14 M 22 ARG 14 M 126 ARG 14 M 126 ARG 14 M 126 ARG 14 M 116 ARG 15 N 61 TRP 15 N 115 ASN 16 O 6 GLN 17 P 9 ARG 17 P 25 PHE 17 P 96 TYR 17 P 125 THR 19 R 30 LYS 19 R 102 LYS 20 S <td< td=""><td>12</td><td>K</td><td>102</td><td>THR</td></td<>	12	K	102	THR
12 K 109 THR 13 L 9 ARG 13 L 64 LYS 14 M 5 ILE 14 M 22 ARG 14 M 14 ARG 14 M 14 ARG 14 M 12 ARG 14 M 14 ARG 14 M 16 ARG 15 N 61 TRP 15 N 115 ASN 16 O 6 GLN 17 P 9 ARG 17 P 25 PHE 17 P 45 ILE 17 P 125 THR 19 R 30 LYS 19 R 102 LYS 19 R 102 LYS 20 S 9 THR 20 S 112 LEU 21	$\frac{12}{12}$	K	104	ARG
12 11 130 1110 13 L 9 ARG 13 L 64 LYS 14 M 5 ILE 14 M 14 ARG 14 M 22 ARG 14 M 12 ARG 14 M 16 ARG 15 N 61 TRP 15 N 115 ASN 16 O 6 GLN 17 P 9 ARG 17 P 9 ARG 17 P 9 ARG 17 P 25 PHE 17 P 45 ILE 17 P 125 THR 19 R 30 LYS 19 R 102 LYS 19 R 102 LYS 20 S 9 THR 20 S 112 LEU 21	12 12	K	109	THR
13 L 64 LYS 14 M 5 ILE 14 M 14 ARG 14 M 14 ARG 14 M 22 ARG 14 M 116 ARG 15 N 61 TRP 15 N 115 ASN 16 O 6 GLN 16 O 10 LYS 17 P 9 ARG 17 P 25 PHE 17 P 45 ILE 17 P 96 TYR 17 P 125 THR 19 R 30 LYS 19 R 80 LYS 19 R 102 LYS 20 S 9 THR 20 S 112 LEU 21 T 55<	13	I.	9	ARG
13 14 M 5 ILE 14 M 14 ARG 14 M 14 ARG 14 M 12 ARG 14 M 116 ARG 15 N 61 TRP 15 N 61 TRP 15 N 115 ASN 16 O 6 GLN 16 O 10 LYS 17 P 9 ARG 17 P 25 PHE 17 P 45 ILE 17 P 45 ILE 17 P 125 THR 19 R 30 LYS 19 R 102 LYS 20 S 9 THR 20 S 112 LEU 21 T 55 ARG 21 T<	13	L	64	IYS
14 M 14 ARG 14 M 14 ARG 14 M 116 ARG 14 M 116 ARG 15 N 61 TRP 15 N 115 ASN 16 O 6 GLN 16 O 10 LYS 17 P 9 ARG 17 P 25 PHE 17 P 45 ILE 17 P 96 TYR 17 P 96 TYR 17 P 30 LYS 19 R 30 LYS 19 R 80 LYS 19 R 102 LYS 20 S 9 THR 20 S 112 LEU 21 T 55 ARG 21 T 78 PHE 22 U 10 LYS 22	14	M	5	ILE
14 M 22 ARG 14 M 116 ARG 15 N 61 TRP 15 N 115 ASN 16 O 6 GLN 17 P 9 ARG 17 P 9 ARG 17 P 25 PHE 17 P 25 PHE 17 P 45 ILE 17 P 96 TYR 17 P 125 THR 19 R 30 LYS 19 R 30 LYS 19 R 102 LYS 20 S 9 THR 20 S 112 LEU 21 T 55 ARG 21 T 78 PHE 22 U 10 LYS 22 U 40 ARG 23 V 44 ARG	14	M	14	ARG
14 M 116 ARG 15 N 61 TRP 15 N 115 ASN 16 O 6 GLN 16 O 10 LYS 17 P 9 ARG 17 P 25 PHE 17 P 45 ILE 17 P 96 TYR 17 P 96 TYR 17 P 30 LYS 17 P 30 LYS 17 P 30 LYS 17 P 30 LYS 19 R 30 LYS 19 R 102 LYS 20 S 9 THR 20 S 112 LEU 21 T 55 ARG 21 T 78 PHE 22 U 10<	14	M	22	ARG
11 11 110 1100 15 N 61 TRP 15 N 115 ASN 16 O 6 GLN 16 O 10 LYS 17 P 9 ARG 17 P 25 PHE 17 P 45 ILE 17 P 96 TYR 17 P 96 TYR 17 P 125 THR 19 R 30 LYS 19 R 70 GLU 19 R 102 LYS 20 S 9 THR 20 S 112 LEU 21 T 55 ARG 21 T 78 PHE 22 U 10 LYS 22 U 40 ARG 23 V	14	M	116	ARG
15 N 115 ASN 15 N 115 ASN 16 O 6 GLN 16 O 10 LYS 17 P 9 ARG 17 P 25 PHE 17 P 45 ILE 17 P 45 ILE 17 P 96 TYR 17 P 125 THR 17 P 30 LYS 17 P 30 LYS 19 R 30 LYS 19 R 102 LYS 20 S 9 THR 20 S 112 LEU 21 T 55 ARG 21 T 78 PHE 22 U 10 LYS 22 U 40 ARG 22 U 48	15	N	61	TRP
16O 6 GLN 16 O 10 LYS 17 P9ARG 17 P 25 PHE 17 P 45 ILE 17 P 96 TYR 17 P 96 TYR 17 P 125 THR 19 R 30 LYS 19 R 70 GLU 19 R 102 LYS 20 S9THR 20 S112LEU 21 T 55 ARG 21 T 78 PHE 22 U 40 ARG 22 U 40 ARG 23 V 44 ARG	15	N	115	ASN
16 O 10 LYS 17 P 9 ARG 17 P 25 PHE 17 P 45 ILE 17 P 96 TYR 17 P 96 TYR 17 P 96 TYR 17 P 125 THR 17 P 125 THR 19 R 30 LYS 19 R 80 LYS 19 R 102 LYS 20 S 9 THR 20 S 112 LEU 21 T 55 ARG 21 T 78 PHE 22 U 10 LYS 22 U 40 ARG 23 V 44 ARG	16	0	6	GLN
17 P 9 ARG 17 P 25 PHE 17 P 45 ILE 17 P 96 TYR 17 P 96 TYR 17 P 125 THR 17 P 125 THR 19 R 30 LYS 19 R 70 GLU 19 R 102 LYS 20 S 9 THR 20 S 112 LEU 21 T 55 ARG 21 T 78 PHE 22 U 10 LYS 22 U 40 ARG 22 U 40 ARG 23 V 44 ARG	16	0	10	LYS
17 P 25 PHE 17 P 45 ILE 17 P 96 TYR 17 P 125 THR 17 P 125 THR 19 R 30 LYS 19 R 80 LYS 19 R 102 LYS 20 S 9 THR 20 S 112 LEU 21 T 55 ARG 21 T 78 PHE 22 U 10 LYS 22 U 40 ARG 23 V 44 ARG	17	P	9	ARG
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	17	P	25	PHE
17 P 96 TYR 17 P 125 THR 19 R 30 LYS 19 R 70 GLU 19 R 80 LYS 19 R 102 LYS 20 S 9 THR 20 S 112 LEU 21 T 55 ARG 21 T 78 PHE 22 U 10 LYS 22 U 40 ARG 23 V 44 ARG	17	Р	45	ILE
17 P 125 THR 19 R 30 LYS 19 R 70 GLU 19 R 80 LYS 19 R 102 LYS 20 S 9 THR 20 S 112 LEU 21 T 55 ARG 21 T 78 PHE 22 U 10 LYS 22 U 40 ARG 23 V 44 ARG	17	Р	96	TYR
19 R 30 LYS 19 R 70 GLU 19 R 80 LYS 19 R 102 LYS 20 S 9 THR 20 S 112 LEU 21 T 55 ARG 22 U 10 LYS 22 U 40 ARG 22 U 48 LYS 23 V 44 ARG	17	Р	125	THR
19 R 70 GLU 19 R 80 LYS 19 R 102 LYS 20 S 9 THR 20 S 112 LEU 21 T 55 ARG 21 T 78 PHE 22 U 40 ARG 22 U 48 LYS 23 V 44 ARG	19	R	30	LYS
19 R 80 LYS 19 R 102 LYS 20 S 9 THR 20 S 112 LEU 21 T 55 ARG 21 T 78 PHE 22 U 10 LYS 22 U 40 ARG 22 U 48 LYS 23 V 44 ARG	19	R	70	GLU
19 R 102 LYS 20 S 9 THR 20 S 112 LEU 21 T 55 ARG 21 T 78 PHE 22 U 10 LYS 22 U 40 ARG 22 U 48 LYS 23 V 44 ARG	19	R	80	LYS
20 S 9 THR 20 S 112 LEU 21 T 55 ARG 21 T 78 PHE 22 U 10 LYS 22 U 40 ARG 22 U 48 LYS 23 V 44 ARG	19	R	102	LYS
20 S 112 LEU 21 T 55 ARG 21 T 78 PHE 22 U 10 LYS 22 U 40 ARG 22 U 48 LYS 23 V 44 ARG	20	S	9	THR
21 T 55 ARG 21 T 78 PHE 22 U 10 LYS 22 U 40 ARG 22 U 48 LYS 23 V 44 ARG	20	S	112	LEU
21 T 78 PHE 22 U 10 LYS 22 U 40 ARG 22 U 48 LYS 23 V 44 ARG	21	Т	55	ARG
22 U 10 LYS 22 U 40 ARG 22 U 48 LYS 23 V 44 ARG	21	Т	78	PHE
22 U 40 ARG 22 U 48 LYS 23 V 44 ARG	22	U	10	LYS
22 U 48 LYS 23 V 44 ARG	22	U	40	ARG
23 V 44 ARG	22	U	48	LYS
	23	V	44	ARG



COnti	писи јтоп	i preui	ous puye
Mol	Chain	\mathbf{Res}	Type
24	W	4	LYS
25	Ζ	16	ARG
26	1	50	PHE
26	1	54	LYS
27	2	4	THR
28	3	4	MET
28	3	44	LYS
28	3	52	LYS
28	3	61	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
3	А	76	ASN
3	А	118	ASN
3	А	220	HIS
3	А	227	ASN
4	В	92	ASN
5	С	3	GLN
5	С	34	GLN
5	С	163	ASN
5	С	176	ASN
6	D	37	ASN
6	D	129	ASN
8	G	140	GLN
8	G	164	GLN
10	Ι	103	ASN
19	R	15	HIS
24	W	49	HIS
25	Z	56	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Х	2686/2880~(93%)	750 (27%)	76~(2%)
2	Y	121/123~(98%)	33~(27%)	4(3%)
All	All	2807/3003~(93%)	783 (27%)	80 (2%)

All (783) RNA backbone outliers are listed below:



Mol	Chain	Res	Type
1	Х	3	U
1	Х	10	А
1	Х	12	U
1	Х	13	А
1	Х	14	А
1	Х	15	G
1	Х	23	G
1	Х	26	G
1	Х	27	G
1	Х	28	А
1	Х	34	U
1	Х	39	С
1	Х	42	G
1	X	45	С
1	Х	46	С
1	Х	47	G
1	Х	48	А
1	Х	49	U
1	Х	50	G
1	Х	51	А
1	Х	57	G
1	Х	59	G
1	Х	69	G
1	Х	70	А
1	Х	71	А
1	Х	72	А
1	Х	73	А
1	Х	74	G
1	X	83	A
1	X	89	A
1	X	91	A
1	X	95	G
1	Х	99	U
1	X	100	G
1	Х	101	А
1	X	102	C
1	X	108	G
1	X	109	A
1	X	111	G
1	X	116	A
1	X	117	A
1	X	118	U
1	X	119	G



Mol	Chain	Res	Type
1	Х	120	G
1	Х	123	A
1	Х	126	С
1	Х	127	С
1	Х	129	A
1	Х	132	U
1	Х	133	С
1	Х	134	G
1	Х	135	U
1	Х	137	А
1	Х	143	A
1	Х	147	G
1	Х	148	С
1	Х	149	A
1	Х	150	А
1	Х	157	G
1	Х	158	А
1	Х	164	G
1	Х	169	С
1	Х	173	А
1	Х	176	А
1	Х	192	G
1	Х	193	А
1	Х	199	A
1	Х	200	А
1	Х	201	G
1	Х	206	U
1	Х	207	U
1	Х	210	А
1	Х	218	A
1	Х	219	G
1	Х	220	U
1	Х	222	G
1	Х	225	G
1	Х	226	С
1	Х	229	G
1	Х	241	С
1	Х	242	A
1	Х	243	G
1	Х	244	С
1	Х	245	С
1	Х	247	A



Mol	Chain	Res	Type
1	Х	249	A
1	Х	250	С
1	Х	252	G
1	Х	254	A
1	Х	255	A
1	Х	256	С
1	Х	257	G
1	Х	259	U
1	Х	260	U
1	Х	261	G
1	Х	262	С
1	Х	264	U
1	Х	265	U
1	Х	266	U
1	Х	267	С
1	Х	268	G
1	Х	270	G
1	Х	272	U
1	Х	273	U
1	Х	274	G
1	Х	275	U
1	Х	276	А
1	Х	280	С
1	Х	281	С
1	Х	282	А
1	Х	304	А
1	Х	305	А
1	Х	310	А
1	Х	322	А
1	Х	340	G
1	Х	342	G
1	Х	343	A
1	Х	344	G
1	Х	349	G
1	Х	358	С
1	Х	360	A
1	Х	362	С
1	Х	384	A
1	Х	385	G
1	Х	386	U
1	Х	387	A
1	Х	388	G



Mol	Chain	Res	Type
1	Х	398	С
1	Х	399	G
1	Х	400	U
1	Х	401	G
1	Х	403	A
1	Х	404	A
1	Х	408	U
1	Х	409	G
1	Х	416	U
1	Х	418	С
1	Х	419	G
1	Х	424	G
1	Х	425	A
1	Х	441	A
1	Х	448	С
1	Х	456	C
1	Х	459	А
1	Х	461	А
1	Х	463	С
1	Х	467	U
1	Х	475	U
1	Х	476	G
1	Х	483	A
1	Х	484	G
1	Х	492	G
1	Х	493	A
1	Х	504	G
1	Х	506	G
1	Х	514	G
1	Х	515	A
1	X	516	G
1	X	518	A
1	X	519	С
1	Х	520	С
1	X	527	C
1	X	536	A
1	X	537	C
1	X	538	A
1	X	540	G
1	X	541	C
1	X	542	A
1	X	543	G



Mol	Chain	Res	Type
1	X	552	C
1	X	554	U
1	X	555	U
1	X	556	A
1	X	559	С
1	X	560	G
1	X	572	G
1	Х	578	U
1	Х	582	G
1	Х	584	A
1	Х	591	G
1	Х	595	A
1	Х	600	G
1	Х	601	A
1	Х	602	C
1	Х	603	C
1	Х	605	G
1	Х	613	А
1	Х	614	G
1	Х	624	А
1	Х	625	А
1	Х	626	А
1	Х	627	А
1	Х	628	А
1	Х	631	G
1	Х	632	А
1	Х	636	G
1	Х	642	А
1	Х	645	G
1	X	646	C
1	X	648	A
1	X	649	G
1	X	655	A
1	X	657	A
1	X	664	C
1	X	665	A
1	X	666	U
1	X	667	U
1	X	668	A
1	X	682	G
1	X	690	A
1	X	699	G



Mol	Chain	Res	Type
1	Х	719	A
1	Х	741	G
1	Х	743	A
1	Х	747	A
1	Х	752	G
1	Х	760	U
1	Х	766	А
1	Х	774	А
1	Х	775	U
1	Х	777	А
1	Х	778	G
1	Х	781	G
1	Х	782	U
1	Х	788	G
1	Х	789	G
1	Х	790	A
1	Х	795	A
1	Х	797	A
1	Х	798	G
1	Х	802	А
1	Х	803	С
1	Х	805	G
1	Х	806	А
1	Х	807	А
1	Х	813	А
1	Х	818	G
1	Х	820	U
1	Х	825	С
1	Х	832	A
1	Х	837	U
1	Х	840	U
1	Х	841	G
1	Х	859	U
1	Х	860	U
1	Х	872	G
1	Х	877	G
1	Х	879	A
1	Х	887	G
1	Х	890	U
1	Х	891	A
1	Х	913	A
1	Х	922	A



\mathbf{Mol}	Chain	Res	Type
1	Х	924	С
1	Х	939	С
1	Х	940	G
1	Х	944	A
1	Х	949	G
1	Х	952	A
1	Х	957	G
1	Х	958	G
1	Х	969	U
1	Х	970	A
1	Х	971	A
1	Х	972	С
1	Х	973	U
1	Х	985	G
1	Х	994	A
1	Х	995	A
1	Х	1006	С
1	Х	1007	А
1	Х	1016	С
1	Х	1018	С
1	Х	1019	U
1	Х	1021	А
1	Х	1022	А
1	Х	1023	U
1	Х	1024	G
1	Х	1028	G
1	Х	1033	G
1	Х	1034	U
1	Х	1036	G
1	X	1038	U
1	X	1043	A
1	Х	1044	U
1	X	$10\overline{45}$	G
1	X	$10\overline{47}$	G
1	Х	1049	С
1	X	1054	C
1	X	1055	A
1	Х	1056	U
1	X	1057	A
1	X	1058	G
1	X	1060	C
1	X	1064	C



Mol	Chain	Res	Type
1	Х	1069	G
1	Х	1070	G
1	Х	1072	U
1	Х	1073	G
1	Х	1075	С
1	Х	1076	U
1	Х	1077	U
1	Х	1081	А
1	Х	1082	G
1	Х	1083	С
1	Х	1084	А
1	X	1085	G
1	Х	1086	С
1	X	1087	C
1	X	1089	C
1	X	1090	C
1	Х	1094	С
1	Х	1096	А
1	Х	1097	А
1	Х	1098	G
1	Х	1099	А
1	Х	1101	U
1	Х	1102	G
1	Х	1105	U
1	Х	1106	А
1	Х	1114	А
1	Х	1122	А
1	Х	1123	G
1	Х	1124	U
1	Х	1127	C
1	Х	1128	G
1	Х	1129	A
1	X	1130	U
1	Х	1139	A
1	X	1141	U
1	X	1143	A
1	Х	1146	G
1	X	1148	G
1	X	1149	G
1	X	1152	C
1	X	1153	A
1	X	1154	A



Mol	Chain	Res	Type
1	Х	1156	U
1	Х	1161	U
1	Х	1165	G
1	Х	1166	A
1	Х	1180	А
1	Х	1182	U
1	Х	1183	С
1	Х	1192	А
1	Х	1207	G
1	Х	1224	А
1	Х	1226	А
1	Х	1227	А
1	X	1234	С
1	X	1242	A
1	X	1249	G
1	X	1251	G
1	Х	1266	G
1	Х	1269	G
1	Х	1275	А
1	Х	1278	А
1	Х	1282	А
1	Х	1284	G
1	Х	1285	А
1	Х	1288	А
1	Х	1289	А
1	Х	1298	G
1	Х	1302	С
1	Х	1311	С
1	Х	1313	U
1	X	1314	A
1	Х	1315	A
1	X	1321	A
1	Х	1325	U
1	Х	1331	G
1	Х	1334	A
1	Х	1342	U
1	X	1351	G
1	Х	1354	A
1	X	1359	G
1	Х	1365	U
1	X	1370	U
1	Х	1378	А



Mol	Chain	Res	Type
1	Х	1379	A
1	Х	1381	G
1	Х	1391	A
1	Х	1392	U
1	Х	1398	G
1	Х	1401	G
1	Х	1404	С
1	Х	1408	А
1	Х	1409	U
1	Х	1412	С
1	Х	1413	U
1	Х	1428	G
1	Х	1430	G
1	Х	1432	G
1	Х	1433	A
1	Х	1434	U
1	Х	1435	G
1	Х	1440	G
1	Х	1441	A
1	Х	1442	С
1	Х	1443	G
1	Х	1460	G
1	Х	1465	G
1	Х	1467	U
1	Х	1468	A
1	Х	1469	U
1	Х	1470	G
1	Х	1474	A
1	Х	1476	G
1	Х	1482	U
1	Х	1483	G
1	Х	1490	U
1	Х	1497	C
1	Х	1498	G
1	Х	1499	A
1	Х	1500	U
1	Х	1501	C
1	Х	1505	U
1	Х	1506	C
1	Х	1509	A
1	Х	1510	A
1	Х	1513	U



Mol	Chain	Res	Type
1	Х	1519	G
1	X	1531	С
1	Х	1545	G
1	Х	1562	G
1	Х	1571	G
1	Х	1574	A
1	Х	1575	С
1	Х	1582	A
1	Х	1585	A
1	Х	1587	A
1	Х	1593	С
1	Х	1594	U
1	Х	1601	U
1	Х	1602	G
1	Х	1603	A
1	Х	1604	A
1	Х	1610	А
1	Х	1623	С
1	Х	1624	А
1	Х	1625	А
1	Х	1626	А
1	Х	1634	А
1	Х	1636	G
1	Х	1642	G
1	Х	1647	U
1	Х	1648	С
1	Х	1650	А
1	Х	1651	U
1	Х	1657	А
1	Х	1665	С
1	X	1668	G
1	X	1671	A
1	Х	1673	С
1	Х	1681	A
1	Х	1688	U
1	Х	1689	U
1	Х	1691	G
1	Х	1692	С
1	X	1693	A
1	Х	1695	U
1	X	1698	C
1	X	1699	A



Mol	Chain	Res	Type
1	Х	1708	C
1	X	1710	U
1	Х	1713	G
1	X	1714	A
1	X	1717	A
1	Х	1718	A
1	Х	1719	G
1	Х	1747	G
1	Х	1753	A
1	Х	1754	G
1	Х	1755	G
1	Х	1760	G
1	Х	1764	A
1	Х	1766	U
1	Х	1771	А
1	Х	1773	C
1	Х	1779	С
1	Х	1788	С
1	Х	1790	G
1	Х	1791	С
1	Х	1792	С
1	Х	1793	А
1	Х	1798	G
1	Х	1799	А
1	Х	1800	А
1	Х	1801	С
1	Х	1802	А
1	Х	1807	А
1	Х	1808	С
1	X	1811	A
1	X	1819	U
1	X	1821	A
1	X	1825	C
1	X	1826	U
1	X	1827	G
1	X	1830	C
1	Х	1831	G
1	Х	1839	A
1	X	1840	A
1	Х	1850	G
1	X	1852	G
1	Х	1855	G



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1 X	1867	A
1 X	1871	G
1 X	1872	A
1 X	1883	A
1 X	1886	G
1 X	1889	G
1 X	1891	С
1 X	1909	U
1 X	1910	A
1 X	1911	A
1 X	1912	G
1 X	1913	G
1 X	1920	A
1 X	1921	A
1 X	1922	U
1 X	1928	G
1 X	1938	U
1 X	1939	U
1 X	1943	A
1 X	1946	U
1 X	1947	G
1 X	1949	A
1 X	1950	С
1 X	1953	A
1 X	1954	A
1 X	1955	G
1 X	1958	G
1 X	1959	U
1 X	1965	U
1 X	1975	G
1 X	1977	C
1 X	1980	A
1 X	2006	G
1 X	2011	U
1 X	2014	A
1 X	2015	G
1 X	2019	C
1 X	2026	C
1 X	2033	C
1 X	2035	G
1 X	2038	C
1 X	2039	G



Mol	Chain	Res	Type
1	Х	2043	A
1	Х	2044	G
1	Х	2045	A
1	X	2046	С
1	X	2052	G
1	Х	2063	A
1	Х	2066	G
1	Х	2075	U
1	Х	2076	G
1	Х	2077	G
1	Х	2079	A
1	Х	2082	С
1	Х	2084	G
1	X	2085	G
1	Х	2086	U
1	Х	2088	U
1	Х	2089	C
1	Х	2090	U
1	Х	2167	A
1	Х	2168	A
1	Х	2170	С
1	Х	2171	U
1	Х	2172	U
1	Х	2176	U
1	Х	2181	A
1	Х	2188	A
1	Х	2189	A
1	Х	2190	A
1	Х	2191	A
1	Х	2192	U
1	Х	2196	U
1	Х	2197	U
1	Х	2198	U
1	Х	2199	C
1	Х	2200	G
1	Х	2204	A
1	Х	2205	C
1	Х	2217	G
1	Х	2222	U
1	Х	2246	A
1	Х	2247	A
1	Х	2262	C
	· · · ·	· -	



1 X 2264 C 1 X 2265 A 1 X 2266 A 1 X 2268 G 1 X 2274 C 1 X 2275 U 1 X 2277 A 1 X 2284 U 1 X 2285 U 1 X 2287 G 1 X 2287 G 1 X 2290 A 1 X 2291 U 1 X 2298 U 1 X 2301 A 1 X 2304 G 1 X 2304 G 1 X 2313 A 1 X 2313 A 1 X 2323 U 1 X 2323 U<	Mol	Chain	Res	Type
1 X 2265 A 1 X 2266 A 1 X 2274 C 1 X 2275 U 1 X 2277 A 1 X 2284 U 1 X 2285 U 1 X 2287 G 1 X 2287 G 1 X 2287 G 1 X 2290 A 1 X 2291 U 1 X 2298 U 1 X 2301 A 1 X 2304 G 1 X 2306 A 1 X 2307 A 1 X 2313 G 1 X 2313 G 1 X 2322 U 1 X 2323 U 1 X 2323 U 1 X	1	Х	2264	C
1 X 2266 A 1 X 2268 G 1 X 2274 C 1 X 2275 U 1 X 2277 A 1 X 2284 U 1 X 2285 U 1 X 2287 G 1 X 2287 G 1 X 2290 A 1 X 2290 A 1 X 2290 A 1 X 2290 A 1 X 2291 U 1 X 2301 A 1 X 2304 G 1 X 2307 A 1 X 2313 G 1 X 2313 G 1 X 2322 U 1 X 2323 U 1 X 2323 U 1 X	1	Х	2265	A
1 X 2268 G 1 X 2274 C 1 X 2275 U 1 X 2277 A 1 X 2284 U 1 X 2285 U 1 X 2285 U 1 X 2287 G 1 X 2290 A 1 X 2291 U 1 X 2293 U 1 X 2293 A 1 X 2299 A 1 X 2301 A 1 X 2304 G 1 X 2307 A 1 X 2304 G 1 X 2313 G 1 X 2323 U 1 X 2323 U 1 X 2324 G<	1	Х	2266	A
1X 2274 C1X 2275 U1X 2277 A1X 2284 U1X 2285 U1X 2286 G1X 2287 G1X 2290 A1X 2290 A1X 2291 U1X 2299 A1X 2299 A1X 2209 A1X 2209 A1X 2301 A1X 2304 G1X 2304 G1X 2307 A1X 2307 A1X 2313 G1X 2322 U1X 2323 U1X 2323 U1X 2323 U1X 2323 U1X 2323 U1X 2323 G1X 2331 A1X 2355 A1X 2355 A1X 2364 C1X 2364 C1X 2364 C1X 2364 C1X 2369 U1X 2369 U1X 2369 U1X 2369	1	X	2268	G
1X 2275 U1X 2277 A1X 2284 U1X 2285 U1X 2286 G1X 2287 G1X 2290 A1X 2290 A1X 2291 U1X 2299 A1X 2299 A1X 2299 A1X 2301 A1X 2304 G1X 2307 A1X 2307 A1X 2313 G1X 2322 U1X 2323 U1X 2323 U1X 2323 U1X 2323 U1X 2323 U1X 2323 U1X 2324 G1X 2333 A1X 2333 A1X 2355 A1X 2355 A1X 2364 C1X 2364 C1X 2363 G1X 2364 C1X 2364 C1X 2368 G1X 2370 G1X 2375 G1X 2382	1	X	2274	С
1 X 2277 A 1 X 2284 U 1 X 2285 U 1 X 2287 G 1 X 2287 G 1 X 2290 A 1 X 2290 A 1 X 2291 U 1 X 2299 A 1 X 2209 A 1 X 2209 A 1 X 2203 U 1 X 2304 G 1 X 2306 A 1 X 2307 A 1 X 2313 G 1 X 2322 U 1 X 2323 U 1 X 2323 U 1 X 2331 A 1 X </td <td>1</td> <td>X</td> <td>2275</td> <td>U</td>	1	X	2275	U
1X2284U1X2285U1X2286G1X2287G1X2290A1X2291U1X2299A1X2299A1X2301A1X2304G1X2307A1X2307A1X2313G1X2322U1X2323U1X2323U1X2324G1X2329C1X2331A1X2355A1X2355A1X2361G1X2362G1X2363G1X2364C1X2367A1X2367A1X2367A1X2367A1X2367A1X2369U1X2369U1X2375G1X2382C	1	Х	2277	A
1X2285U1X2286G1X2287G1X2290A1X2291U1X2299A1X2299A1X2301A1X2304G1X2306A1X2307A1X2307A1X2313G1X2315A1X2322U1X2323U1X2323U1X2326C1X2331A1X2333A1X2355A1X2355A1X2361G1X2363G1X2363G1X2364C1X2367A1X2368G1X2369U1X2369U1X2370G1X2375G1X2382C	1	Х	2284	U
1 X 2286 G 1 X 2287 G 1 X 2290 A 1 X 2291 U 1 X 2298 U 1 X 2299 A 1 X 2301 A 1 X 2304 G 1 X 2306 A 1 X 2307 A 1 X 2303 G 1 X 2313 G 1 X 2313 G 1 X 2322 U 1 X 2323 U 1 X 2323 U 1 X 2324 G 1 X 2329 C 1 X 2331 A 1 X 2333 A 1 X 2333 A 1 X 2355 A 1 X	1	Х	2285	U
1 X 2287 G 1 X 2290 A 1 X 2291 U 1 X 2298 U 1 X 2299 A 1 X 2301 A 1 X 2304 G 1 X 2306 A 1 X 2307 A 1 X 2313 G 1 X 2313 G 1 X 2313 G 1 X 2313 G 1 X 2322 U 1 X 2323 U 1 X 2323 U 1 X 2324 G 1 X 2329 C 1 X 2331 A 1 X 2333 A 1 X 2333 A 1 X 2355 A 1 X	1	X	2286	G
1X2290A1X2291U1X2298U1X2299A1X2301A1X2304G1X2306A1X2307A1X2313G1X2315A1X2322U1X2323U1X2323U1X2326C1X2329C1X2333A1X2339A1X2355A1X2358C1X2363G1X2363G1X2363G1X2364C1X2367A1X2368G1X2369U1X2370G1X2375G1X2375G1X2382C	1	Х	2287	G
1X2291U1X2298U1X2299A1X2301A1X2304G1X2306A1X2307A1X2313G1X2315A1X2322U1X2323U1X2323U1X2323U1X2324G1X2329C1X2331A1X2333A1X2355A1X2355A1X2361G1X2363G1X2363G1X2364C1X2367A1X2369U1X2370G1X2370G1X2375G1X2375G1X2375G1X2375G1X2375G1X2375G1X2382C	1	Х	2290	A
1X2298U1X2299A1X2301A1X2304G1X2306A1X2307A1X2315A1X2315A1X2322U1X2323U1X2323U1X2324G1X2326C1X2331A1X2333A1X2333A1X2355A1X2355A1X2361G1X2362G1X2363G1X2364C1X2367A1X2369U1X2370G1X2375G1X2375G1X2375G1X2375G1X2375G1X2375G1X2375G1X2382C	1	X	2291	U
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	X	2298	U
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	X	2299	A
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	X	2301	A
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	X	2304	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	X	2306	A
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Х	2307	A
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Х	2313	G
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	X	2315	A
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Х	2322	U
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	Х	2323	U
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	Х	2324	G
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	Х	2326	С
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	Х	2329	С
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	Х	2331	A
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	Х	2333	A
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	Х	2339	A
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	Х	2351	G
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	Х	2355	A
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	Х	2358	C
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	Х	2361	G
1 X 2363 G 1 X 2364 C 1 X 2367 A 1 X 2367 A 1 X 2368 G 1 X 2369 U 1 X 2370 G 1 X 2375 G 1 X 2382 C	1	Х	2362	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Х	2363	G
1 X 2367 A 1 X 2368 G 1 X 2369 U 1 X 2370 G 1 X 2375 G 1 X 2382 C	1	Х	2364	C
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Х	2367	A
1 X 2369 U 1 X 2370 G 1 X 2375 G 1 X 2382 C	1	Х	2368	G
1 X 2370 G 1 X 2375 G 1 X 2382 C	1	Х	2369	U
1 X 2375 G 1 X 2382 C	1	Х	2370	G
1 X 2382 C	1	Х	2375	G
· / / / / / / / / / / / / / / / / / / / / / / / / / /	1	Х	2382	C



Mol	Chain	Res	Type
1	Х	2385	U
1	Х	2386	G
1	Х	2389	G
1	X	2398	U
1	Х	2402	U
1	Х	2403	С
1	Х	2404	A
1	Х	2408	G
1	Х	2409	A
1	Х	2410	U
1	Х	2415	G
1	Х	2419	С
1	Х	2420	C
1	Х	2426	G
1	Х	2427	A
1	Х	2429	A
1	Х	2436	U
1	Х	2437	G
1	Х	2438	А
1	Х	2452	U
1	Х	2453	С
1	Х	2455	А
1	Х	2457	А
1	Х	2458	U
1	Х	2459	С
1	Х	2460	G
1	Х	2461	G
1	Х	2468	G
1	Х	2469	G
1	Х	2470	U
1	X	2471	U
1	X	2477	С
1	X	2480	C
1	Х	2481	G
1	X	2484	G
1	X	2485	U
1	X	2491	C
1	X	2492	G
1	X	2497	A
1	X	2508	G
1	Х	2509	A
1	X	2521	A



Mol	Chain	Res	Type
1	Х	2529	G
1	X	2538	С
1	X	2542	U
1	X	2543	A
1	X	2545	A
1	X	2546	G
1	X	2548	G
1	Х	2551	A
1	Х	2553	G
1	Х	2556	A
1	Х	2560	G
1	X	2561	G
1	X	2562	G
1	X	2563	U
1	X	2564	U
1	X	2565	C
1	Х	2578	G
1	Х	2588	U
1	Х	2591	С
1	Х	2594	U
1	Х	2613	A
1	Х	2621	G
1	X	2633	A
1	Х	2664	G
1	Х	2668	U
1	Х	2679	G
1	Х	2684	A
1	Х	2692	A
1	Х	2693	U
1	Х	2699	G
1	Х	2706	U
1	Х	2707	G
1	Х	2713	A
1	Х	2724	G
1	Х	2728	A
1	Х	2731	G
1	Х	2732	С
1	Х	2736	U
1	Х	2737	A
1	Х	2738	A
1	Х	2744	A
1	Х	2745	A
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Mol	Chain	Res	Type
1	Х	2757	G
1	Х	2758	A
1	Х	2759	U
1	Х	2769	С
1	Х	2771	С
1	Х	2772	U
1	Х	2773	G
1	Х	2781	G
1	Х	2783	U
1	Х	2787	A
1	Х	2792	С
1	Х	2793	G
1	Х	2795	A
1	Х	2796	A
1	Х	2798	A
1	Х	2807	U
1	Х	2808	U
1	Х	2809	A
1	Х	2810	A
1	Х	2815	С
1	Х	2842	С
1	Х	2843	А
1	Х	2847	G
1	Х	2848	A
1	Х	2849	С
1	Х	2850	U
1	Х	2851	G
1	Х	2854	G
1	Х	2858	А
1	Х	2861	A
1	Х	2864	C
1	Х	2867	G
1	Х	2868	G
1	X	2869	U
1	X	2877	A
2	Y	3	A
2	Y	6	C
2	Y	14	С
2	Y	15	A
2	Y	16	U
2	Y	17	A
2	Y	18	G



Mol	Chain	Res	Type
2	Y	26	G
2	Y	27	А
2	Y	28	А
2	Y	29	С
2	Y	30	С
2	Y	37	С
2	Y	40	С
2	Y	42	U
2	Y	43	G
2	Y	44	С
2	Y	49	С
2	Y	52	G
2	Y	54	U
2	Y	58	G
2	Y	59	А
2	Y	69	G
2	Y	84	G
2	Y	95	U
2	Y	99	G
2	Y	102	A
2	Y	108	G
2	Y	112	A
2	Y	115	G
2	Y	121	G
2	Y	122	U
2	Y	123	U

All (80) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	Х	38	G
1	Х	48	А
1	Х	50	G
1	Х	70	А
1	Х	100	G
1	Х	219	G
1	Х	259	U
1	Х	265	U
1	Х	341	А
1	Х	383	G
1	Х	400	U
1	Х	483	А



Mol	Chain	Res	Type
1	Х	490	A
1	Х	518	A
1	Х	537	С
1	Х	540	G
1	Х	559	С
1	Х	600	G
1	Х	751	G
1	Х	759	С
1	Х	788	G
1	Х	789	G
1	Х	797	А
1	Х	806	А
1	Х	843	G
1	X	859	U
1	X	872	G
1	X	969	U
1	Х	972	С
1	Х	994	А
1	Х	1023	U
1	Х	1053	G
1	Х	1074	G
1	Х	1086	С
1	Х	1096	А
1	Х	1122	А
1	Х	1145	С
1	Х	1153	А
1	Х	1225	G
1	Х	1288	А
1	Х	1391	A
1	Х	1403	U
1	X	1408	A
1	X	1412	С
1	Х	1433	A
1	Х	1439	G
1	Х	1473	U
1	Х	1475	U
1	Х	1602	G
1	Х	1625	A
1	X	1712	G
1	Х	1753	A
1	X	1790	G
1	Х	1800	A


Mol	Chain	Res	Type
1	Х	1810	U
1	Х	1909	U
1	Х	1910	А
1	Х	1920	А
1	Х	2043	А
1	Х	2180	U
1	Х	2190	А
1	Х	2237	С
1	Х	2312	А
1	Х	2322	U
1	Х	2323	U
1	Х	2325	А
1	Х	2330	G
1	Х	2402	U
1	Х	2437	G
1	Х	2460	G
1	Х	2485	U
1	Х	2705	А
1	Х	2782	G
1	Х	2807	U
1	Х	2846	G
1	Х	2848	A
2	Y	14	С
2	Y	36	A
2	Y	58	G
2	Y	68	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 388 ligands modelled in this entry, 374 are monoatomic - leaving 14 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	Tuno	Chain	Pog	Tink	Bo	ond leng	ths	E	Bond ang	gles
	туре	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	SPD	Х	3243	1	$9,\!9,\!9$	0.63	0	8,8,8	1.12	0
31	SPD	Х	3242	1	9, 9, 9	0.60	0	8,8,8	0.93	0
32	MPD	Х	3245	-	7,7,7	0.57	0	9,10,10	0.40	0
29	QU2	X	2901	-	53, 53, 53	1.00	4 (7%)	66,76,76	1.65	11 (16%)
34	EOH	Х	3250	-	2,2,2	0.50	0	$1,\!1,\!1$	0.11	0
31	SPD	Х	3238	1	9,9,9	0.85	0	8,8,8	2.07	<mark>3 (37%)</mark>
32	MPD	Х	3248	-	7,7,7	0.62	0	9,10,10	0.40	0
31	SPD	Х	3240	1	$9,\!9,\!9$	0.67	0	8,8,8	1.36	1 (12%)
31	SPD	Х	3241	1	$9,\!9,\!9$	0.31	0	8,8,8	0.79	0
32	MPD	Х	3246	-	7,7,7	0.55	0	9,10,10	1.14	0
32	MPD	Х	3247	-	7,7,7	0.39	0	9,10,10	0.73	0
31	SPD	Х	3244	1	9,9,9	0.27	0	8,8,8	0.82	0
31	SPD	X	3239	1	9,9,9	0.67	0	8,8,8	1.86	2 (25%)
31	SPD	X	3237	1	9,9,9	0.68	0	8,8,8	1.18	1 (12%)

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
31	SPD	Х	3243	1	-	3/7/7/7	-
31	SPD	Х	3242	1	-	1/7/7/7	-
32	MPD	Х	3245	-	-	1/5/5/5	-
29	QU2	Х	2901	-	-	21/57/98/98	0/3/4/4
31	SPD	Х	3238	1	-	2/7/7/7	-
32	MPD	Х	3248	-	-	3/5/5/5	-
31	SPD	Х	3240	1	-	1/7/7/7	-
31	SPD	Х	3241	1	-	2/7/7/7	-
32	MPD	Х	3246	-	-	2/5/5/5	-
32	MPD	Х	3247	-	-	3/5/5/5	_
31	SPD	Х	3244	1	-	2/7/7/7	-
31	SPD	X	3239	1	-	2/7/7/7	-
31	SPD	X	3237	1	_	4/7/7/7	-



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
29	Х	2901	QU2	C32-C31	3.95	1.60	1.52
29	Х	2901	QU2	C7-C8	3.04	1.62	1.54
29	Х	2901	QU2	C7-C6	2.27	1.57	1.54
29	Х	2901	QU2	O6-C32	2.05	1.47	1.42

All (4) bond length outliers are listed below:

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
29	Х	2901	QU2	C5-C4-C3	5.21	126.35	109.52
31	Х	3238	SPD	C7-N6-C5	4.51	134.73	113.45
29	Х	2901	QU2	O8-C22-C23	4.08	118.67	108.10
29	Х	2901	QU2	C36-O6-C32	3.98	124.97	114.52
29	Х	2901	QU2	O5-C31-C30	-3.87	99.93	111.04
31	Х	3239	SPD	C4-C5-N6	3.83	122.48	112.14
29	Х	2901	QU2	O3-C21-C14	3.45	118.83	110.04
29	Х	2901	QU2	O12-C12-C11	3.40	123.79	115.37
31	Х	3240	SPD	C7-N6-C5	3.01	127.67	113.45
29	Х	2901	QU2	C19-C6-C7	-2.99	106.20	110.69
31	Х	3237	SPD	C7-C8-C9	-2.75	104.21	114.28
29	Х	2901	QU2	C37-O5-C31	2.58	121.31	114.52
31	Х	3239	SPD	C7-N6-C5	2.54	125.44	113.45
29	Х	2901	QU2	O4-C30-C31	2.31	114.09	109.51
29	Х	2901	QU2	C22-C23-C24	2.26	112.89	109.19
29	X	2901	QU2	C23-C24-N1	2.17	117.12	110.83
31	Х	3238	SPD	C3-C4-C5	2.04	123.22	113.56
31	Х	3238	SPD	C7-C8-C9	2.03	121.72	114.28

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	Х	2901	QU2	C10-C11-C12-C13
29	Х	2901	QU2	C10-C11-C12-O12
29	Х	2901	QU2	C12-C13-C14-C15
29	Х	2901	QU2	O12-C13-C14-C15
29	Х	2901	QU2	O12-C13-C14-C21
29	Х	2901	QU2	C13-C14-C21-O3
29	Х	2901	QU2	C15-C14-C21-O3
29	Х	2901	QU2	C23-C24-N1-C29
29	Х	2901	QU2	C25-C24-N1-C28
29	Х	2901	QU2	C25-C24-N1-C29



Mol	Chain	Res	Type	Atoms
29	Х	2901	QU2	O4-C30-O3-C21
29	Х	2901	QU2	C20-C8-C9-C10
29	Х	2901	QU2	C20-C8-C9-O11
31	Х	3239	SPD	C8-C7-N6-C5
31	Х	3237	SPD	N6-C7-C8-C9
29	Х	2901	QU2	C33-C32-O6-C36
31	Х	3237	SPD	C8-C7-N6-C5
31	Х	3240	SPD	C2-C3-C4-C5
31	Х	3238	SPD	C4-C5-N6-C7
31	Х	3243	SPD	C4-C5-N6-C7
31	Х	3239	SPD	C2-C3-C4-C5
29	Х	2901	QU2	C31-C30-O3-C21
29	Х	2901	QU2	C13-C14-C15-O2
32	Х	3248	MPD	O2-C2-C3-C4
29	Х	2901	QU2	C19-C6-C7-C8
32	Х	3245	MPD	C2-C3-C4-C5
32	Х	3248	MPD	C2-C3-C4-C5
32	Х	3247	MPD	CM-C2-C3-C4
31	Х	3244	SPD	N6-C7-C8-C9
31	Х	3243	SPD	C2-C3-C4-C5
29	Х	2901	QU2	C5-C6-C7-C8
31	Х	3241	SPD	C2-C3-C4-C5
31	Х	3237	SPD	C7-C8-C9-N10
32	Х	3246	MPD	O2-C2-C3-C4
32	Х	3247	MPD	O2-C2-C3-C4
31	Х	3243	SPD	N1-C2-C3-C4
31	Х	3237	SPD	C3-C4-C5-N6
31	Х	3242	SPD	C4-C5-N6-C7
31	Х	3244	SPD	C8-C7-N6-C5
29	Х	2901	QU2	O8-C5-C6-C7
32	Х	3246	MPD	C2-C3-C4-C5
32	Х	3247	MPD	C2-C3-C4-C5
31	Х	3241	SPD	C4-C5-N6-C7
29	Х	2901	QU2	C14-C21-O3-C30
32	Х	3248	MPD	C2-C3-C4-O4
29	Х	2901	QU2	C31-C32-O6-C36
31	X	3238	SPD	C2-C3-C4-C5

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There are no ring outliers.

8 monomers are involved in 20 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	Х	3243	SPD	5	0
31	Х	3242	SPD	1	0
31	Х	3238	SPD	5	0
32	Х	3248	MPD	1	0
31	Х	3240	SPD	3	0
32	Х	3246	MPD	1	0
31	Х	3244	SPD	1	0
31	Х	3239	SPD	3	0

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



5.7 Other polymers (i)

There are no such residues in this entry.



5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	Х	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Х	724:C	O3'	725:C	Р	4.40



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	# RSRZ > 2	$OWAB(A^2)$	Q<0.9
1	Х	2699/2880~(93%)	-0.55	38 (1%) 75 64	74, 122, 216, 317	2(0%)
2	Y	122/123~(99%)	-0.44	3 (2%) 57 44	131, 174, 197, 204	0
3	А	272/274~(99%)	0.37	19 (6%) 16 10	102, 146, 172, 180	0
4	В	206/206~(100%)	0.07	9 (4%) 34 22	83, 99, 121, 130	0
5	С	196/205~(95%)	0.22	13 (6%) 18 11	94, 144, 175, 183	0
6	D	177/177~(100%)	1.12	50 (28%) 0 0	197, 222, 244, 253	0
7	Е	171/171~(100%)	0.16	12 (7%) 16 10	130, 176, 217, 223	0
8	G	142/143~(99%)	0.19	9 (6%) 20 11	92, 121, 139, 144	0
9	Н	134/134~(100%)	-0.46	1 (0%) 87 82	86, 93, 104, 108	0
10	Ι	137/137~(100%)	0.73	25~(18%) 1 1	112, 159, 177, 179	0
11	J	135/136~(99%)	0.75	22~(16%) 1 1	133, 156, 174, 182	0
12	K	115/116~(99%)	-0.27	1 (0%) 84 76	76, 81, 91, 93	0
13	L	104/104~(100%)	0.94	20~(19%) 1 0	158, 170, 176, 179	0
14	М	118/166~(71%)	-0.25	1 (0%) 86 79	90, 98, 118, 124	0
15	Ν	117/117~(100%)	-0.17	1 (0%) 84 76	87, 118, 147, 154	0
16	Ο	98/98~(100%)	-0.13	1 (1%) 82 73	105, 139, 163, 169	0
17	Р	129/134~(96%)	0.09	4 (3%) 49 34	83, 92, 118, 135	0
18	Q	92/93~(98%)	0.44	12 (13%) 3 2	114, 137, 155, 161	0
19	R	110/110~(100%)	0.52	10 (9%) 9 5	128, 135, 177, 198	0
20	S	175/175~(100%)	0.83	32 (18%) 1 0	161, 189, 202, 208	0
21	Т	74/91~(81%)	0.99	14 (18%) 1 0	129, 139, 146, 151	0
22	U	74/74 (100%)	0.75	10 (13%) 3 2	129, 164, 191, 198	0
23	V	54/61~(88%)	0.23	6 (11%) 5 3	149, 159, 187, 199	0
24	W	$55/55\ \overline{(100\%)}$	1.56	22~(40%) 0 0	130, 137, 144, 146	0



Mol	Chain	Analysed	<RSRZ $>$	$\# RSRZ {>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
25	Z	57/58~(98%)	-0.32	1 (1%) 68 56	76, 91, 115, 122	0
26	1	49/49~(100%)	1.26	11 (22%) 0 0	158,163,167,170	0
27	2	46/47~(97%)	0.38	2 (4%) 35 23	94, 110, 119, 123	0
28	3	63/63~(100%)	1.47	21 (33%) 0 0	136, 142, 153, 154	0
All	All	5921/6197~(95%)	-0.06	370 (6%) 20 12	74, 133, 212, 317	2(0%)

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All (370) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	Ι	67	ASN	9.5
1	Х	774	А	8.9
28	3	63	PRO	8.2
10	Ι	68	VAL	7.3
6	D	162	THR	6.8
26	1	24	THR	6.4
22	U	8	THR	6.3
23	V	66	GLN	6.1
1	Х	1086	С	6.1
21	Т	71	ASN	6.1
6	D	108	LEU	6.0
13	L	52	ALA	5.9
1	Х	2198	U	5.9
6	D	141	ILE	5.9
20	S	68	ALA	5.8
13	L	40	ALA	5.6
28	3	22	VAL	5.6
10	Ι	72	TYR	5.5
13	L	63	ASN	5.5
20	S	81	VAL	5.5
24	W	6	VAL	5.5
6	D	73	SER	5.4
6	D	120	ASN	5.4
11	J	37	ALA	5.3
6	D	107	GLY	5.3
6	D	139	PRO	5.2
11	J	21	ASP	5.1
20	S	22	VAL	5.1
5	С	189	ASP	5.1
5	С	193	LEU	5.0
28	3	14	ILE	5.0
8	G	97	ASP	5.0



Mol	Chain	Res	Type RSR	
20	S	69	VAL	5.0
21	Т	20	TYR	5.0
28	3	64	ARG	5.0
4	В	206	ALA	4.9
13	L	53	ALA	4.8
20	S	23	ALA	4.8
13	L	62	GLY	4.8
26	1	35	LEU	4.6
1	Х	282	А	4.6
22	U	7	LEU	4.6
5	С	180	ILE	4.6
19	R	84	VAL	4.6
28	3	62	LEU	4.6
6	D	156	ILE	4.5
20	S	80	HIS	4.5
10	Ι	65	PHE	4.5
6	D	165	GLU	4.4
23	V	36	GLN	4.4
23	V	65	GLU	4.4
1	Х	362	С	4.3
10	Ι	88	PHE	4.3
5	С	16	GLU	4.3
13	L	54	ALA	4.3
28	3	48	PHE	4.3
11	J	140	GLU	4.3
24	W	50	LEU	4.3
22	U	6	TYR	4.2
6	D	103	LEU	4.2
6	D	176	PRO	4.2
10	Ι	66	ASN	4.2
13	L	61	SER	4.2
3	А	249	PRO	4.2
8	G	96	ASP	4.1
7	Е	156	ALA	4.1
1	Х	1191	G	4.1
6	D	142	THR	4.1
26	1	25	THR	4.1
28	3	20	GLY	4.1
10	Ι	92	THR	4.1
1	Х	1111	С	4.1
24	W	33	GLU	4.0
11	J	104	MET	4.0



Mol	Chain	Res	Type	RSRZ
24	W	4	LYS	4.0
10	Ι	87	THR	4.0
2	Y	2	С	4.0
10	Ι	15	ASP	4.0
26	1	54	LYS	4.0
13	L	30	SER	4.0
6	D	175	LEU	3.9
13	L	33	ARG	3.9
20	S	83	PHE	3.9
6	D	136	LEU	3.8
1	Х	1095	А	3.8
13	L	39	TYR	3.7
11	J	101	GLY	3.7
22	U	62	LEU	3.7
21	Т	45	PHE	3.7
18	Q	66	GLY	3.7
3	А	251	GLY	3.7
28	3	61	MET	3.7
20	S	21	ALA	3.7
22	U	26	ALA	3.6
28	3	60	LEU	3.6
13	L	55	SER	3.6
21	Т	52	GLY	3.6
6	D	109	PRO	3.6
11	J	119	PHE	3.6
24	W	7	ARG	3.6
6	D	31	ILE	3.6
11	J	105	PHE	3.6
6	D	138	PHE	3.5
3	А	35	GLU	3.5
1	Х	1104	G	3.5
21	Т	42	GLY	3.5
6	D	94	GLU	3.5
3	A	254	THR	3.5
13	L	12	ARG	3.5
20	S	74	ARG	3.5
1	X	2045	A	3.4
28	3	51	ALA	3.4
6	D	135	GLN	3.4
20	S	77	ALA	3.4
1	Х	2581	A	3.4
6	D	157	VAL	3.4



Mol	Chain	Res	Type	RSRZ
26	1	21	TYR	3.4
19	R	100	ASP	3.4
1	Х	1057	А	3.3
24	W	26	ARG	3.3
6	D	36	VAL	3.3
1	Х	2166	G	3.3
1	Х	1087	С	3.3
20	S	70	GLN	3.3
24	W	1	MET	3.3
5	С	190	ALA	3.3
6	D	34	ILE	3.3
10	Ι	83	LEU	3.3
11	J	63	GLY	3.3
10	Ι	63	ARG	3.2
20	S	82	ASP	3.2
11	J	22	ALA	3.2
17	Р	133	ASN	3.2
28	3	49	VAL	3.2
3	А	190	TYR	3.2
20	S	171	VAL	3.2
19	R	81	VAL	3.2
24	W	34	VAL	3.2
3	А	268	ARG	3.2
18	Q	64	ARG	3.2
4	В	135	HIS	3.1
7	Е	57	ASP	3.1
11	J	100	PRO	3.1
2	Y	123	U	3.1
8	G	44	VAL	3.1
21	Т	41	ARG	3.1
6	D	99	PHE	3.1
1	Х	2089	С	3.1
8	G	166	LEU	3.1
1	Х	2165	А	3.1
24	W	53	VAL	3.1
6	D	172	SER	3.0
24	W	10	ILE	3.0
10	Ι	16	ARG	3.0
28	3	9	MET	3.0
28	3	37	SER	3.0
1	X	1085	G	3.0
21	Т	59	LEU	3.0



Mol	Chain	Res	Type	RSRZ
18	Q	27	PHE	3.0
21	Т	22	GLY	3.0
3	А	38	PRO	3.0
6	D	69	LYS	3.0
13	L	89	PHE	3.0
26	1	18	THR	3.0
13	L	42	ILE	2.9
6	D	163	ASP	2.9
6	D	112	ARG	2.9
1	Х	2780	A	2.9
13	L	57	ALA	2.9
24	W	3	ILE	2.9
11	J	20	GLY	2.9
1	X	2090	U	2.9
18	Q	67	ARG	2.9
3	А	110	GLY	2.9
7	Е	155	ASP	2.9
10	Ι	18	ARG	2.9
20	S	86	VAL	2.9
1	Х	1753	А	2.9
3	А	2	ALA	2.8
20	S	15	ASP	2.8
3	А	8	PRO	2.8
24	W	17	VAL	2.8
19	R	82	ALA	2.8
20	S	20	ALA	2.8
11	J	98	VAL	2.8
19	R	55	THR	2.8
13	L	51	LEU	2.8
6	D	161	LYS	2.8
7	Е	37	TYR	2.8
11	J	36	ILE	2.8
11	J	139	ASP	2.8
11	J	19	THR	2.8
28	3	23	MET	2.8
1	X	1602	G	2.7
7	Е	62	ARG	2.7
13	L	34	SER	2.7
6	D	32	GLU	2.7
11	J	55	MET	2.7
3	А	231	HIS	2.7
5	С	45	THR	2.7



\mathbf{Mol}	Chain	Res Type		RSRZ
7	Е	153	LYS	2.7
5	С	172	VAL	2.7
24	W	20	VAL	2.7
28	3	52	LYS	2.7
6	D	173	MET	2.7
1	Х	2083	G	2.7
3	А	111	LEU	2.7
21	Т	21	LEU	2.7
21	Т	15	ASP	2.7
6	D	72	LYS	2.7
10	Ι	31	GLY	2.7
2	Y	14	С	2.7
4	В	1	MET	2.7
28	3	21	LYS	2.6
13	L	29	LEU	2.6
4	В	3	GLY	2.6
6	D	74	ILE	2.6
10	Ι	41	SER	2.6
1	Х	1110	G	2.6
6	D	113	ASP	2.6
6	D	164	GLU	2.6
20	S	160	LEU	2.6
18	Q	71	GLN	2.6
20	S	92	VAL	2.6
1	Х	1090	С	2.6
18	Q	9	ALA	2.6
4	В	169	ASN	2.6
3	А	69	ARG	2.6
20	S	155	PRO	2.6
6	D	137	ILE	2.6
10	Ι	115	SER	2.6
28	3	16	ILE	2.5
6	D	81	GLN	2.5
23	V	62	ARG	2.5
8	G	148	LEU	2.5
27	2	22	MET	2.5
22	U	14	VAL	2.5
10	I	105	PRO	2.5
17	Р	118	LYS	2.5
20	S	122	ILE	2.5
6	D	169	LEU	2.5
18	Q	93	GLY	2.5



Mol	Chain	Res Type		RSRZ
10	Ι	48	PHE	2.5
8	G	99	VAL	2.4
8	G	58	ILE	2.4
18	Q	56	MET	2.4
4	В	84	PHE	2.4
6	D	121	ALA	2.4
11	J	108	ALA	2.4
8	G	114	THR	2.4
1	Х	1077	U	2.4
6	D	65	PRO	2.4
19	R	83	LEU	2.4
3	А	184	ARG	2.4
21	Т	47	ALA	2.4
19	R	62	MET	2.4
10	Ι	61	PRO	2.4
11	J	38	MET	2.4
22	U	61	TRP	2.4
1	Х	1037	U	2.4
21	Т	53	MET	2.4
23	V	64	GLY	2.4
11	J	117	GLU	2.4
1	Х	281	С	2.4
26	1	52	GLU	2.3
28	3	24	ALA	2.3
20	S	4	THR	2.3
26	1	50	PHE	2.3
12	K	69	ASP	2.3
10	Ι	60	LEU	2.3
4	В	12	THR	2.3
6	D	83	MET	2.3
20	S	72	ASP	2.3
17	Р	103	LEU	2.3
20	S	162	ALA	2.3
1	Х	1072	U	2.3
1	Х	2169	А	2.3
27	2	40	HIS	2.3
24	W	51	LEU	2.3
24	W	25	LEU	2.3
4	В	34	VAL	2.3
10	Ι	30	ALA	2.3
7	Е	168	GLN	2.3
20	S	134	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
18	Q	77	LYS	2.3
24	W	49	HIS	2.3
19	R	12	ASP	2.3
4	В	205	SER	2.3
24	W	32	ARG	2.3
11	J	42	TRP	2.3
20	S	73	LYS	2.3
25	Ζ	26	THR	2.3
5	С	17	LEU	2.3
11	J	118	ALA	2.3
26	1	14	SER	2.3
22	U	16	ASN	2.2
19	R	44	GLN	2.2
22	U	60	VAL	2.2
6	D	140	GLU	2.2
7	Е	61	HIS	2.2
10	Ι	69	GLY	2.2
6	D	88	LYS	2.2
26	1	53	LYS	2.2
11	J	109	GLY	2.2
20	S	66	VAL	2.2
14	М	115	ALA	2.2
5	С	10	ASN	2.2
1	Х	2088	U	2.2
1	Х	1091	С	2.2
20	S	154	LEU	2.2
10	Ι	99	VAL	2.2
1	Х	2779	А	2.2
7	Е	173	ALA	2.2
1	Х	1094	С	2.2
9	Н	19	ILE	2.2
3	A	72	LYS	2.2
28	3	39	ASP	2.2
1	X	1056	U	2.2
5	С	21	GLU	2.2
18	Q	74	ASP	2.2
10	Ι	33	GLY	2.2
28	3	50	LEU	2.1
5	С	121	ASP	2.1
13	L	41	GLN	2.1
24	W	5	LEU	2.1
13	L	109	GLU	2.1



Mol	Chain	Res	Type	RSRZ
1	Х	1093	U	2.1
3	А	104	TYR	2.1
6	D	145	MET	2.1
23	V	35	GLY	2.1
21	Т	10	SER	2.1
28	3	15	LYS	2.1
7	Е	123	PHE	2.1
1	Х	2170	С	2.1
19	R	73	GLU	2.1
3	А	26	LYS	2.1
21	Т	72	LYS	2.1
1	Х	2087	U	2.1
6	D	87	ILE	2.1
20	S	94	VAL	2.1
17	Р	105	ARG	2.1
3	А	103	ARG	2.1
18	Q	70	GLY	2.1
20	S	120	LEU	2.1
24	W	2	LYS	2.1
26	1	10	VAL	2.1
6	D	82	GLY	2.1
7	Е	41	LEU	2.1
6	D	20	PHE	2.1
16	0	45	THR	2.1
5	С	188	ILE	2.1
7	Е	114	ILE	2.1
6	D	152	MET	2.1
22	U	11	LYS	2.1
20	S	173	PRO	2.1
3	А	246	PRO	2.0
6	D	154	ILE	2.0
6	D	144	ASP	2.0
10	Ι	54	SER	2.0
24	W	55	GLU	2.0
8	G	80	VAL	2.0
5	С	119	ALA	2.0
20	S	123	VAL	2.0
24	W	9	VAL	2.0
20	S	148	THR	2.0
18	Q	72	ARG	2.0
1	Х	408	U	2.0
15	N	91	ASN	2.0



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Mol	Chain	\mathbf{Res}	Type	RSRZ
24	W	54	GLN	2.0
6	D	62	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} extsf{-}\mathbf{B} extsf{-}\mathbf{factors}(\mathbf{\AA}^2)$	Q<0.9
30	MG	Х	3190	1/1	0.37	0.91	$183,\!183,\!183,\!183$	0
30	MG	Х	3130	1/1	0.41	0.73	$143,\!143,\!143,\!143$	0
30	MG	Х	3211	1/1	0.52	0.56	111,111,111,111	0
30	MG	Y	210	1/1	0.54	0.58	$149,\!149,\!149,\!149$	0
30	MG	Х	3143	1/1	0.58	0.53	$95,\!95,\!95,\!95$	0
30	MG	Х	3155	1/1	0.59	0.48	99,99,99,99	0
30	MG	Х	3057	1/1	0.60	0.85	$131,\!131,\!131,\!131$	0
30	MG	Х	3087	1/1	0.65	0.65	82,82,82,82	0
30	MG	Х	2983	1/1	0.66	1.13	121,121,121,121	0
30	MG	Y	213	1/1	0.66	0.96	$131,\!131,\!131,\!131$	0
30	MG	Х	3107	1/1	0.68	0.91	122,122,122,122	0
30	MG	Х	3117	1/1	0.68	0.77	$130,\!130,\!130,\!130$	0
30	MG	Х	3210	1/1	0.68	0.74	99,99,99,99	0
30	MG	Х	3227	1/1	0.69	0.44	98,98,98,98	0
30	MG	Х	3086	1/1	0.69	0.62	112,112,112,112	0
30	MG	Х	3002	1/1	0.69	0.58	$107,\!107,\!107,\!107$	0
30	MG	Х	3224	1/1	0.70	2.02	$133,\!133,\!133,\!133$	0
30	MG	Х	3083	1/1	0.70	0.53	104,104,104,104	0
30	MG	X	3110	1/1	0.70	0.53	127,127,127,127	0
30	MG	X	3176	1/1	0.70	0.45	106, 106, 106, 106, 106	0



7	40	S

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Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	\mathbf{RSR}	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	$\mathbf{Q}{<}0.9$
30	MG	Х	3120	1/1	0.71	0.58	110, 110, 110, 110	0
30	MG	Х	2924	1/1	0.72	0.95	78,78,78,78	0
30	MG	Х	3231	1/1	0.72	0.16	99,99,99,99	0
30	MG	Х	3196	1/1	0.73	0.90	$86,\!86,\!86,\!86$	0
30	MG	Х	3207	1/1	0.73	0.44	$102,\!102,\!102,\!102$	0
30	MG	Х	3050	1/1	0.73	0.31	91,91,91,91	0
30	MG	Y	214	1/1	0.73	1.13	122,122,122,122	0
30	MG	2	102	1/1	0.73	0.32	116, 116, 116, 116	0
30	MG	Y	205	1/1	0.74	1.25	123, 123, 123, 123	0
30	MG	Х	3191	1/1	0.74	0.33	146, 146, 146, 146	0
30	MG	Х	3023	1/1	0.74	1.01	91,91,91,91	0
30	MG	Х	2985	1/1	0.74	0.61	101, 101, 101, 101	0
30	MG	Х	2975	1/1	0.74	1.03	79,79,79,79	0
30	MG	Х	3232	1/1	0.75	0.78	87,87,87,87	0
30	MG	Х	3051	1/1	0.75	0.54	$79,\!79,\!79,\!79$	0
30	MG	Х	2953	1/1	0.75	1.05	125,125,125,125	0
30	MG	Х	3156	1/1	0.76	0.30	121,121,121,121	0
30	MG	Х	3115	1/1	0.76	0.72	$108,\!108,\!108,\!108$	0
30	MG	Х	3214	1/1	0.76	0.83	94,94,94,94	0
30	MG	Х	3041	1/1	0.76	0.33	88,88,88,88	0
30	MG	Х	3139	1/1	0.77	0.37	99,99,99,99	0
30	MG	Ι	201	1/1	0.77	0.49	$105,\!105,\!105,\!105$	0
30	MG	Х	3183	1/1	0.77	0.43	92,92,92,92	0
30	MG	Х	3146	1/1	0.78	0.50	97,97,97,97	0
30	MG	K	201	1/1	0.78	0.41	89,89,89,89	0
30	MG	Х	2978	1/1	0.78	0.93	$95,\!95,\!95,\!95$	0
30	MG	Х	3065	1/1	0.79	0.81	$102,\!102,\!102,\!102$	0
30	MG	Х	3134	1/1	0.79	0.52	82,82,82,82	0
30	MG	Х	3072	1/1	0.79	0.90	123,123,123,123	0
30	MG	Х	3141	1/1	0.79	0.29	87,87,87,87	0
32	MPD	Х	3245	8/8	0.79	0.46	128,128,128,128	0
30	MG	Х	3079	1/1	0.80	0.42	$106,\!106,\!106,\!106$	0
30	MG	Х	3111	1/1	0.80	0.58	100, 100, 100, 100	0
30	MG	Х	3215	1/1	0.80	0.51	$105,\!105,\!105,\!105$	0
30	MG	X	3209	1/1	0.80	0.51	81,81,81,81	0
31	SPD	X	3243	10/10	0.80	$0.\overline{39}$	96,96,96,96	0
31	SPD	X	3244	10/10	0.80	0.31	137, 137, 137, 137, 137	0
30	MG	X	3112	1/1	0.80	1.67	128, 128, 128, 128, 128	0
30	MG	N	203	1/1	0.81	0.59	98,98,98,98	0
30	MG	Х	3043	1/1	0.81	0.81	120,120,120,120	0
30	MG	X	2994	1/1	0.81	0.56	86,86,86,86	0



7	40	\mathbf{S}

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Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	\mathbf{RSR}	$\mathbf{B} extsf{-}\mathbf{factors}(\mathbf{A}^2)$	$\mathbf{Q}{<}0.9$
30	MG	Y	207	1/1	0.81	0.93	$131,\!131,\!131,\!131$	0
30	MG	Х	2989	1/1	0.81	1.05	111, 111, 111, 111	0
30	MG	Х	3225	1/1	0.82	0.30	$132,\!132,\!132,\!132$	0
30	MG	Y	216	1/1	0.82	0.60	$152,\!152,\!152,\!152$	0
30	MG	Х	3161	1/1	0.82	0.39	$107,\!107,\!107,\!107$	0
30	MG	Х	2982	1/1	0.82	0.69	83,83,83,83	0
30	MG	Х	3181	1/1	0.82	0.24	91,91,91,91	0
30	MG	Х	3025	1/1	0.82	1.06	$109,\!109,\!109,\!109$	0
30	MG	Х	2928	1/1	0.82	0.36	127, 127, 127, 127, 127	0
30	MG	Х	2955	1/1	0.82	0.67	80,80,80,80	0
30	MG	Х	3067	1/1	0.82	0.47	85,85,85,85	0
35	CA	Х	3251	1/1	0.82	0.32	78,78,78,78	0
30	MG	Х	3185	1/1	0.83	0.40	92,92,92,92	0
30	MG	Х	3189	1/1	0.83	0.64	153, 153, 153, 153	0
30	MG	Х	3152	1/1	0.83	0.46	88,88,88,88	0
30	MG	Х	3160	1/1	0.83	0.53	$108,\!108,\!108,\!108,\!108$	0
30	MG	Х	3019	1/1	0.83	0.88	82,82,82,82	0
30	MG	Х	2954	1/1	0.84	0.30	115, 115, 115, 115	0
30	MG	Х	3182	1/1	0.84	0.32	87,87,87,87	0
30	MG	Х	3223	1/1	0.84	1.86	137,137,137,137	0
30	MG	X	3103	1/1	0.84	0.69	145,145,145,145	0
30	MG	Х	3169	1/1	0.84	0.92	112,112,112,112	0
30	MG	X	3009	1/1	0.84	0.72	123,123,123,123	0
30	MG	X	3178	1/1	0.84	0.26	95,95,95,95	0
30	MG	A	302	1/1	0.84	1.29	104,104,104,104	0
30	MG	Х	2950	1/1	0.85	0.77	122,122,122,122	0
30	MG	X	3233	1/1	0.85	0.86	68,68,68,68	0
30	MG	Y	201	1/1	0.85	1.01	126,126,126,126	0
30	MG	X	3037	1/1	0.85	1.48	95,95,95,95	0
30	MG	X	2917	1/1	0.85	1.17	79,79,79,79	0
30	MG	Х	3164	1/1	0.85	0.48	149,149,149,149	0
30	MG	Х	2948	1/1	0.85	1.06	103, 103, 103, 103	0
30	MG	X	3187	1/1	0.85	0.82	120,120,120,120	0
30	MG	X	3024	1/1	0.85	0.87	122,122,122,122	0
30	MG	X	3014	1/1	0.86	0.24	96,96,96,96	0
30	MG	X	3042	1/1	0.86	0.33	89.89.89.89	0
30	MG	X	3074	1/1	0.86	1.05	106,106,106,106	0
30	MG	X	2969	1/1	0.86	0.52	96,96,96,96	0
30	MG	X	2906	1/1	0.86	0.59	94,94,94,94	0
30	MG	X	2944	1/1	0.86	0.53	101,101,101.101	0
31	SPD	X	3242		0.86	0.32	95.95.95.95	0
30	MG	X	2946	1/1	0.86	0.54	75,75,75,75	0
$\begin{array}{r} 30\\ 30\\ 30\\ 30\\ 30\\ 30\\ 30\\ 30\\ 30\\ 30\\$	MG MG MG MG MG MG MG MG MG MG MG MG MG M	X X X X X X Y X X X X X X X X X X X X X	3169 3009 3178 302 2950 3233 201 3037 2917 3164 2948 3187 3024 3014 3024 3014 3042 3074 2969 2906 2944 3242 2946	$\begin{array}{c} 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 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\\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\ 1/1 \\$	$\begin{array}{c} 0.84\\ 0.84\\ 0.84\\ 0.84\\ 0.85\\ 0.85\\ 0.85\\ 0.85\\ 0.85\\ 0.85\\ 0.85\\ 0.85\\ 0.85\\ 0.85\\ 0.85\\ 0.85\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 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0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\ 0.86\\$	$\begin{array}{c} 0.92\\ 0.72\\ 0.26\\ 1.29\\ 0.77\\ 0.86\\ 1.01\\ 1.48\\ 1.17\\ 0.48\\ 1.06\\ 0.82\\ 0.87\\ 0.24\\ 0.33\\ 1.05\\ 0.52\\ 0.59\\ 0.53\\ 0.32\\ 0.54\\ \end{array}$	$\begin{array}{r} 112,112,112,112\\ 123,123,123,123\\ 95,95,95,95\\ 104,104,104,104\\ 122,122,122,122\\ 68,68,68,68\\ 126,126,126,126\\ 95,95,95,95\\ 79,79,79,79\\ 149,149,149,149\\ 103,103,103,103\\ 120,120,120,120\\ 122,122,122,122\\ 96,96,96,96\\ 89,89,89,89\\ 106,106,106,106\\ 96,96,96,96\\ 94,94,94,94\\ 101,101,101,101\\ 95,95,95,95\\ 75,75,75,75,75\\ \end{array}$	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0



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$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	30	MG	X	3059	1/1	0.86	0.40	149, 149, 149, 149	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	30	MG	Х	2913	1/1	0.86	0.58	85,85,85,85	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	30	MG	Х	3140	1/1	0.86	0.36	$98,\!98,\!98,\!98$	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	30	MG	Х	2965	1/1	0.87	0.72	99,99,99,99	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	30	MG	Х	3118	1/1	0.87	0.72	$98,\!98,\!98,\!98$	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	30	MG	А	303	1/1	0.87	0.51	113, 113, 113, 113	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	30	MG	Х	3005	1/1	0.87	0.52	120, 120, 120, 120	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	30	MG	Х	3124	1/1	0.87	0.27	$95,\!95,\!95,\!95$	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	30	MG	Х	3104	1/1	0.87	0.53	97,97,97,97	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	30	MG	Х	3036	1/1	0.87	0.34	89,89,89,89	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	30	MG	Х	3179	1/1	0.87	0.46	75,75,75,75	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	30	MG	Y	208	1/1	0.87	0.49	180, 180, 180, 180, 180	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	30	MG	Х	3116	1/1	0.87	0.56	115, 115, 115, 115	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	30	MG	Х	3204	1/1	0.87	0.41	161, 161, 161, 161	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	30	MG	Х	3226	1/1	0.87	0.58	79,79,79,79	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	30	MG	Х	3168	1/1	0.88	0.37	135, 135, 135, 135, 135	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	30	MG	Х	3206	1/1	0.88	0.21	102, 102, 102, 102	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	30	MG	Х	2996	1/1	0.88	0.59	71,71,71,71	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	30	MG	2	101	1/1	0.88	0.59	$103,\!103,\!103,\!103$	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	30	MG	Х	3208	1/1	0.88	0.79	104, 104, 104, 104	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	30	MG	Х	2992	1/1	0.88	0.29	91,91,91,91	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	30	MG	Х	3068	1/1	0.88	0.36	83,83,83,83	0
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	30	MG	Х	3017	1/1	0.88	0.58	93,93,93,93	0
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	30	MG	Х	3101	1/1	0.88	0.76	128,128,128,128	0
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	34	EOH	Х	3250	3/3	0.88	0.42	88,88,88,88	0
29 QU2 X 2901 50/50 0.89 0.37 80,80,80,80 0 30 MG X 2941 1/1 0.89 0.47 81,81,81,81 0 30 MG X 3216 1/1 0.89 0.18 135,135,135,135 0	30	MG	Х	2968	1/1	0.88	0.48	114,114,114,114	0
30 MG X 2941 1/1 0.89 0.47 81,81,81,81 0 30 MG X 3216 1/1 0.89 0.18 135,135,135,135 0	29	QU2	Х	2901	50/50	0.89	0.37	80,80,80,80	0
30 MG X 3216 1/1 0.89 0.18 135,135,135 0 30 MG X 3216 1/1 0.89 0.18 135,135,135 0	30	MG	Х	2941	1/1	0.89	0.47	81,81,81,81	0
	30	MG	Х	3216	1/1	0.89	0.18	$135,\!135,\!135,\!135,\!135$	0
30 MG X 3217 1/1 0.89 1.01 83,83,83,83 0 - 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.01 1.	30	MG	Х	3217	1/1	0.89	1.01	83,83,83,83	0
30 MG X 3012 1/1 0.89 1.23 101,101,101,101 0	30	MG	Х	3012	1/1	0.89	1.23	101,101,101,101	0
30 MG X 3094 1/1 0.89 0.40 84,84,84,84 0	30	MG	Х	3094	1/1	0.89	0.40	84,84,84,84	0
30 MG X 2925 1/1 0.89 0.53 99,99,99,99 0	30	MG	Х	2925	1/1	0.89	0.53	99,99,99,99	0
30 MG X 3048 1/1 0.89 0.55 112,112,112,112 0	30	MG	Х	3048	1/1	0.89	0.55	112,112,112,112	0
30 MG X 3166 1/1 0.89 0.77 139,139,139,139 0	30	MG	Х	3166	1/1	0.89	0.77	139,139,139,139	0
30 MG X 3029 1/1 0.89 0.22 87,87,87,87 0	30	MG	X	3029	1/1	0.89	0.22	87,87,87,87	0
30 MG X 2991 1/1 0.89 0.55 90,90,90,90 0	30	MG	X	2991	1/1	0.89	0.55	90,90,90,90	0
30 MG X 3078 1/1 0.89 0.96 86,86,86,86 0	30	MG	X	3078	1/1	0.89	0.96	86,86,86,86	0
30 MG X 3236 1/1 0.89 0.53 88,88,88,88 0	30	MG	X	3236	1/1	0.89	0.53	88,88,88,88	0
30 MG X 3055 1/1 0.89 0.79 111,111,111,111 0	30	MG	X	3055	1/1	0.89	0.79	111,111,111,111	0
30 MG X 3142 1/1 0.89 0.18 94.94.94.94 0	30	MG	X	3142	1/1	0.89	0.18	94,94,94.94	0
30 MG X 3080 1/1 0.89 0.22 98,98,98,98 0	30	MG	X	3080	1/1	0.89	0.22	98,98,98,98	0



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Mol	Type	Chain	Res	Atoms	RSCC	\mathbf{RSR}	${f B} ext{-factors}({f A}^2)$	$\mathbf{Q}{<}0.9$
30	MG	Х	3081	1/1	0.89	0.33	$123,\!123,\!123,\!123$	0
30	MG	Х	2997	1/1	0.90	0.74	97,97,97,97	0
30	MG	Х	2961	1/1	0.90	0.54	$70,\!70,\!70,\!70$	0
30	MG	Х	3088	1/1	0.90	0.54	87,87,87,87	0
30	MG	Х	3228	1/1	0.90	0.38	109, 109, 109, 109	0
30	MG	Х	2963	1/1	0.90	0.79	94,94,94,94	0
30	MG	Х	3095	1/1	0.90	0.80	$106,\!106,\!106,\!106$	0
30	MG	Х	3098	1/1	0.90	0.65	$69,\!69,\!69,\!69$	0
30	MG	Х	2942	1/1	0.90	0.58	$73,\!73,\!73,\!73$	0
30	MG	Х	3071	1/1	0.90	0.06	155, 155, 155, 155, 155	0
30	MG	Y	202	1/1	0.90	0.56	122,122,122,122	0
30	MG	Y	204	1/1	0.90	0.84	$140,\!140,\!140,\!140$	0
30	MG	Х	3144	1/1	0.90	0.39	$108,\!108,\!108,\!108$	0
30	MG	Y	206	1/1	0.90	0.56	$148,\!148,\!148,\!148$	0
30	MG	Х	3192	1/1	0.90	0.41	88,88,88,88	0
30	MG	Х	3030	1/1	0.90	1.01	83,83,83,83	0
30	MG	Х	3148	1/1	0.90	0.52	88,88,88,88	0
30	MG	Х	3126	1/1	0.91	0.30	107, 107, 107, 107	0
30	MG	Х	3128	1/1	0.91	0.15	92,92,92,92	0
30	MG	Х	2930	1/1	0.91	0.66	87,87,87,87	0
30	MG	Y	209	1/1	0.91	0.88	140, 140, 140, 140	0
30	MG	Х	2964	1/1	0.91	0.73	85,85,85,85	0
30	MG	Х	3076	1/1	0.91	0.43	108, 108, 108, 108, 108	0
30	MG	Х	3052	1/1	0.91	0.75	121,121,121,121	0
30	MG	Х	3106	1/1	0.91	0.30	$79,\!79,\!79,\!79$	0
30	MG	Х	3032	1/1	0.91	0.80	56, 56, 56, 56	0
30	MG	Х	3108	1/1	0.91	0.57	112,112,112,112	0
30	MG	Х	2940	1/1	0.91	0.81	89,89,89,89	0
30	MG	Х	3145	1/1	0.91	0.46	106, 106, 106, 106	0
30	MG	Х	2958	1/1	0.91	0.62	$79,\!79,\!79,\!79$	0
30	MG	Х	3060	1/1	0.91	0.21	84,84,84,84	0
30	MG	Х	3114	1/1	0.91	0.84	105, 105, 105, 105, 105	0
31	SPD	Х	3240	10/10	0.91	0.26	75,75,75,75	0
30	MG	Х	3064	1/1	0.91	0.54	82,82,82,82	0
30	MG	Х	2998	1/1	0.91	0.56	84,84,84,84	0
30	MG	X	2959	1/1	0.91	0.89	79,79,79,79	0
30	MG	Х	3090	1/1	0.91	0.34	78,78,78,78	0
30	MG	X	3004	1/1	0.91	0.85	105,105,105,105	0
30	MG	X	2921	1/1	0.91	0.30	97,97,97,97	0
35	CA	X	3253	1/1	0.91	0.38	72,72,72,72	0
30	MG	X	3180	1/1	0.92	0.34	76,76,76,76	0
30	MG	X	3003	1/1	0.92	0.37	82,82,82,82	0



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Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	\mathbf{RSR}	B -factors (A^2)	$\mathbf{Q}{<}0.9$
30	MG	Х	3077	1/1	0.92	0.58	118, 118, 118, 118	0
30	MG	Х	2915	1/1	0.92	0.46	83,83,83,83	0
30	MG	N	202	1/1	0.92	0.31	$95,\!95,\!95,\!95$	0
30	MG	Х	3047	1/1	0.92	0.92	100, 100, 100, 100	0
30	MG	Х	3070	1/1	0.92	1.17	$105,\!105,\!105,\!105$	0
30	MG	Х	3167	1/1	0.92	0.25	117,117,117,117	0
31	SPD	Х	3237	10/10	0.92	0.30	82,82,82,82	0
30	MG	Х	2920	1/1	0.92	0.77	67,67,67,67	0
30	MG	Х	3082	1/1	0.92	0.18	$110,\!110,\!110,\!110$	0
30	MG	Х	3172	1/1	0.92	0.61	$98,\!98,\!98,\!98$	0
30	MG	Х	3195	1/1	0.92	0.55	$91,\!91,\!91,\!91$	0
30	MG	Х	3174	1/1	0.92	0.82	$115,\!115,\!115,\!115$	0
32	MPD	Х	3246	8/8	0.92	0.17	93,93,93,93	0
30	MG	Х	3026	1/1	0.92	0.64	107, 107, 107, 107, 107	0
30	MG	Х	3137	1/1	0.92	0.30	78,78,78,78	0
30	MG	Х	2976	1/1	0.92	0.48	81,81,81,81	0
30	MG	Х	3015	1/1	0.93	0.57	72,72,72,72	0
30	MG	Х	2905	1/1	0.93	0.57	84,84,84,84	0
30	MG	Х	2974	1/1	0.93	0.84	86,86,86,86	0
30	MG	Х	3221	1/1	0.93	0.62	82,82,82,82	0
30	MG	Х	3127	1/1	0.93	0.60	83,83,83,83	0
30	MG	Х	3157	1/1	0.93	0.47	97,97,97,97	0
30	MG	Х	3159	1/1	0.93	0.52	$143,\!143,\!143,\!143$	0
30	MG	Ι	202	1/1	0.93	0.42	143, 143, 143, 143	0
30	MG	Х	3085	1/1	0.93	0.39	127,127,127,127	0
30	MG	Х	3058	1/1	0.93	0.36	$156,\!156,\!156,\!156$	0
30	MG	Х	3109	1/1	0.93	1.03	77,77,77,77	0
30	MG	Х	3073	1/1	0.93	0.78	$137,\!137,\!137,\!137$	0
30	MG	Х	3046	1/1	0.93	0.24	94,94,94,94	0
30	MG	Х	3202	1/1	0.93	0.53	$156,\!156,\!156,\!156$	0
31	SPD	Х	3238	10/10	0.93	0.30	79,79,79,79	0
30	MG	Х	3031	1/1	0.93	0.94	$69,\!69,\!69,\!69$	0
30	MG	Х	3205	1/1	0.93	0.12	186, 186, 186, 186	0
30	MG	Х	3113	1/1	0.93	0.50	86,86,86,86	0
30	MG	Х	3091	1/1	0.93	0.24	85,85,85,85	0
30	MG	Х	3062	1/1	0.93	0.47	110, 110, 110, 110	0
30	MG	Х	2926	1/1	0.93	0.45	99,99,99,99	0
32	MPD	Х	3248	8/8	0.93	0.31	94,94,94,94	0
30	MG	Х	2904	1/1	0.93	0.63	62,62,62,62	0
30	MG	Х	2995	1/1	0.93	0.39	76,76,76,76	0
30	MG	X	3147	1/1	0.93	0.14	93,93,93,93	0
30	MG	Х	3044	1/1	0.94	0.63	82,82,82,82	0



7	40	\mathbf{S}

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Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	RSR	${f B} ext{-factors}({f A}^2)$	Q < 0.9
30	MG	Х	3045	1/1	0.94	0.25	$124,\!124,\!124,\!124$	0
30	MG	Y	211	1/1	0.94	0.33	$173,\!173,\!173,\!173$	0
30	MG	Y	212	1/1	0.94	0.62	$186,\!186,\!186,\!186$	0
30	MG	Х	3089	1/1	0.94	0.59	89,89,89,89	0
30	MG	Х	3133	1/1	0.94	0.78	$70,\!70,\!70,\!70$	0
30	MG	Х	2910	1/1	0.94	0.68	$70,\!70,\!70,\!70$	0
30	MG	Х	3135	1/1	0.94	0.07	90,90,90,90	0
30	MG	Х	3219	1/1	0.94	0.44	$103,\!103,\!103,\!103$	0
30	MG	Х	3186	1/1	0.94	0.52	$105,\!105,\!105,\!105$	0
30	MG	Х	3136	1/1	0.94	0.54	77,77,77,77	0
30	MG	J	201	1/1	0.94	0.09	$134,\!134,\!134,\!134$	0
30	MG	Х	3188	1/1	0.94	0.71	131, 131, 131, 131	0
30	MG	Х	2987	1/1	0.94	0.79	107, 107, 107, 107, 107	0
30	MG	Х	2988	1/1	0.94	0.47	100, 100, 100, 100	0
30	MG	Х	3049	1/1	0.94	0.92	$106,\!106,\!106,\!106$	0
30	MG	Х	3096	1/1	0.94	0.42	$90,\!90,\!90,\!90$	0
30	MG	3	101	1/1	0.94	0.78	103, 103, 103, 103	0
30	MG	Х	3229	1/1	0.94	0.17	112,112,112,112	0
30	MG	Х	3038	1/1	0.94	0.35	80,80,80,80	0
31	SPD	Х	3239	10/10	0.94	0.27	78,78,78,78	0
30	MG	Х	3039	1/1	0.94	0.42	76,76,76,76	0
30	MG	Х	3200	1/1	0.94	0.17	116, 116, 116, 116	0
30	MG	Х	3201	1/1	0.94	0.37	104,104,104,104	0
30	MG	Х	3170	1/1	0.94	0.65	127,127,127,127	0
30	MG	Х	3069	1/1	0.94	0.17	131,131,131,131	0
30	MG	Х	3173	1/1	0.94	0.22	191,191,191,191	0
30	MG	Х	3007	1/1	0.94	0.64	100, 100, 100, 100	0
30	MG	Х	2927	1/1	0.94	0.80	77,77,77,77	0
30	MG	Х	3177	1/1	0.94	0.21	97,97,97,97	0
30	MG	Х	3010	1/1	0.94	0.63	97,97,97,97	0
30	MG	Х	2990	1/1	0.95	0.76	89,89,89,89	0
30	MG	Х	2911	1/1	0.95	0.56	59,59,59,59	0
30	MG	В	301	1/1	0.95	0.18	72,72,72,72	0
30	MG	Х	3006	1/1	0.95	0.16	108,108,108,108	0
30	MG	X	2977	1/1	0.95	0.67	82,82,82,82	0
30	MG	X	3230	1/1	0.95	0.52	119,119,119,119	0
30	MG	X	2993	1/1	0.95	0.33	95,95,95,95	0
30	MG	X	2956	1/1	0.95	0.34	107,107,107,107	0
30	MG	X	3011	1/1	0.95	0.53	87,87,87,87	0
30	MG	X	3234	1/1	0.95	0.42	75,75,75.75	0
30	MG	X	3034	1/1	0.95	0.35	99,99.99.99	0
30	MG	X	2951	1/1	0.95	0.92	115,115,115,115	0
30 30 30 30 30 30	MG MG MG MG	X X X X X	2950 3011 3234 3034 2951	$ \frac{1/1}{1/1} \\ \frac{1/1}{1/1} \\ \frac{1/1}{1/1} \\ 1/1 $	0.95 0.95 0.95 0.95 0.95	$\begin{array}{r} 0.34 \\ \hline 0.53 \\ \hline 0.42 \\ \hline 0.35 \\ \hline 0.92 \end{array}$	$\begin{array}{r} 107,107,107,107\\ 87,87,87,87\\ \hline 75,75,75,75\\ 99,99,99,99\\ 115,115,115,115\end{array}$	0 0 0 0 0



7	40	\mathbf{S}

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Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	RSR	${f B} ext{-factors}({f A}^2)$	Q < 0.9	
30	MG	Х	3054	1/1	0.95	0.76	$93,\!93,\!93,\!93$	0	
30	MG	Х	3123	1/1	0.95	0.18	$104,\!104,\!104,\!104$	0	
30	MG	Х	2919	1/1	0.95	1.04	89,89,89,89	0	
30	MG	Х	3056	1/1	0.95	0.79	$149,\!149,\!149,\!149$	0	
30	MG	Х	2960	1/1	0.95	0.71	$74,\!74,\!74,\!74$	0	
30	MG	Х	2970	1/1	0.95	0.68	88,88,88,88	0	
30	MG	Х	3129	1/1	0.95	0.66	$76,\!76,\!76,\!76$	0	
30	MG	Х	3018	1/1	0.95	0.12	89,89,89,89	0	
30	MG	Х	3131	1/1	0.95	0.36	83,83,83,83	0	
32	MPD	Х	3247	8/8	0.95	0.17	$103,\!103,\!103,\!103$	0	
30	MG	Х	3132	1/1	0.95	0.88	$75,\!75,\!75,\!75$	0	
30	MG	Х	2923	1/1	0.95	0.72	89,89,89,89	0	
30	MG	Х	3061	1/1	0.95	0.33	82,82,82,82	0	
35	CA	Х	3252	1/1	0.95	0.45	100, 100, 100, 100	0	
30	MG	Х	2962	1/1	0.95	0.82	89,89,89,89	0	
30	MG	Х	3102	1/1	0.96	1.71	$98,\!98,\!98,\!98$	0	
30	MG	Y	217	1/1	0.96	0.52	161, 161, 161, 161	0	
30	MG	Х	2922	1/1	0.96	0.53	95,95,95,95	0	
30	MG	Х	2908	1/1	0.96	0.69	49,49,49,49	0	
30	MG	Х	2916	1/1	0.96	0.32	80,80,80,80	0	
30	MG	Х	2914	1/1	0.96	0.70	79,79,79,79	0	
30	MG	Х	2935	1/1	0.96	0.62	76,76,76,76	0	
30	MG	Х	2947	1/1	0.96	0.57	89,89,89,89	0	
30	MG	Х	3028	1/1	0.96	0.48	101,101,101,101	0	
30	MG	Х	3193	1/1	0.96	0.79	68,68,68,68	0	
30	MG	Х	3165	1/1	0.96	0.39	144,144,144,144	0	
30	MG	Х	2980	1/1	0.96	0.29	92,92,92,92	0	
30	MG	Х	3199	1/1	0.96	0.47	163, 163, 163, 163	0	
30	MG	Х	2966	1/1	0.96	0.67	89,89,89,89	0	
30	MG	Х	2967	1/1	0.96	0.52	97,97,97,97	0	
30	MG	Х	3138	1/1	0.96	0.24	85,85,85,85	0	
30	MG	Х	3203	1/1	0.96	0.48	157,157,157,157	0	
30	MG	X	2938	1/1	0.96	0.49	104,104,104,104	0	
31	SPD	X	3241	10/10	0.96	0.27	160,160,160,160	0	
30	MG	X	3013	1/1	0.96	0.49	74,74,74,74	0	
30	MG	X	3092	1/1	0.96	0.41	91,91,91,91	0	
30	MG	X	2949	1/1	0.96	0.21	91,91,91,91	0	
30	MG	X	3000	1/1	0.96	0.68	98,98,98,98	0	
30	MG	X	3016	1/1	0.96	0.39	116,116,116,116	0	
30	MG	X	3122	1/1	0.96	0.32	97,97.97.97	0	
30	MG	X	3001	$\frac{1}{1}$	0.96	0.96	128,128.128.128	0	
30	MG	X	3099	1/1	0.96	0.38	101,101,101,101	0	
30	MG	Х	3099	1/1	0.96	0.38	101, 101, 101, 101	0	



7	40	\mathbf{S}

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{A}^2)$	$\mathbf{Q}{<}0.9$	
30	MG	Х	3040	1/1	0.96	0.10	$143,\!143,\!143,\!143$	0	
30	MG	Х	3149	1/1	0.96	0.56	100, 100, 100, 100	0	
30	MG	Х	3150	1/1	0.96	0.26	$158,\!158,\!158,\!158,\!158$	0	
35	CA	Х	3255	1/1	0.96	0.23	$78,\!78,\!78,\!78$	0	
30	MG	Х	2986	1/1	0.97	0.57	$101,\!101,\!101,\!101$	0	
30	MG	Х	2907	1/1	0.97	0.48	75,75,75,75	0	
30	MG	Х	2932	1/1	0.97	0.24	94,94,94,94	0	
30	MG	Х	2971	1/1	0.97	0.66	$149,\!149,\!149,\!149$	0	
30	MG	Х	2933	1/1	0.97	0.30	81,81,81,81	0	
30	MG	Х	3063	1/1	0.97	0.36	88,88,88,88	0	
30	MG	Х	3212	1/1	0.97	0.22	95,95,95,95	0	
30	MG	Х	3213	1/1	0.97	0.75	99,99,99,99	0	
30	MG	Y	215	1/1	0.97	0.11	$130,\!130,\!130,\!130$	0	
30	MG	Х	3008	1/1	0.97	0.30	110, 110, 110, 110	0	
30	MG	Х	2957	1/1	0.97	0.57	72,72,72,72	0	
30	MG	А	301	1/1	0.97	0.41	$105,\!105,\!105,\!105$	0	
30	MG	Х	3235	1/1	0.97	0.48	80,80,80,80	0	
30	MG	Х	3121	1/1	0.97	0.44	$103,\!103,\!103,\!103$	0	
30	MG	Х	3066	1/1	0.97	0.45	94,94,94,94	0	
30	MG	Х	2984	1/1	0.97	0.41	88,88,88,88	0	
33	NA	Х	3249	1/1	0.97	0.23	91,91,91,91	0	
30	MG	Y	203	1/1	0.97	0.67	101, 101, 101, 101	0	
30	MG	Х	3022	1/1	0.97	0.67	120, 120, 120, 120, 120	0	
30	MG	Х	3171	1/1	0.97	0.77	116, 116, 116, 116	0	
30	MG	М	201	1/1	0.97	0.26	90,90,90,90	0	
35	CA	Х	3254	1/1	0.97	0.24	82,82,82,82	0	
30	MG	Х	2918	1/1	0.97	0.47	97,97,97,97	0	
30	MG	Х	3198	1/1	0.98	0.53	132,132,132,132	0	
30	MG	Х	3097	1/1	0.98	0.62	132,132,132,132	0	
30	MG	Х	2999	1/1	0.98	0.20	$105,\!105,\!105,\!105$	0	
30	MG	Х	2936	1/1	0.98	0.39	87,87,87,87	0	
30	MG	Х	3100	1/1	0.98	0.45	88,88,88,88	0	
30	MG	N	201	1/1	0.98	0.53	108, 108, 108, 108	0	
30	MG	Х	3027	1/1	0.98	0.22	107, 107, 107, 107	0	
30	MG	Х	2952	1/1	0.98	0.70	78,78,78,78	0	
30	MG	X	3125	1/1	0.98	0.09	94,94,94,94	0	
30	MG	Х	2979	1/1	0.98	0.31	95,95,95,95	0	
30	MG	X	2945	1/1	0.98	0.52	96,96,96,96	0	
30	MG	Х	3105	1/1	0.98	0.35	105, 105, 105, 105	0	
30	MG	X	3151	1/1	0.98	0.25	157,157,157,157	0	
30	MG	X	2981	1/1	0.98	0.54	103,103,103,103	0	
30	MG	Х	3154	1/1	0.98	0.09	106, 106, 106, 106	0	



Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B} ext{-factors}({f A}^2)$	$\mathbf{Q}{<}0.9$
30	MG	Х	2912	1/1	0.98	0.51	80,80,80,80	0
30	MG	Х	3033	1/1	0.98	0.16	119, 119, 119, 119	0
30	MG	Х	2939	1/1	0.98	0.54	93,93,93,93	0
30	MG	Х	3035	1/1	0.98	0.27	80,80,80,80	0
30	MG	Х	2972	1/1	0.98	0.71	$106,\!106,\!106,\!106$	0
30	MG	Х	3020	1/1	0.98	0.29	85,85,85,85	0
30	MG	Х	3162	1/1	0.98	0.07	112,112,112,112	0
30	MG	Х	3021	1/1	0.98	0.44	90,90,90,90	0
30	MG	Х	3222	1/1	0.98	0.30	$109,\!109,\!109,\!109$	0
30	MG	Х	3093	1/1	0.98	0.26	89,89,89,89	0
30	MG	Х	2929	1/1	0.98	0.32	79,79,79,79	0
30	MG	Х	3194	1/1	0.98	0.38	85,85,85,85	0
30	MG	Х	2934	1/1	0.98	0.39	$95,\!95,\!95,\!95$	0
30	MG	Х	2902	1/1	0.98	0.48	$105,\!105,\!105,\!105$	0
30	MG	Х	3197	1/1	0.98	0.16	94,94,94,94	0
36	K	Х	3256	1/1	0.98	0.24	89,89,89,89	0
30	MG	Х	3119	1/1	0.99	0.10	102, 102, 102, 102	0
30	MG	Х	2931	1/1	0.99	0.38	93,93,93,93	0
30	MG	Х	3158	1/1	0.99	0.49	67,67,67,67	0
30	MG	Х	3184	1/1	0.99	0.10	75,75,75,75	0
30	MG	Х	2943	1/1	0.99	0.38	87,87,87,87	0
30	MG	Х	2909	1/1	0.99	0.34	$68,\!68,\!68,\!68$	0
30	MG	Х	3075	1/1	0.99	0.45	100, 100, 100, 100	0
30	MG	Х	2903	1/1	0.99	0.40	89,89,89,89	0
30	MG	Х	3175	1/1	0.99	0.07	89,89,89,89	0
30	MG	Х	3218	1/1	0.99	0.26	88,88,88,88	0
30	MG	Х	3163	1/1	0.99	0.20	71,71,71,71	0
30	MG	Х	3220	1/1	0.99	0.38	88,88,88,88	0
30	MG	X	3084	1/1	0.99	0.12	$1\overline{28,128,128,128},128$	0
30	MG	X	3153	1/1	0.99	0.41	110,110,110,110	0
30	MG	Х	2937	1/1	0.99	0.32	80,80,80,80	0
30	MG	X	3053	1/1	0.99	0.09	$1\overline{10,110,110,110}$	0
30	MG	X	2973	1/1	1.00	0.30	$107,\!107,\!107,\!107$	0

6.5 Other polymers (i)

There are no such residues in this entry.

