Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 01:15 PM EST

PDB ID	:	3J7Z
EMDB ID	:	EMD-6057
Title	:	Structure of the E. coli 50S subunit with ErmCL nascent chain
Authors	:	Arenz, S.; Meydan, S.; Starosta, A.L.; Berninghausen, O.; Beckmann, R.; Vazquez-Laslop, N.; Wilson, D.N.
Deposited on	:	2014-08-27
Resolution	:	3.90 Å(reported)
Based on initial model	:	4KIX

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

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

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

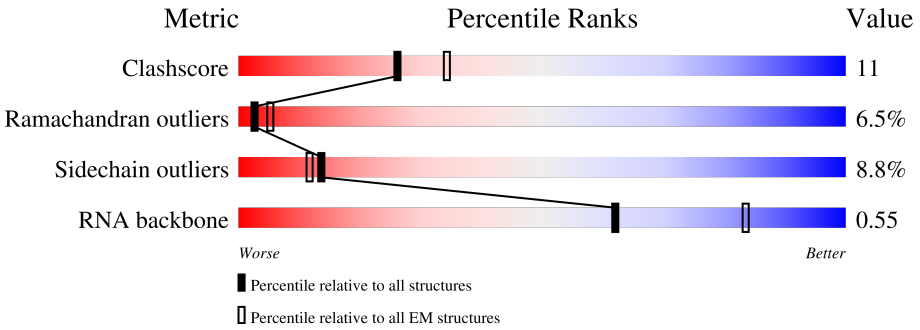
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.90 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	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	57	23% 75% 19%
2	1	55	87% 58% 25% 7% 9%
3	2	46	7% 78% 20%
4	3	65	6% 77% 17% 5%
5	4	38	18% 55% 39%
6	5	165	89% 25% 38% 18% 8% 10%
7	6	121	25% 17% 6% 75%

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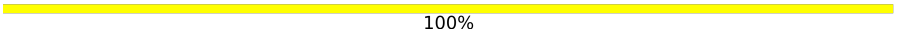
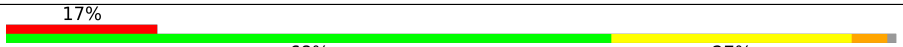
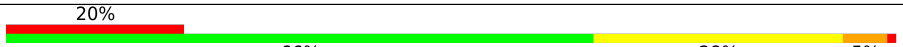
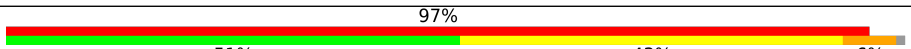
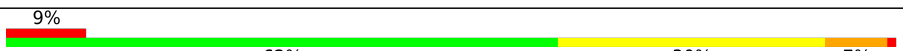
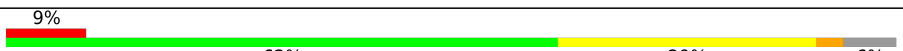
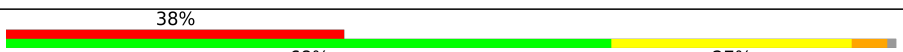
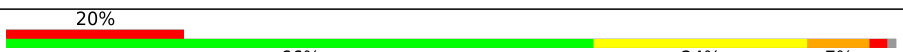
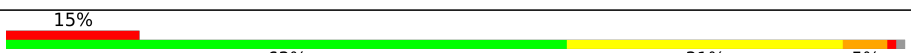
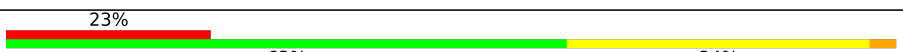
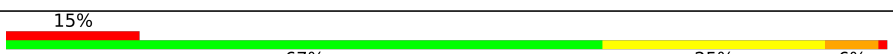
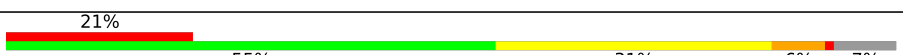
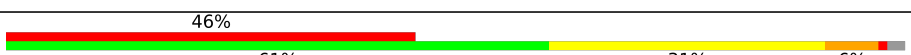
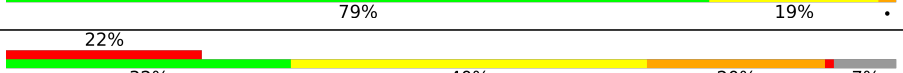
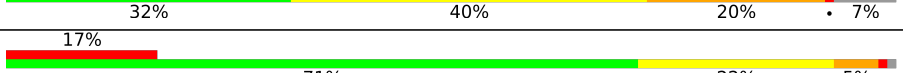
Mol	Chain	Length	Quality of chain
8	7	3	
9	A	2903	
10	B	118	
11	C	273	
12	D	209	
13	E	201	
14	F	179	
15	G	177	
16	H	149	
17	I	142	
18	J	142	
19	K	123	
20	L	144	
21	M	136	
22	N	127	
23	O	117	
24	P	115	
25	Q	118	
26	R	103	
27	S	110	
28	T	100	
29	U	104	
30	V	94	
31	W	85	
32	X	78	

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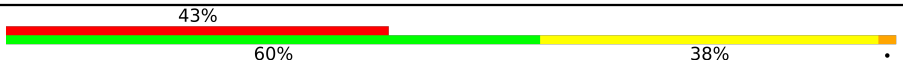
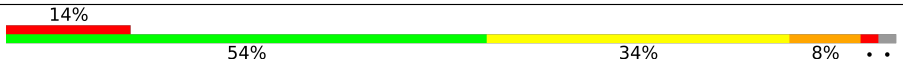
Mol	Chain	Length	Quality of chain
33	Y	63	
34	Z	59	
35	a	19	

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 90700 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	56	444	269	94	80	1	0	0

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1	50	409	263	75	71	0	0

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	46	377	228	90	57	2	0	0

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	64	504	323	105	74	2	0	0

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	38	302	185	65	48	4	0	0

- Molecule 6 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	148	1117	705	196	209	7	0	0

- Molecule 7 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	30	Total	C	N	O	S	0	0
			227	144	33	47	3		

- Molecule 8 is a RNA chain called P-tRNA CCA-end.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	3	Total	C	N	O	P	0	0
			58	28	11	17	2		

- Molecule 9 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	2854	Total	C	N	O	P	0	0
			61274	27334	11279	19807	2854		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 11 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 12 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 13 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 14 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 15 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 16 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	50	Total	C	N	O	S	0	0
			384	247	68	68	1		

- Molecule 17 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 18 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 19 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 20 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 21 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 22 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 23 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	O	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 24 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 25 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Q	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 26 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 27 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 28 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 29 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	U	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 30 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 31 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	79	Total	C	N	O	S	0	0
			596	367	120	108	1		

- Molecule 32 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	X	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 33 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

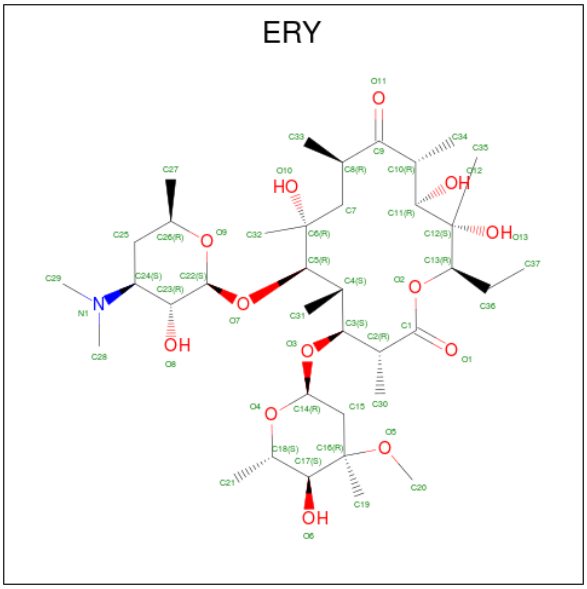
- Molecule 34 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 35 is a protein called ErmCL nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	a	7	Total	C	N	O	0	3
			36	27	4	5		

- Molecule 36 is ERYTHROMYCIN A (three-letter code: ERY) (formula: $C_{37}H_{67}NO_{13}$).



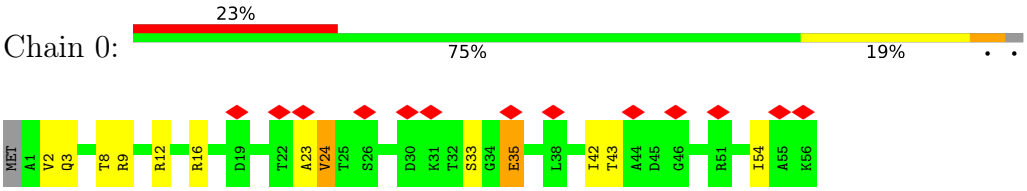
Mol	Chain	Residues	Atoms				AltConf
36	A	1	Total	C	N	O	0
			51	37	1	13	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

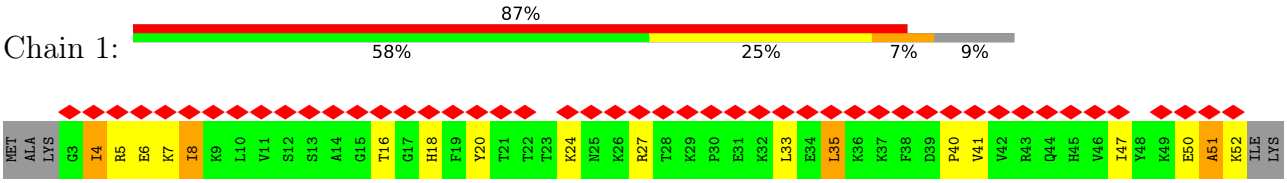
• Molecule 1: 50S ribosomal protein L32

Chain 0:



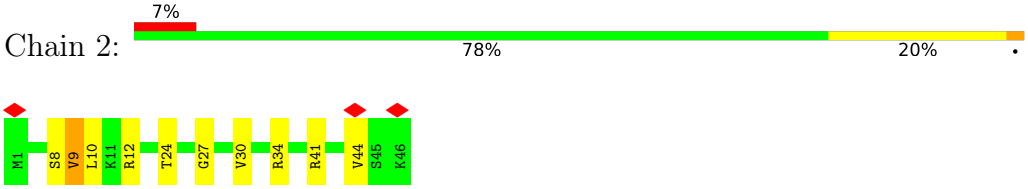
• Molecule 2: 50S ribosomal protein L33

Chain 1:



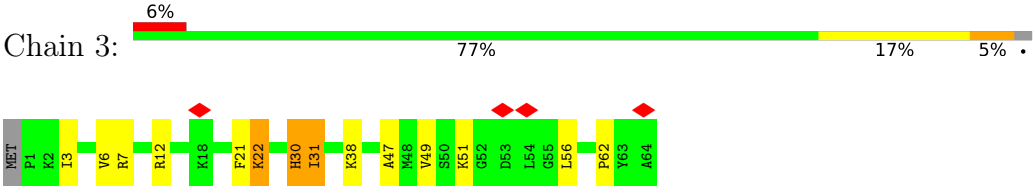
• Molecule 3: 50S ribosomal protein L34

Chain 2:



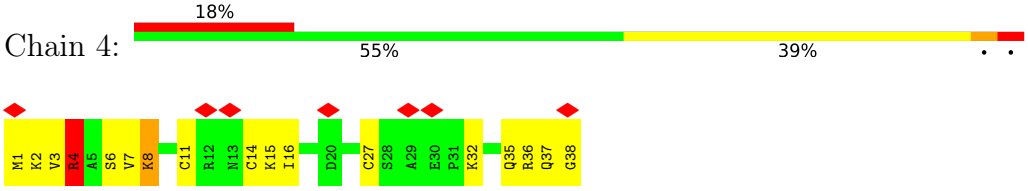
• Molecule 4: 50S ribosomal protein L35

Chain 3:



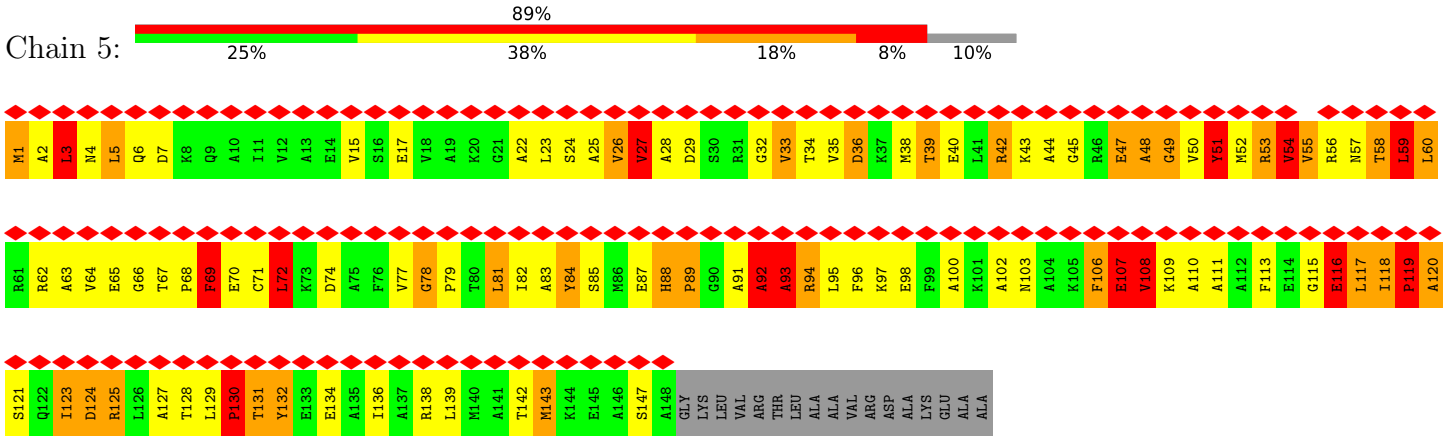
• Molecule 5: 50S ribosomal protein L36

Chain 4:



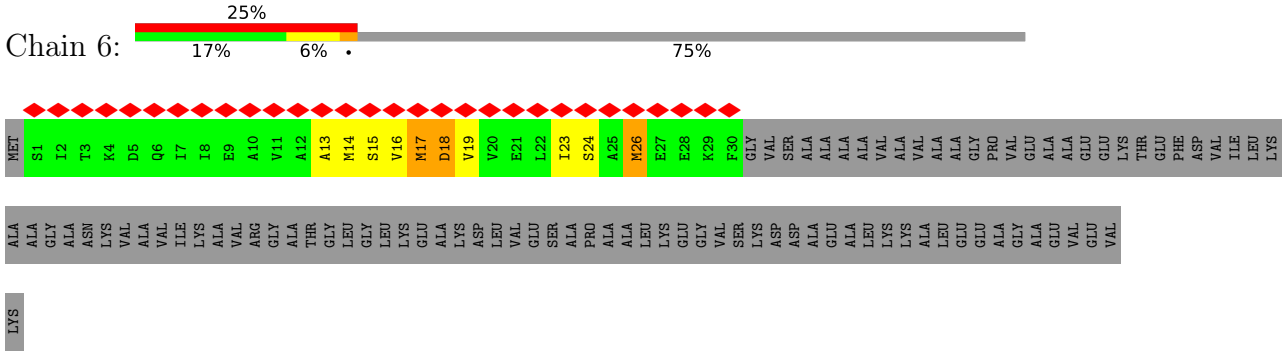
• Molecule 6: 50S ribosomal protein L10

Chain 5:



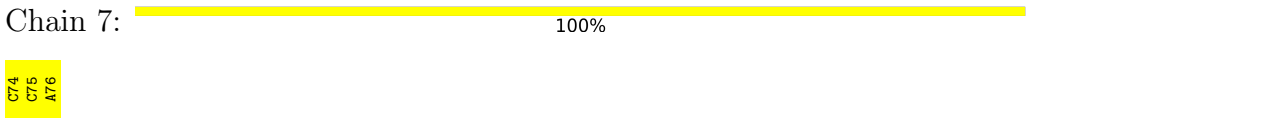
• Molecule 7: 50S ribosomal protein L7/L12

Chain 6:



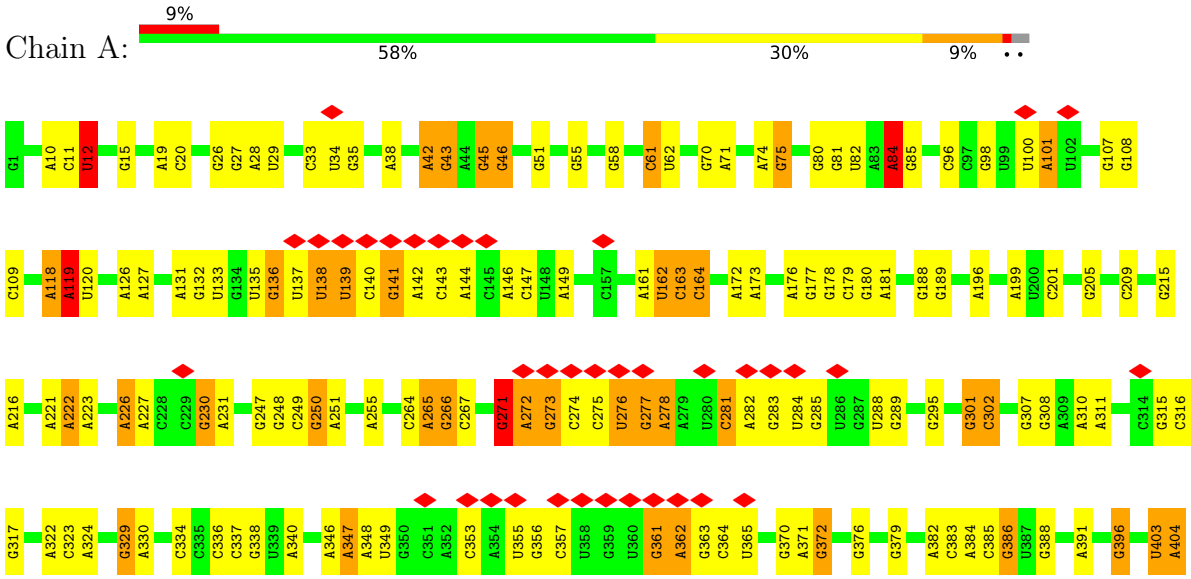
• Molecule 8: P-tRNA CCA-end

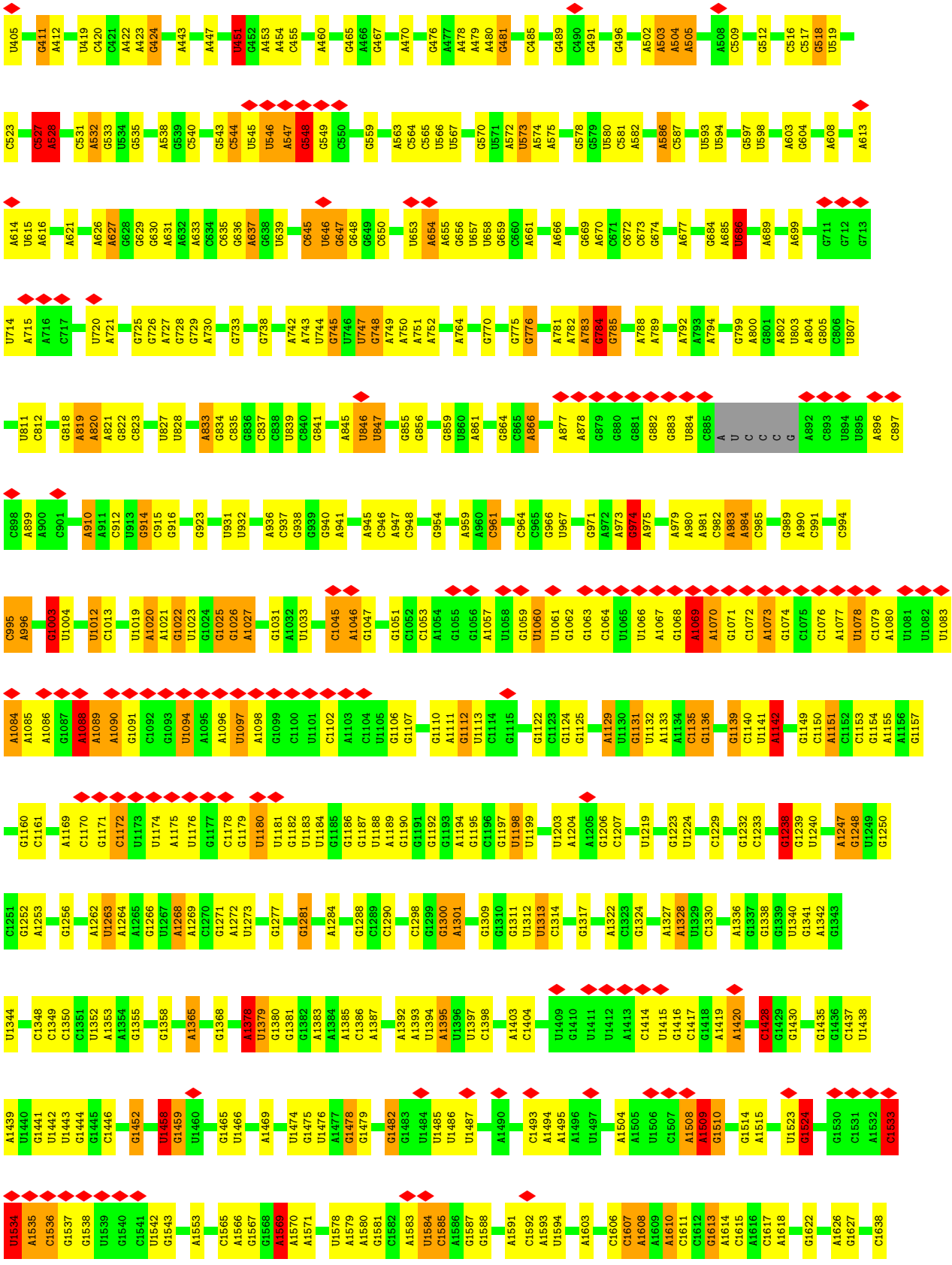
Chain 7:

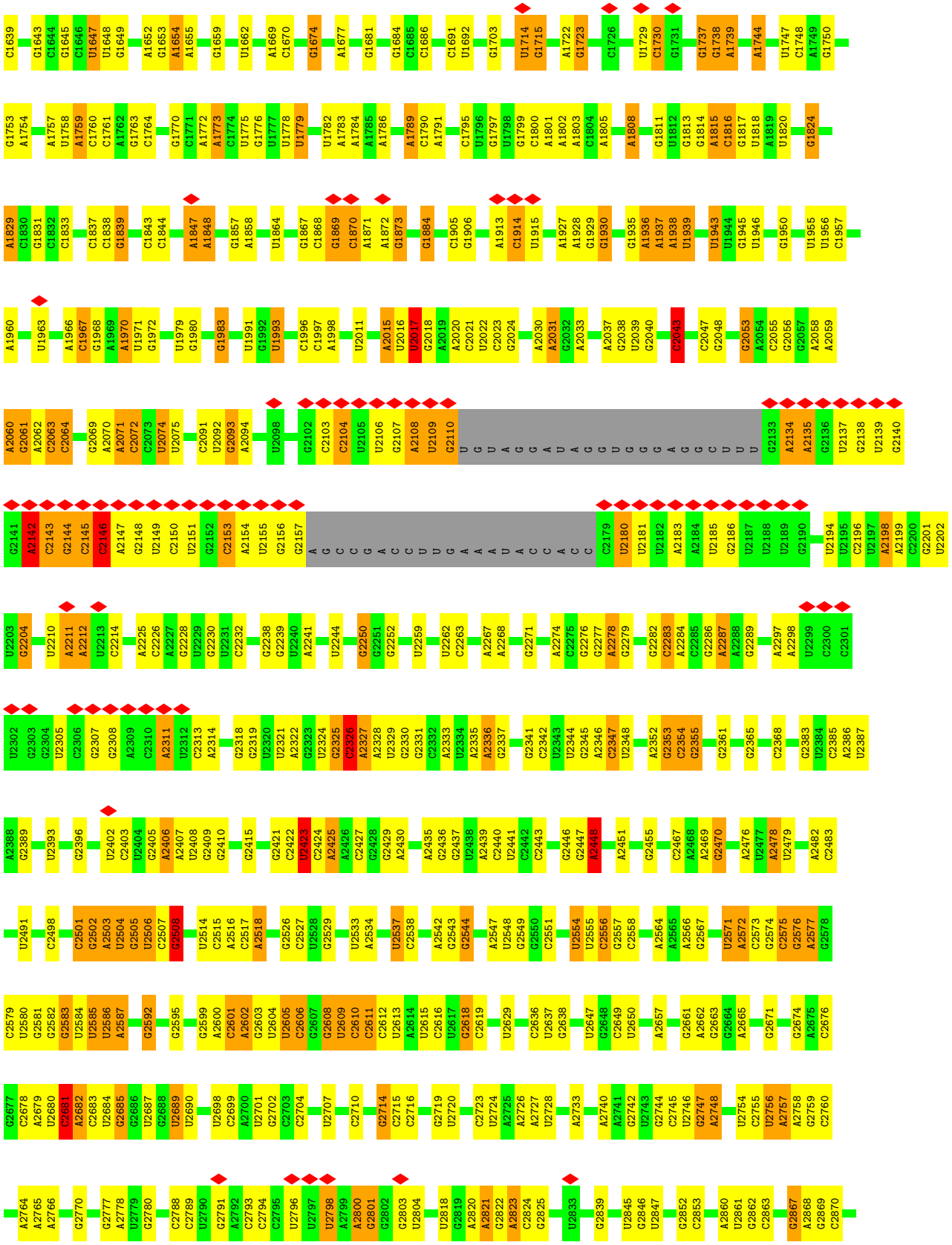


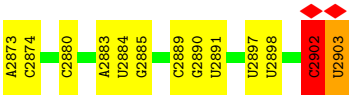
• Molecule 9: 23S rRNA

Chain A:



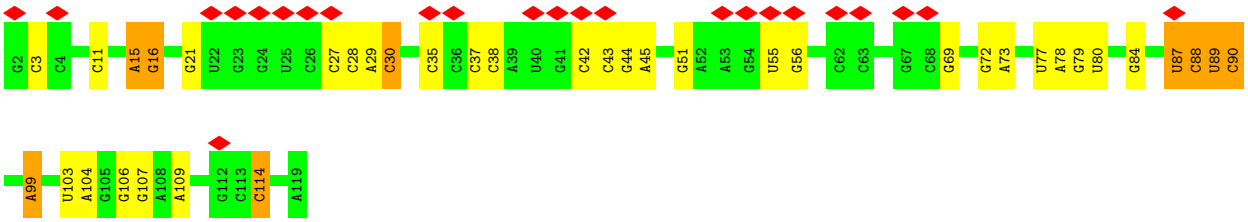

U405 G411 A412 U419 C420 C421 A422 A423 G424 A443 A447 U451 G452 A453 A454 C455 A460 G465 A466 G467 A470 G476 A477 A478 A479 A480 G481 C485 G489 C490 G491 G496 A502 A503 A504 A505 A508 C509 G512 C516 C517 G518 U519
C523 C527 A528 C531 A532 G533 U534 G535 A538 G539 C540 G543 C544 U545 U546 A547 G548 G549 C550 G559 A563 C564 C565 U566 U567 G570 U571 A572 U573 A574 A575 G578 G579 U580 C581 A582 A586 C587 U593 U594 G597 U598 A603 G604 A608 A613
A614 U615 A616 A621 A626 A627 G628 G629 G630 A631 A632 A633 C634 C635 G636 A637 G638 U639 C645 U646 G647 G648 G649 C650 U653 A654 A655 G656 U657 U658 G659 C660 A661 A666 G669 A670 C671 C672 C673 G674 A677 G684 A685 U686 A689 A699 G711 G712 G713
U714 A715 A716 C717 U720 A721 G725 G726 A727 G728 G729 A730 G733 G738 A742 A743 U744 G745 U746 U747 G748 A749 A750 A751 A752 A764 G770 G775 G776 A781 A782 A783 G784 G785 A788 A789 A792 A793 A794 G799 A800 G801 A802 U803 A804 G805 C806 U807
U811 C812 G818 A819 A820 A821 G822 C823 U827 U828 A833 G834 C835 G836 C837 C838 U839 C840 G841 A845 U846 U847 G855 G856 G859 U860 A861 G864 C865 A866 A877 A878 G879 G880 G881 G882 G883 U884 C885 A U C C C G A892 G893 U894 U895 A896 C897
C898 A899 A900 C901 A910 A911 C912 U913 G914 C915 G916 G923 U931 U932 A936 C937 G938 G939 G940 A941 A945 C946 A947 C948 G954 A959 A960 C961 C964 G965 G966 U967 G971 A972 A973 G974 A975 A979 A980 A981 C982 A983 A984 C985 G989 A990 C991 C994
C995 A996 G1003 U1004 U1012 C1013 U1019 A1020 A1021 G1022 U1023 G1024 G1025 G1026 A1027 G1031 A1032 U1033 C1045 A1046 G1047 G1051 C1052 C1053 A1054 G1055 G1056 A1057 U1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 A1080 U1081 U1082 U1083
A1084 A1085 A1086 G1087 A1088 A1089 A1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 G1110 A1111 G1112 U1113 C1114 G1115 G1122 C1123 G1124 G1125 A1129 U1130 G1131 U1132 A1133 A1134 C1135 G1136 G1139 C1140 U1141 A1142 G1149 C1150 A1151 C1152 C1153 G1154 A1155 A1156 G1157
G1160 C1161 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1181 G1182 U1183 U1184 G1185 G1186 G1187 U1188 A1189 G1190 G1191 G1192 G1193 A1194 G1195 C1196 G1197 U1198 U1199 U1203 A1204 A1205 G1206 C1207 U1219 G1223 U1224 C1229 G1232 C1233 G1238 G1239 U1240 A1247 G1248 U1249 G1250
C1251 G1252 A1253 G1256 A1262 U1263 A1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 G1277 G1281 A1284 G1288 C1289 C1290 C1298 G1299 G1300 A1301 G1309 G1310 G1311 U1312 U1313 C1314 G1317 A1322 C1323 G1324 A1327 A1328 U1329 C1330 A1336 G1337 G1338 G1339 U1340 G1341 A1342 G1343
U1344 C1348 C1349 C1350 C1351 U1352 A1353 A1354 G1355 G1358 A1365 G1368 A1378 U1379 G1380 G1381 G1382 A1383 A1384 A1385 C1386 A1387 A1392 A1393 U1394 A1395 U1396 U1397 C1398 A1403 C1404 U1409 G1410 U1411 U1412 A1413 C1414 U1415 G1416 C1417 G1418 A1419 A1420 C1423 G1429 G1430 G1435 G1436 C1437 U1438
A1439 U1440 G1441 U1442 U1443 G1444 G1445 C1446 G1452 U1458 G1459 U1460 G1465 U1466 A1469 U1474 G1475 U1476 A1477 G1478 G1479 G1482 G1483 U1484 U1485 U1486 U1487 A1490 C1493 A1494 A1495 A1496 U1497 A1504 A1505 U1506 C1507 A1508 A1509 G1510 G1514 A1515 U1523 G1524 G1530 C1531 A1532 G1533
U1534 A1535 C1536 G1537 G1538 U1539 G1540 C1541 U1542 G1543 A1553 C1565 A1566 G1567 G1568 A1569 A1570 A1571 U1578 A1579 A1580 G1581 C1582 A1583 U1584 C1585 A1586 G1587 G1588 A1591 C1592 A1593 U1594 A1603 C1606 C1607 A1608 A1609 A1610 C1611 C1612 G1613 A1614 C1615 A1616 C1617 A1618 G1622 A1626 G1627 C1638





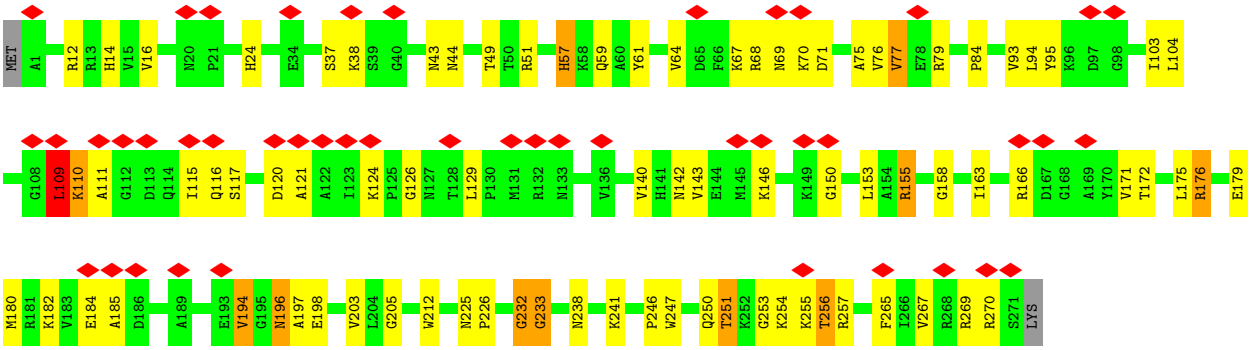
• Molecule 10: 5S rRNA

Chain B:



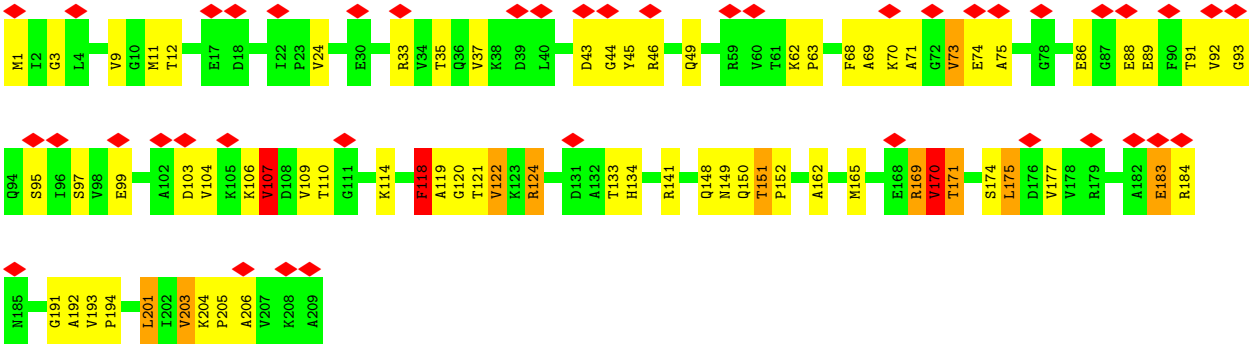
• Molecule 11: 50S ribosomal protein L2

Chain C:



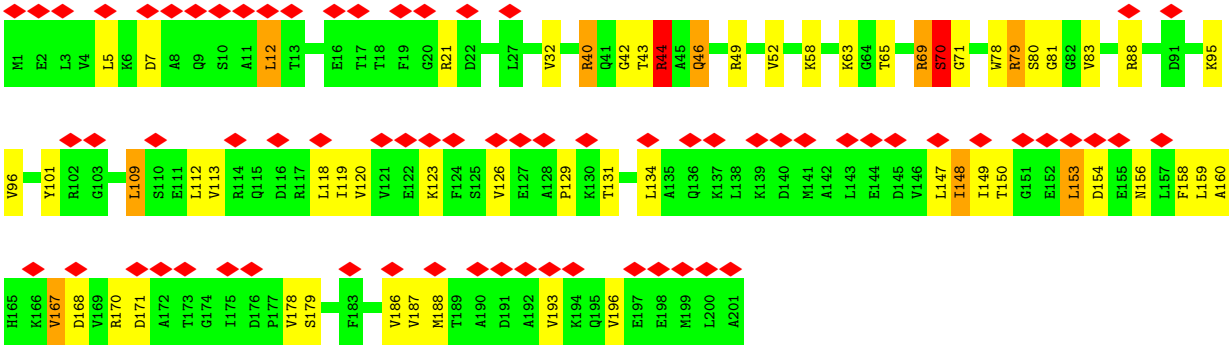
• Molecule 12: 50S ribosomal protein L3

Chain D:



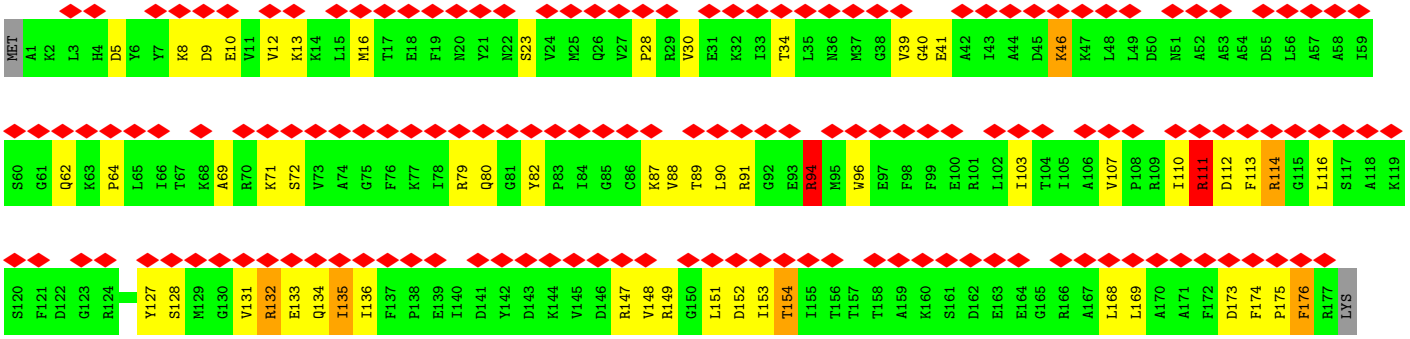
• Molecule 13: 50S ribosomal protein L4

Chain E:



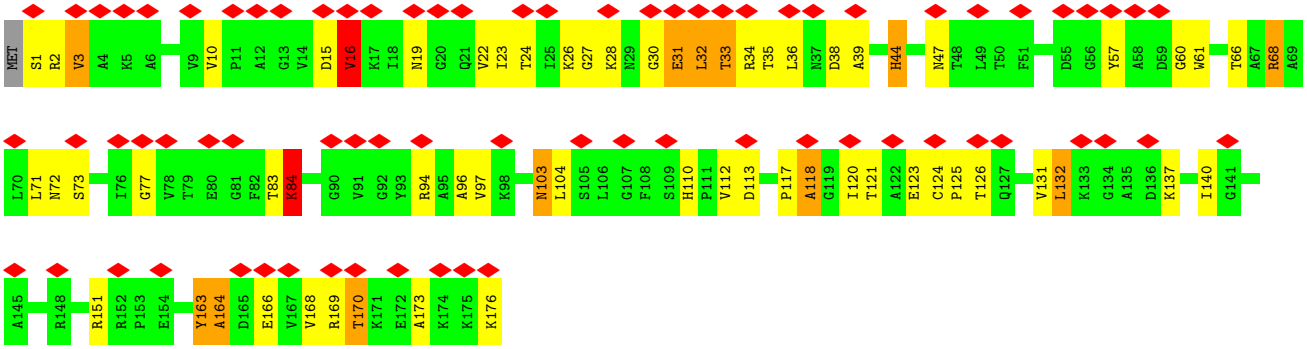
• Molecule 14: 50S ribosomal protein L5

Chain F:



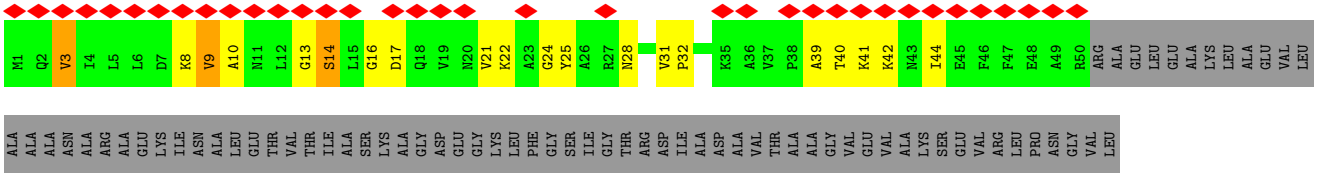
• Molecule 15: 50S ribosomal protein L6

Chain G:



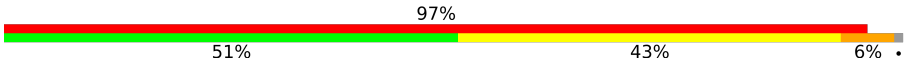
• Molecule 16: 50S ribosomal protein L9

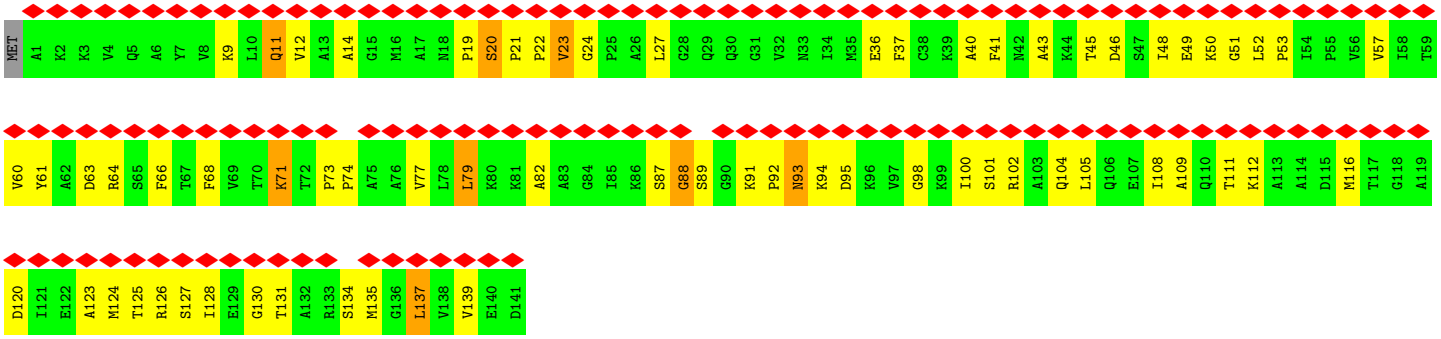
Chain H:



• Molecule 17: 50S ribosomal protein L11

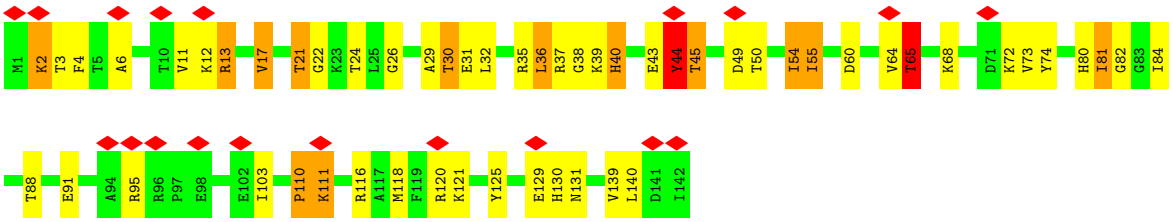
Chain I:





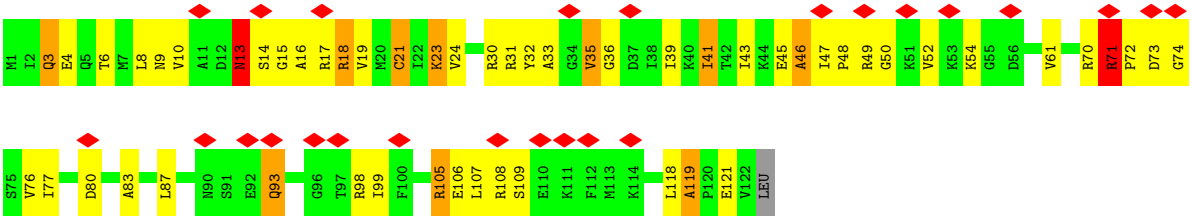
• Molecule 18: 50S ribosomal protein L13

Chain J:



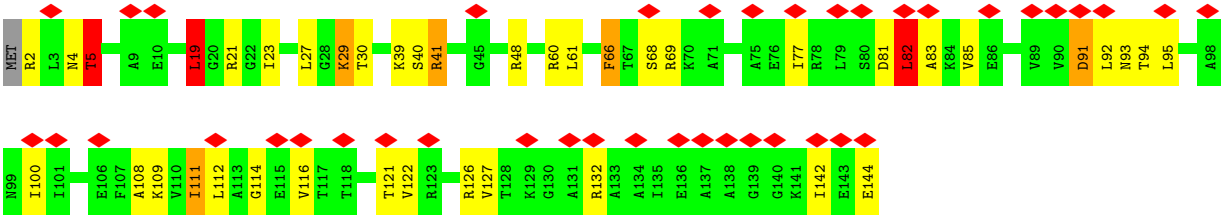
• Molecule 19: 50S ribosomal protein L14

Chain K:



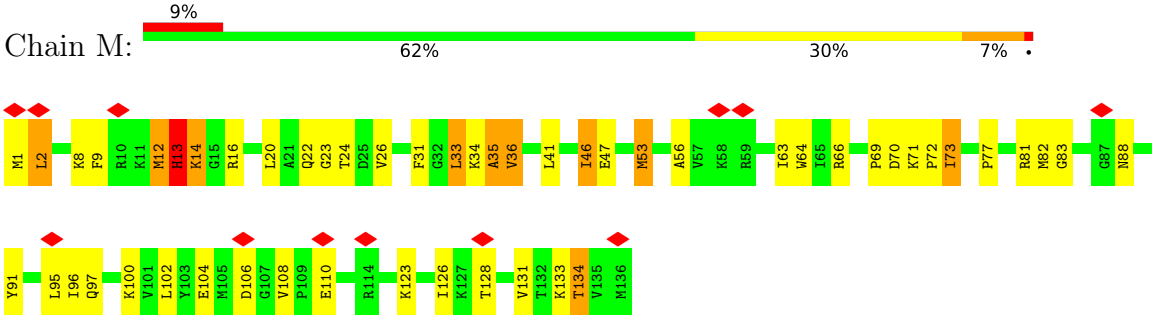
• Molecule 20: 50S ribosomal protein L15

Chain L:



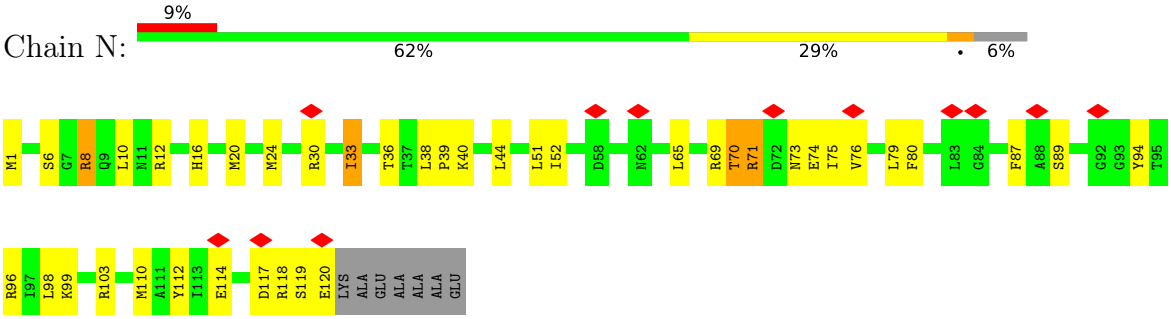
• Molecule 21: 50S ribosomal protein L16

Chain M:



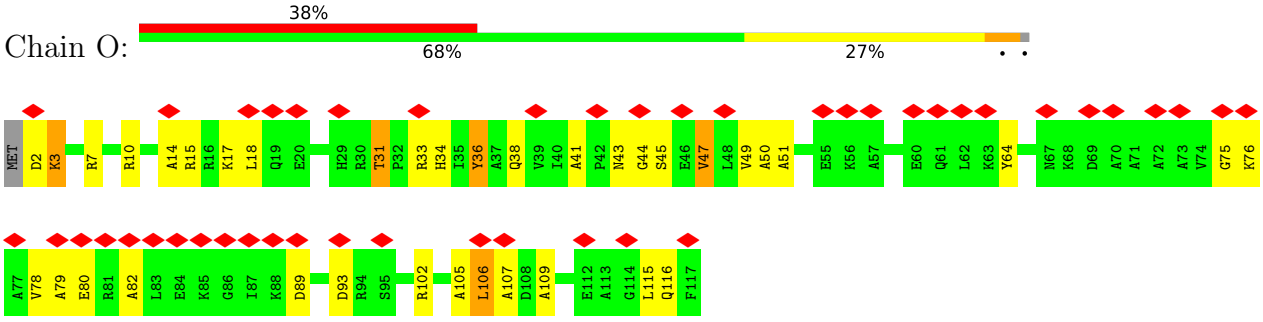
• Molecule 22: 50S ribosomal protein L17

Chain N:



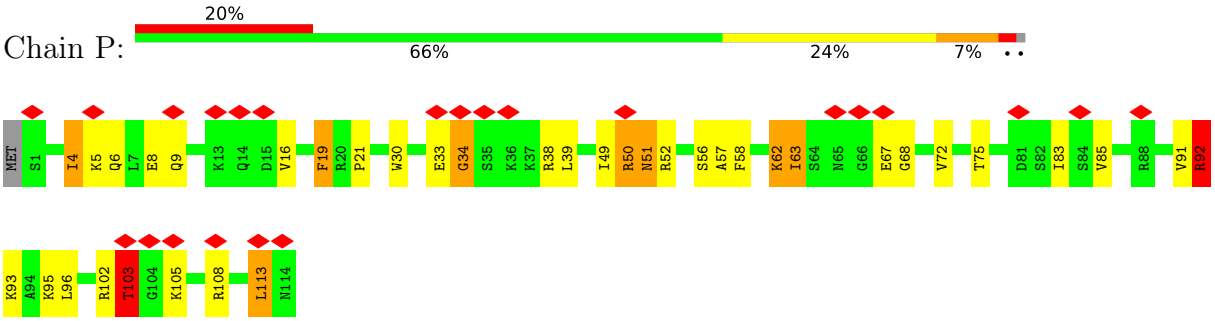
• Molecule 23: 50S ribosomal protein L18

Chain O:



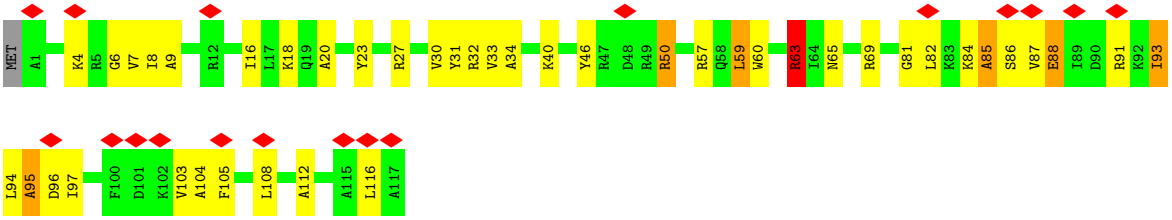
• Molecule 24: 50S ribosomal protein L19

Chain P:

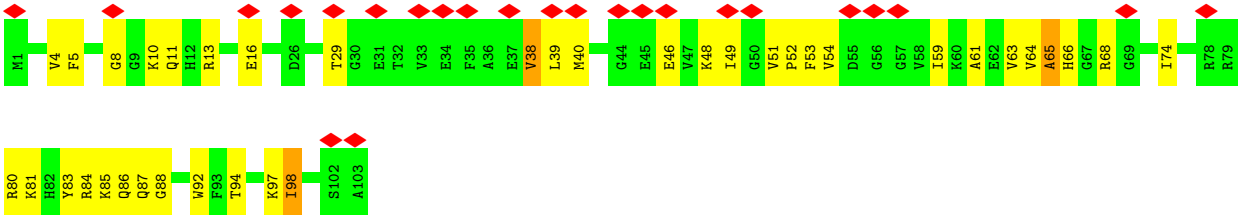


• Molecule 25: 50S ribosomal protein L20

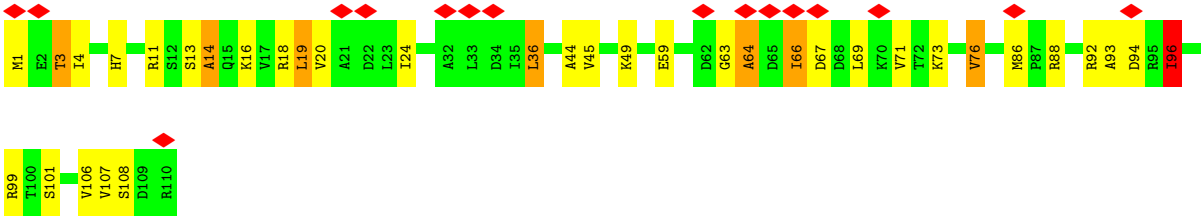
Chain Q:



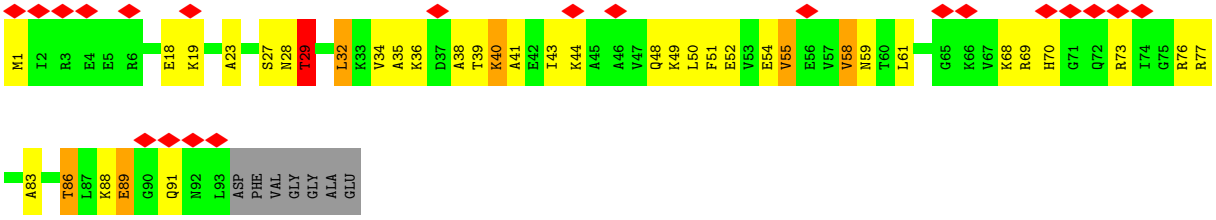
• Molecule 26: 50S ribosomal protein L21



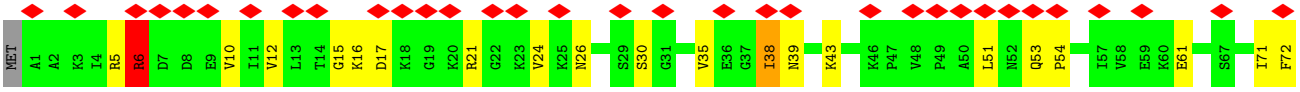
• Molecule 27: 50S ribosomal protein L22

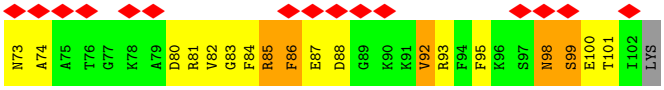


• Molecule 28: 50S ribosomal protein L23



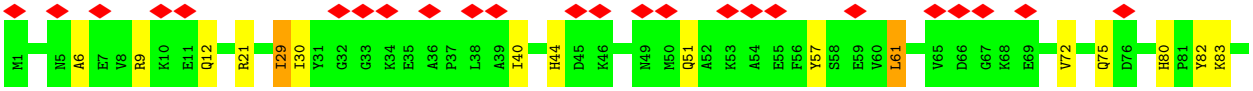
• Molecule 29: 50S ribosomal protein L24

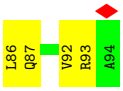




• Molecule 30: 50S ribosomal protein L25

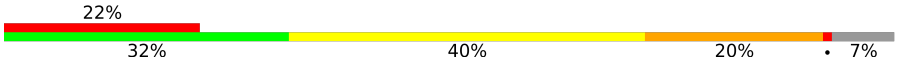
Chain V:

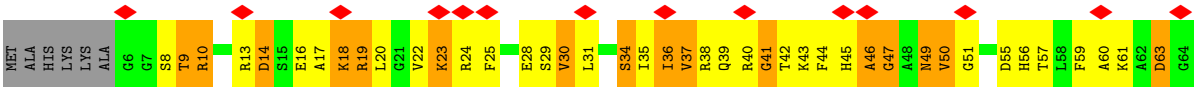


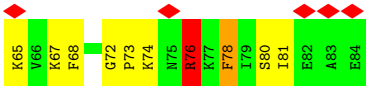


• Molecule 31: 50S ribosomal protein L27

Chain W:

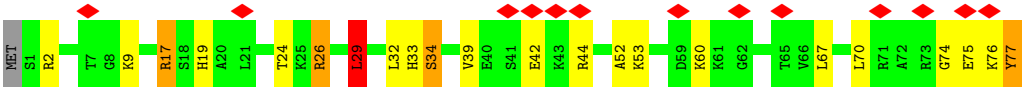






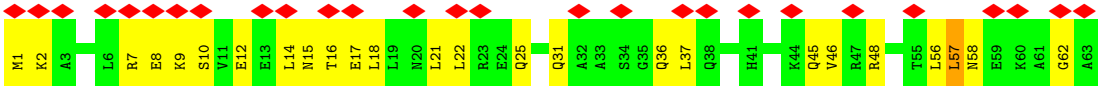
• Molecule 32: 50S ribosomal protein L28

Chain X:



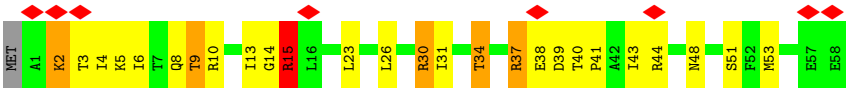
• Molecule 33: 50S ribosomal protein L29

Chain Y:



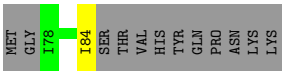
• Molecule 34: 50S ribosomal protein L30

Chain Z:



• Molecule 35: ErmCL nascent chain

Chain a:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	269163	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	defocus groups	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	125085	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.019	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.003	Depositor
Map size (Å)	196.11601, 202.764, 255.94801	wwPDB
Map dimensions	177, 183, 231	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.108, 1.108, 1.108	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ERY

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	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.54	0/450	0.70	0/599
2	1	0.53	0/416	0.74	0/554
3	2	0.53	0/380	0.70	0/498
4	3	0.53	0/513	0.75	0/676
5	4	0.59	0/303	0.84	0/397
6	5	0.74	0/1131	1.32	26/1524 (1.7%)
7	6	0.59	0/227	0.65	0/304
8	7	0.16	0/64	0.54	0/97
9	A	0.80	15/68626 (0.0%)	1.22	301/107056 (0.3%)
10	B	0.66	0/2828	1.10	2/4410 (0.0%)
11	C	0.54	0/2121	0.79	3/2852 (0.1%)
12	D	0.57	0/1586	0.77	1/2134 (0.0%)
13	E	0.53	0/1571	0.76	2/2113 (0.1%)
14	F	0.50	0/1434	0.71	1/1926 (0.1%)
15	G	0.55	0/1343	0.73	0/1816
16	H	0.53	0/389	0.73	0/523
17	I	0.62	0/1046	0.84	1/1410 (0.1%)
18	J	0.63	1/1152 (0.1%)	0.78	0/1551
19	K	0.65	1/947 (0.1%)	0.77	0/1268
20	L	0.56	0/1054	0.79	2/1403 (0.1%)
21	M	0.61	0/1093	0.77	0/1460
22	N	0.51	0/973	0.68	0/1301
23	O	0.46	0/902	0.70	0/1209
24	P	0.52	0/929	0.78	1/1242 (0.1%)
25	Q	0.62	0/960	0.71	1/1278 (0.1%)
26	R	0.61	1/829 (0.1%)	0.76	0/1107
27	S	0.54	0/864	0.73	0/1156
28	T	0.55	0/744	0.85	1/994 (0.1%)
29	U	0.56	0/787	0.78	0/1051
30	V	0.48	0/766	0.67	1/1025 (0.1%)
31	W	0.69	0/603	1.00	1/797 (0.1%)
32	X	0.50	0/635	0.79	1/848 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Y	0.46	0/510	0.75	0/677
34	Z	0.54	0/453	0.84	1/605 (0.2%)
35	a	0.86	0/32	1.43	1/40 (2.5%)
All	All	0.74	18/98661 (0.0%)	1.12	347/147901 (0.2%)

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
6	5	0	1
11	C	0	1
12	D	0	1
18	J	0	1
19	K	0	1
All	All	0	5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	984	A	N9-C4	-8.36	1.32	1.37
9	A	528	A	N9-C4	-6.60	1.33	1.37
9	A	1142	A	N9-C4	-6.51	1.33	1.37
9	A	783	A	N9-C4	-6.27	1.34	1.37
9	A	1569	A	N9-C4	-6.16	1.34	1.37
9	A	783	A	N3-C4	-5.96	1.31	1.34
9	A	2606	C	N1-C6	-5.84	1.33	1.37
9	A	1073	A	C5-C6	5.82	1.46	1.41
9	A	2508	G	O3'-P	-5.60	1.54	1.61
18	J	44	TYR	CD2-CE2	-5.59	1.30	1.39
9	A	528	A	N3-C4	-5.47	1.31	1.34
26	R	86	GLN	CB-CG	5.41	1.67	1.52
9	A	1142	A	C5-C6	-5.32	1.36	1.41
9	A	2478	A	N9-C4	-5.29	1.34	1.37
9	A	2053	G	C6-O6	5.26	1.28	1.24
9	A	783	A	N7-C5	-5.24	1.36	1.39
19	K	21	CYS	CB-SG	-5.23	1.73	1.81
9	A	783	A	C5-C6	-5.02	1.36	1.41

All (347) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1073	A	N1-C6-N6	-20.00	106.60	118.60
9	A	1073	A	C5-C6-N6	14.06	134.95	123.70
9	A	2053	G	N1-C6-O6	13.89	128.23	119.90
9	A	984	A	C2-N3-C4	-12.15	104.53	110.60
9	A	961	C	O5'-P-OP2	-11.75	95.12	105.70
9	A	2053	G	C6-C5-N7	-11.60	123.44	130.40
9	A	1073	A	C6-C5-N7	11.45	140.32	132.30
9	A	2053	G	C5-C6-N1	-11.39	105.80	111.50
9	A	1073	A	C4-C5-N7	-11.28	105.06	110.70
9	A	783	A	C5-N7-C8	-10.82	98.49	103.90
9	A	974	G	C6-C5-N7	-10.52	124.09	130.40
9	A	2053	G	C4-C5-C6	10.22	124.93	118.80
9	A	974	G	C4-C5-N7	9.91	114.76	110.80
9	A	783	A	N7-C8-N9	9.65	118.63	113.80
6	5	92	ALA	C-N-CA	9.60	145.71	121.70
9	A	1534	U	C2-N1-C1'	9.34	128.91	117.70
9	A	1073	A	C5-N7-C8	9.30	108.55	103.90
9	A	528	A	C2-N3-C4	-9.13	106.03	110.60
6	5	93	ALA	C-N-CA	9.06	144.35	121.70
9	A	1950	G	N1-C6-O6	8.81	125.19	119.90
9	A	465	G	C8-N9-C4	-8.69	102.92	106.40
9	A	1533	C	N1-C2-O2	8.66	124.09	118.90
9	A	783	A	C8-N9-C4	-8.64	102.35	105.80
9	A	1073	A	N9-C4-C5	8.61	109.24	105.80
9	A	2074	U	O5'-P-OP2	-8.55	98.00	105.70
9	A	2534	A	N1-C6-N6	8.53	123.72	118.60
9	A	1936	A	C2-N3-C4	-8.52	106.34	110.60
9	A	974	G	C4-N9-C1'	8.44	137.47	126.50
9	A	2572	A	N1-C6-N6	8.41	123.65	118.60
9	A	1533	C	C2-N1-C1'	8.40	128.04	118.80
9	A	1142	A	C2-N3-C4	-8.35	106.42	110.60
6	5	27	VAL	CG1-CB-CG2	8.20	124.02	110.90
9	A	586	A	O5'-P-OP1	-8.12	98.39	105.70
12	D	151	THR	C-N-CD	8.00	145.20	128.40
9	A	1533	C	C6-N1-C2	-7.99	117.10	120.30
9	A	783	A	C4-C5-N7	7.82	114.61	110.70
9	A	984	A	N3-C4-C5	7.76	132.23	126.80
9	A	1478	G	N1-C6-O6	7.75	124.55	119.90
9	A	1795	C	C6-N1-C2	-7.73	117.21	120.30
6	5	51	TYR	C-N-CA	7.70	140.95	121.70
9	A	2053	G	C4-N9-C1'	7.68	136.48	126.50
9	A	2606	C	C5-C6-N1	-7.68	117.16	121.00
9	A	783	A	N1-C6-N6	7.66	123.19	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	2053	G	C2-N3-C4	-7.65	108.07	111.90
6	5	49	GLY	C-N-CA	7.64	140.81	121.70
9	A	974	G	C8-N9-C1'	-7.63	117.09	127.00
6	5	123	ILE	CG1-CB-CG2	7.61	128.13	111.40
9	A	465	G	N3-C4-C5	-7.60	124.80	128.60
6	5	119	PRO	C-N-CA	7.58	140.64	121.70
31	W	76	ARG	NE-CZ-NH2	7.54	124.07	120.30
9	A	783	A	C6-C5-N7	-7.53	127.03	132.30
35	a	84	ILE	CB-CA-C	-7.52	96.55	111.60
9	A	776	G	C5-C6-O6	7.49	133.10	128.60
9	A	1839	G	N1-C6-O6	7.44	124.36	119.90
9	A	2508	G	P-O3'-C3'	-7.43	110.78	119.70
6	5	72	LEU	C-N-CA	7.37	140.14	121.70
13	E	44	ARG	NE-CZ-NH2	7.35	123.98	120.30
9	A	2146	C	N3-C4-C5	-7.35	118.96	121.90
9	A	1533	C	N3-C2-O2	-7.33	116.77	121.90
9	A	2053	G	N1-C2-N3	7.33	128.30	123.90
9	A	974	G	C5-N7-C8	-7.29	100.65	104.30
6	5	81	LEU	CB-CG-CD2	7.28	123.37	111.00
9	A	2250	G	C6-C5-N7	-7.28	126.03	130.40
9	A	1073	A	O5'-P-OP2	7.27	119.42	110.70
9	A	1142	A	N1-C6-N6	7.26	122.96	118.60
9	A	1534	U	C6-N1-C1'	-7.26	111.04	121.20
9	A	1950	G	C6-C5-N7	-7.23	126.06	130.40
9	A	2501	C	C2-N1-C1'	-7.20	110.88	118.80
9	A	2447	G	O5'-P-OP1	-7.19	99.22	105.70
6	5	28	ALA	C-N-CA	7.12	139.50	121.70
9	A	776	G	C5-C6-N1	-7.12	107.94	111.50
9	A	2053	G	C8-N9-C1'	-7.10	117.77	127.00
6	5	47	GLU	C-N-CA	7.02	139.25	121.70
6	5	54	VAL	CG1-CB-CG2	6.99	122.09	110.90
9	A	2423	U	P-O3'-C3'	6.99	128.09	119.70
9	A	2250	G	N1-C6-O6	6.96	124.08	119.90
9	A	1935	G	O5'-P-OP2	-6.94	99.45	105.70
9	A	984	A	N3-C4-N9	-6.92	121.86	127.40
9	A	1284	A	O5'-P-OP2	-6.91	99.48	105.70
9	A	802	A	N1-C6-N6	-6.91	114.45	118.60
9	A	2448	A	N1-C6-N6	6.88	122.73	118.60
9	A	783	A	C2-N3-C4	-6.87	107.17	110.60
9	A	1839	G	C6-C5-N7	-6.84	126.30	130.40
9	A	1654	A	O5'-P-OP1	-6.82	99.56	105.70
9	A	1378	A	P-O3'-C3'	6.82	127.88	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	12	U	N3-C2-O2	-6.81	117.44	122.20
9	A	2681	C	C6-N1-C2	6.79	123.02	120.30
9	A	1311	G	C8-N9-C4	-6.76	103.70	106.40
9	A	503	A	C8-N9-C4	-6.75	103.10	105.80
9	A	974	G	N9-C4-C5	-6.75	102.70	105.40
9	A	974	G	N3-C4-N9	6.74	130.05	126.00
9	A	974	G	N1-C6-O6	6.74	123.94	119.90
9	A	974	G	C5-C6-O6	-6.71	124.57	128.60
9	A	1192	G	C8-N9-C4	6.70	109.08	106.40
20	L	19	LEU	CA-CB-CG	6.70	130.70	115.30
9	A	974	G	N7-C8-N9	6.65	116.43	113.10
14	F	94	ARG	NE-CZ-NH1	6.61	123.60	120.30
11	C	233	GLY	N-CA-C	-6.59	96.62	113.10
9	A	2823	A	C8-N9-C4	-6.58	103.17	105.80
9	A	2508	G	O3'-P-O5'	6.56	116.47	104.00
9	A	2689	U	C5-C4-O4	6.56	129.83	125.90
9	A	528	A	N1-C6-N6	6.55	122.53	118.60
9	A	1263	U	N3-C4-C5	-6.50	110.70	114.60
9	A	984	A	N1-C6-N6	6.49	122.50	118.60
9	A	1815	A	N9-C4-C5	6.48	108.39	105.80
6	5	147	SER	C-N-CA	6.47	137.88	121.70
6	5	84	TYR	C-N-CA	6.46	137.86	121.70
6	5	40	GLU	C-N-CA	6.43	137.78	121.70
9	A	2146	C	C2-N3-C4	6.41	123.11	119.90
9	A	2447	G	N1-C6-O6	6.41	123.75	119.90
9	A	820	A	O5'-P-OP1	-6.40	99.94	105.70
6	5	50	VAL	C-N-CA	6.38	137.65	121.70
9	A	2551	C	OP2-P-O3'	6.37	119.21	105.20
9	A	670	A	O4'-C1'-N9	-6.36	103.11	108.20
9	A	404	A	P-O3'-C3'	6.36	127.33	119.70
9	A	2142	A	OP2-P-O3'	6.34	119.14	105.20
9	A	2267	A	C8-N9-C4	-6.33	103.27	105.80
13	E	44	ARG	NE-CZ-NH1	-6.32	117.14	120.30
9	A	2754	U	N3-C4-O4	6.31	123.82	119.40
9	A	1142	A	N3-C4-C5	6.30	131.21	126.80
9	A	748	G	O4'-C1'-N9	6.28	113.23	108.20
6	5	108	VAL	CG1-CB-CG2	6.27	120.94	110.90
9	A	2770	G	N1-C6-O6	-6.26	116.15	119.90
6	5	60	LEU	CB-CG-CD1	6.22	121.58	111.00
6	5	39	THR	C-N-CA	6.22	137.24	121.70
9	A	1839	G	C5-C6-O6	-6.19	124.89	128.60
9	A	2250	G	C4-C5-N7	6.18	113.27	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1003	G	O5'-P-OP2	-6.18	100.14	105.70
9	A	1125	G	N1-C6-O6	6.18	123.61	119.90
9	A	567	U	N1-C2-O2	-6.17	118.48	122.80
9	A	1142	A	C5-N7-C8	-6.17	100.81	103.90
9	A	2592	G	O5'-P-OP2	-6.16	100.16	105.70
9	A	2606	C	C6-N1-C2	6.16	122.76	120.30
9	A	1950	G	C5-C6-O6	-6.15	124.91	128.60
11	C	109	LEU	CA-CB-CG	6.15	129.45	115.30
9	A	548	G	C8-N9-C4	-6.13	103.95	106.40
9	A	2250	G	C5-N7-C8	-6.12	101.24	104.30
9	A	1142	A	C4-C5-N7	6.12	113.76	110.70
9	A	784	G	O4'-C1'-N9	-6.08	103.34	108.20
9	A	2241	A	C8-N9-C4	-6.07	103.37	105.80
9	A	784	G	P-O3'-C3'	6.06	126.97	119.70
9	A	379	G	N1-C6-O6	6.05	123.53	119.90
9	A	2606	C	N1-C1'-C2'	-6.05	105.35	112.00
6	5	59	LEU	C-N-CA	6.04	136.81	121.70
9	A	1025	G	P-O3'-C3'	6.02	126.92	119.70
20	L	82	LEU	CA-CB-CG	6.01	129.13	115.30
9	A	1328	A	O5'-P-OP2	-5.99	100.31	105.70
9	A	1069	A	OP2-P-O3'	5.98	118.36	105.20
9	A	1073	A	N7-C8-N9	-5.98	110.81	113.80
9	A	2534	A	C4-C5-N7	5.97	113.69	110.70
6	5	53	ARG	C-N-CA	5.96	136.60	121.70
9	A	528	A	C5-C6-N1	-5.93	114.73	117.70
9	A	1779	U	N3-C4-O4	-5.93	115.25	119.40
9	A	2448	A	C6-C5-N7	-5.93	128.15	132.30
9	A	2747	G	OP2-P-O3'	5.93	118.24	105.20
9	A	119	A	O5'-P-OP2	-5.91	100.38	105.70
9	A	2554	U	O5'-P-OP1	-5.91	100.38	105.70
9	A	1428	C	O5'-P-OP1	-5.91	100.39	105.70
9	A	2447	G	C5-C6-O6	-5.89	125.06	128.60
9	A	866	A	N1-C6-N6	5.89	122.13	118.60
9	A	1094	U	N3-C4-C5	-5.89	111.07	114.60
9	A	1069	A	C8-N9-C4	-5.88	103.45	105.80
9	A	527	C	P-O3'-C3'	5.88	126.75	119.70
9	A	2043	C	C6-N1-C2	-5.87	117.95	120.30
9	A	964	C	O5'-P-OP2	-5.86	100.42	105.70
9	A	1509	A	O4'-C1'-N9	5.85	112.88	108.20
9	A	1837	C	O5'-P-OP1	-5.85	100.44	105.70
9	A	1670	C	N1-C2-O2	-5.84	115.39	118.90
9	A	1645	G	N3-C4-C5	-5.80	125.70	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1815	A	C8-N9-C4	-5.80	103.48	105.80
9	A	2715	C	C6-N1-C2	5.80	122.62	120.30
9	A	516	C	O5'-P-OP1	-5.79	100.49	105.70
9	A	1066	U	N3-C2-O2	-5.74	118.18	122.20
6	5	117	LEU	C-N-CA	5.73	136.02	121.70
9	A	1247	A	P-O3'-C3'	5.73	126.57	119.70
9	A	1263	U	C6-N1-C2	-5.73	117.56	121.00
9	A	2534	A	C5-N7-C8	-5.72	101.04	103.90
9	A	1979	U	C6-N1-C2	-5.72	117.57	121.00
9	A	209	C	C6-N1-C2	5.71	122.58	120.30
9	A	1789	A	O5'-P-OP1	-5.71	100.56	105.70
9	A	2508	G	C6-C5-N7	-5.68	126.99	130.40
9	A	2719	G	C5-C6-N1	-5.67	108.66	111.50
9	A	1606	C	C2-N3-C4	-5.66	117.07	119.90
9	A	2719	G	N1-C6-O6	5.65	123.29	119.90
9	A	1358	G	C8-N9-C4	-5.63	104.15	106.40
9	A	271	G	OP1-P-O3'	5.63	117.58	105.20
9	A	2241	A	N9-C4-C5	5.62	108.05	105.80
9	A	1073	A	C4-N9-C1'	-5.62	116.19	126.30
9	A	1534	U	C5-C6-N1	5.62	125.51	122.70
9	A	2605	U	P-O3'-C3'	-5.62	112.96	119.70
9	A	1088	A	O4'-C1'-N9	-5.61	103.71	108.20
9	A	2053	G	N3-C2-N2	-5.57	116.00	119.90
9	A	1157	G	N1-C6-O6	5.57	123.24	119.90
9	A	1509	A	P-O3'-C3'	5.55	126.36	119.70
9	A	626	A	N1-C6-N6	5.55	121.93	118.60
9	A	2271	G	C5-C6-O6	-5.55	125.27	128.60
9	A	2544	G	C6-C5-N7	-5.55	127.07	130.40
9	A	1198	U	O5'-P-OP2	-5.55	100.71	105.70
9	A	532	A	C8-N9-C4	-5.55	103.58	105.80
9	A	1125	G	C6-C5-N7	-5.55	127.07	130.40
9	A	2282	G	C8-N9-C4	-5.53	104.19	106.40
9	A	2501	C	N3-C4-C5	5.53	124.11	121.90
9	A	1611	C	N1-C2-O2	-5.53	115.58	118.90
9	A	2326	C	C5-C4-N4	-5.52	116.33	120.20
9	A	2689	U	N3-C4-O4	-5.52	115.54	119.40
9	A	1192	G	N9-C4-C5	-5.51	103.19	105.40
9	A	2244	U	C5-C4-O4	-5.51	122.59	125.90
9	A	55	G	C5-C6-O6	-5.50	125.30	128.60
9	A	2353	G	N1-C6-O6	-5.50	116.60	119.90
9	A	1069	A	O4'-C1'-N9	5.50	112.60	108.20
9	A	1153	C	N1-C2-O2	-5.50	115.60	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	672	C	N1-C2-O2	5.49	122.20	118.90
9	A	29	U	OP2-P-O3'	5.49	117.28	105.20
9	A	1207	C	C6-N1-C2	-5.48	118.11	120.30
10	B	80	U	N1-C2-N3	5.48	118.19	114.90
9	A	2146	C	C6-N1-C2	-5.48	118.11	120.30
9	A	1027	A	O4'-C1'-N9	-5.47	103.83	108.20
9	A	2446	G	OP2-P-O3'	5.47	117.22	105.20
9	A	984	A	C5-C6-N1	-5.45	114.98	117.70
9	A	451	U	O4'-C1'-N1	5.45	112.56	108.20
9	A	989	G	O4'-C1'-N9	5.44	112.55	108.20
9	A	1073	A	C8-N9-C1'	5.43	137.47	127.70
9	A	598	U	OP2-P-O3'	5.42	117.12	105.20
9	A	1430	G	N1-C6-O6	5.42	123.15	119.90
9	A	1350	C	C6-N1-C2	5.41	122.46	120.30
9	A	1759	A	N1-C6-N6	5.39	121.84	118.60
9	A	2439	A	N1-C6-N6	5.38	121.83	118.60
9	A	2015	A	N1-C6-N6	-5.38	115.38	118.60
9	A	1229	C	C6-N1-C2	5.37	122.45	120.30
9	A	2250	G	C2-N3-C4	-5.37	109.21	111.90
9	A	1950	G	C8-N9-C1'	-5.37	120.02	127.00
9	A	1311	G	N7-C8-N9	5.36	115.78	113.10
9	A	2353	G	C2-N3-C4	5.36	114.58	111.90
9	A	1129	A	O5'-P-OP1	-5.36	100.88	105.70
9	A	548	G	N3-C4-C5	-5.35	125.92	128.60
9	A	250	G	O5'-P-OP2	-5.35	100.88	105.70
9	A	1420	A	O4'-C1'-N9	5.35	112.48	108.20
9	A	1565	C	C6-N1-C2	-5.34	118.16	120.30
9	A	2571	U	C2-N1-C1'	-5.34	111.29	117.70
9	A	1831	G	C8-N9-C4	-5.34	104.27	106.40
24	P	113	LEU	CA-CB-CG	5.33	127.57	115.30
9	A	2544	G	N1-C6-O6	5.33	123.10	119.90
9	A	677	A	OP1-P-O3'	5.33	116.92	105.20
9	A	733	G	C8-N9-C4	-5.33	104.27	106.40
9	A	1190	G	C5-N7-C8	-5.33	101.64	104.30
9	A	2271	G	N1-C6-O6	5.33	123.10	119.90
9	A	940	G	N1-C6-O6	5.33	123.09	119.90
9	A	2508	G	C4-N9-C1'	5.33	133.42	126.50
9	A	1533	C	C5-C6-N1	5.32	123.66	121.00
9	A	2355	G	C8-N9-C4	5.32	108.53	106.40
6	5	50	VAL	CG1-CB-CG2	5.31	119.40	110.90
9	A	837	C	N1-C2-O2	-5.31	115.71	118.90
6	5	131	THR	N-CA-C	-5.31	96.67	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	2153	C	O4'-C1'-N1	5.31	112.45	108.20
9	A	776	G	C4-N9-C1'	5.30	133.39	126.50
9	A	1970	A	C8-N9-C4	-5.30	103.68	105.80
9	A	2015	A	N9-C4-C5	5.30	107.92	105.80
9	A	2250	G	N7-C8-N9	5.29	115.75	113.10
9	A	2470	G	OP2-P-O3'	5.29	116.84	105.20
9	A	2723	C	C6-N1-C2	-5.29	118.18	120.30
9	A	2508	G	O4'-C1'-N9	-5.29	103.97	108.20
9	A	84	A	N1-C6-N6	-5.29	115.43	118.60
9	A	518	G	O5'-P-OP1	-5.29	100.94	105.70
9	A	2071	A	OP2-P-O3'	5.29	116.83	105.20
9	A	2685	G	C5-C6-N1	-5.27	108.86	111.50
6	5	50	VAL	CA-CB-CG1	5.27	118.80	110.90
9	A	1131	G	OP1-P-O3'	5.27	116.80	105.20
9	A	1025	G	N3-C4-C5	-5.26	125.97	128.60
9	A	1458	U	P-O3'-C3'	5.25	126.00	119.70
9	A	2618	G	C5-C6-N1	-5.25	108.87	111.50
9	A	991	C	C6-N1-C2	-5.25	118.20	120.30
9	A	2368	C	C6-N1-C2	5.25	122.40	120.30
9	A	2501	C	C6-N1-C1'	5.24	127.09	120.80
25	Q	63	ARG	NE-CZ-NH2	-5.24	117.68	120.30
9	A	2518	A	N1-C6-N6	5.24	121.75	118.60
9	A	2508	G	C8-N9-C1'	-5.24	120.19	127.00
9	A	1684	G	N3-C4-C5	-5.24	125.98	128.60
34	Z	15	ARG	NE-CZ-NH1	5.24	122.92	120.30
32	X	29	LEU	CA-CB-CG	5.23	127.34	115.30
9	A	1264	A	O5'-P-OP1	-5.23	101.00	105.70
9	A	1355	G	C8-N9-C4	-5.22	104.31	106.40
9	A	2263	C	N3-C4-C5	-5.22	119.81	121.90
9	A	1025	G	C8-N9-C4	-5.21	104.31	106.40
9	A	1206	G	N3-C4-C5	-5.21	125.99	128.60
9	A	833	A	C8-N9-C4	-5.21	103.72	105.80
9	A	2825	G	N3-C4-N9	5.21	129.12	126.00
9	A	1936	A	N3-C4-C5	5.20	130.44	126.80
9	A	2534	A	C5-C6-N6	-5.20	119.54	123.70
9	A	1943	U	C5-C4-O4	5.20	129.02	125.90
9	A	699	A	N1-C6-N6	5.20	121.72	118.60
9	A	2537	U	C5-C4-O4	5.18	129.01	125.90
9	A	1446	C	C6-N1-C2	-5.18	118.23	120.30
9	A	2704	C	C6-N1-C2	5.18	122.37	120.30
9	A	748	G	C4-C5-N7	-5.18	108.73	110.80
9	A	2508	G	P-O5'-C5'	-5.17	112.62	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	119	A	P-O3'-C3'	5.17	125.90	119.70
9	A	465	G	C4-C5-C6	5.17	121.90	118.80
9	A	1395	A	O4'-C1'-N9	5.17	112.33	108.20
9	A	776	G	C4-C5-C6	5.16	121.90	118.80
9	A	1824	G	N9-C4-C5	5.16	107.47	105.40
6	5	130	PRO	CA-N-CD	-5.16	104.28	111.50
9	A	1355	G	N3-C2-N2	-5.16	116.29	119.90
9	A	454	A	O5'-P-OP2	-5.16	101.06	105.70
9	A	1928	A	N1-C6-N6	5.16	121.69	118.60
9	A	916	G	C6-C5-N7	-5.14	127.31	130.40
9	A	984	A	N1-C2-N3	5.14	131.87	129.30
9	A	2037	A	N9-C4-C5	5.14	107.85	105.80
9	A	1524	G	C8-N9-C4	-5.13	104.35	106.40
9	A	1238	G	O5'-P-OP2	-5.12	101.09	105.70
9	A	1639	C	C6-N1-C2	5.12	122.35	120.30
9	A	2198	A	O4'-C1'-N9	5.12	112.29	108.20
9	A	1452	G	C4-C5-N7	5.11	112.84	110.80
9	A	404	A	C8-N9-C4	-5.11	103.76	105.80
30	V	61	LEU	CA-CB-CG	5.11	127.05	115.30
9	A	1538	G	N3-C4-C5	5.11	131.15	128.60
9	A	1534	U	N1-C2-O2	5.10	126.37	122.80
9	A	2443	C	C6-N1-C2	-5.10	118.26	120.30
9	A	2422	C	N1-C2-O2	5.09	121.96	118.90
10	B	114	C	C5-C4-N4	-5.09	116.64	120.20
9	A	376	G	C6-C5-N7	-5.09	127.35	130.40
9	A	1122	G	N3-C4-N9	-5.08	122.95	126.00
17	I	79	LEU	CA-CB-CG	5.08	127.00	115.30
9	A	807	U	N3-C4-O4	5.08	122.96	119.40
9	A	1983	G	C5-C6-N1	-5.08	108.96	111.50
9	A	2537	U	N1-C2-N3	5.08	117.95	114.90
9	A	752	A	C2-N3-C4	-5.07	108.06	110.60
9	A	403	U	P-O3'-C3'	5.07	125.78	119.70
9	A	2455	G	O5'-P-OP2	-5.05	101.16	105.70
9	A	55	G	N1-C6-O6	5.05	122.93	119.90
9	A	467	G	N7-C8-N9	-5.04	110.58	113.10
9	A	1659	G	N3-C4-C5	5.04	131.12	128.60
9	A	686	U	C2-N1-C1'	-5.04	111.65	117.70
9	A	1779	U	C5-C6-N1	-5.04	120.18	122.70
9	A	2278	A	OP2-P-O3'	5.03	116.27	105.20
9	A	1533	C	C6-N1-C1'	-5.02	114.78	120.80
9	A	1979	U	C5-C6-N1	5.02	125.21	122.70
9	A	2396	G	N1-C6-O6	-5.02	116.89	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	2551	C	O5'-P-OP1	-5.02	101.19	105.70
28	T	29	THR	N-CA-C	5.02	124.54	111.00
9	A	1314	C	C5-C4-N4	-5.01	116.69	120.20
9	A	1606	C	P-O3'-C3'	5.01	125.72	119.70
9	A	2017	U	N3-C4-O4	5.01	122.91	119.40
9	A	1314	C	C2-N1-C1'	5.01	124.31	118.80
9	A	2015	A	C5-C6-N6	5.01	127.71	123.70
9	A	2902	C	P-O3'-C3'	5.01	125.71	119.70
9	A	745	G	N3-C4-N9	5.00	129.00	126.00
11	C	155	ARG	CG-CD-NE	5.00	122.31	111.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	5	130	PRO	Peptide
11	C	233	GLY	Peptide
12	D	9	VAL	Peptide
18	J	110	PRO	Peptide
19	K	71	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	444	0	461	16	0
2	1	409	0	440	15	0
3	2	377	0	418	5	0
4	3	504	0	574	10	0
5	4	302	0	340	14	0
6	5	1117	0	1155	123	0
7	6	227	0	237	6	0
8	7	58	0	33	12	0
9	A	61274	0	30817	801	0
10	B	2529	0	1281	20	0
11	C	2082	0	2157	54	0
12	D	1565	0	1616	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	E	1552	0	1619	40	0
14	F	1410	0	1447	44	0
15	G	1323	0	1374	37	0
16	H	384	0	405	12	0
17	I	1032	0	1088	53	0
18	J	1129	0	1162	50	0
19	K	938	0	1012	40	0
20	L	1045	0	1117	37	0
21	M	1074	0	1157	29	0
22	N	960	0	1000	30	0
23	O	892	0	923	21	0
24	P	917	0	965	38	0
25	Q	947	0	1022	52	0
26	R	816	0	839	35	0
27	S	857	0	922	28	0
28	T	738	0	807	33	0
29	U	779	0	834	27	0
30	V	753	0	780	12	0
31	W	596	0	610	80	0
32	X	625	0	655	18	0
33	Y	509	0	543	13	0
34	Z	449	0	491	15	0
35	a	36	0	34	0	0
36	A	51	0	67	8	0
All	All	90700	0	60402	1640	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 11.

All (1640) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:912:C:OP1	21:M:8:LYS:NZ	1.79	1.15
9:A:2062:A:N6	36:A:9000:ERY:H273	1.64	1.13
9:A:2061:G:OP2	13:E:63:LYS:NZ	1.88	1.06
6:5:71:CYS:HB3	6:5:117:LEU:HD12	1.33	1.04
9:A:2579:C:H2'	9:A:2580:U:H5'	1.40	1.03
9:A:2579:C:C2'	9:A:2580:U:H5'	1.88	1.02
9:A:2574:G:C2'	9:A:2575:C:H5'	1.90	1.01
6:5:3:LEU:O	6:5:7:ASP:OD1	1.79	1.00
6:5:26:VAL:HG21	6:5:115:GLY:H	1.23	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2063:C:C5	9:A:2064:C:C5	2.50	1.00
9:A:2574:G:H2'	9:A:2575:C:H5'	1.46	0.98
8:7:74:C:O2	9:A:2252:G:N2	1.97	0.97
9:A:2063:C:H2'	9:A:2064:C:H5'	1.48	0.95
9:A:2582:G:C2	9:A:2583:G:C8	2.55	0.94
6:5:117:LEU:CD2	6:5:120:ALA:HA	1.97	0.94
9:A:2600:A:H2'	9:A:2601:C:H5'	1.48	0.94
6:5:71:CYS:HB3	6:5:117:LEU:CD1	1.98	0.92
9:A:1154:G:OP2	25:Q:57:ARG:NH1	2.03	0.92
9:A:2580:U:H2'	9:A:2581:G:H5'	1.52	0.91
6:5:71:CYS:CB	6:5:117:LEU:HD12	2.00	0.91
9:A:1248:G:OP2	13:E:44:ARG:NH1	2.03	0.91
10:B:43:C:O2	14:F:91:ARG:NH2	2.04	0.90
9:A:2279:G:N7	31:W:10:ARG:NH2	2.20	0.90
29:U:98:ASN:O	29:U:100:GLU:N	2.06	0.89
9:A:1336:A:OP2	28:T:68:LYS:NZ	2.06	0.88
9:A:2582:G:N3	9:A:2583:G:C8	2.41	0.88
9:A:2600:A:C2'	9:A:2601:C:H5'	2.04	0.88
6:5:71:CYS:CB	6:5:117:LEU:CD1	2.50	0.88
9:A:996:A:OP2	25:Q:91:ARG:NH2	2.07	0.88
6:5:24:SER:HB2	6:5:116:GLU:HG2	1.54	0.87
9:A:2505:G:O2'	9:A:2506:U:H5"	1.75	0.87
9:A:2599:G:O2'	9:A:2600:A:H5'	1.74	0.87
9:A:2062:A:H62	36:A:9000:ERY:H273	1.33	0.86
28:T:39:THR:O	28:T:41:ALA:N	2.09	0.86
9:A:1723:G:O6	9:A:1737:G:O2'	1.94	0.85
9:A:2061:G:OP2	13:E:63:LYS:CE	2.24	0.84
6:5:71:CYS:HA	6:5:117:LEU:HD13	1.60	0.84
9:A:2053:G:N2	9:A:2616:C:N3	2.24	0.84
9:A:1069:A:N3	9:A:1073:A:N6	2.26	0.84
6:5:33:VAL:N	6:5:36:ASP:OD2	2.12	0.82
6:5:77:VAL:C	6:5:79:PRO:HD2	2.00	0.82
6:5:71:CYS:HA	6:5:117:LEU:CD1	2.09	0.82
9:A:2603:G:O2'	9:A:2604:U:H5'	1.80	0.82
9:A:504:A:O2'	9:A:505:A:OP1	1.98	0.81
24:P:50:ARG:HB3	24:P:57:ALA:H	1.43	0.81
23:O:34:HIS:O	23:O:102:ARG:NH1	2.14	0.81
6:5:103:ASN:ND2	6:5:107:GLU:O	2.13	0.81
11:C:196:ASN:O	11:C:198:GLU:N	2.12	0.81
9:A:1782:U:O2	9:A:2608:G:O2'	1.97	0.80
9:A:2576:G:O2'	9:A:2577:A:O5'	1.98	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1012:U:OP2	25:Q:69:ARG:NH1	2.14	0.80
9:A:2576:G:N3	9:A:2576:G:H5'	1.97	0.79
9:A:2720:U:OP1	24:P:52:ARG:NH2	2.15	0.79
6:5:33:VAL:HG12	6:5:34:THR:H	1.48	0.79
6:5:43:LYS:NZ	6:5:98:GLU:OE1	2.16	0.79
9:A:2579:C:O2'	9:A:2580:U:H5'	1.82	0.79
9:A:2576:G:H4'	9:A:2577:A:OP1	1.80	0.78
9:A:2585:U:H5'	9:A:2586:U:OP2	1.83	0.78
8:7:76:A:C6	9:A:2451:A:H4'	2.18	0.78
6:5:91:ALA:C	6:5:93:ALA:H	1.87	0.78
9:A:2581:G:O2'	9:A:2610:C:N4	2.15	0.78
19:K:105:ARG:NH1	19:K:106:GLU:OE2	2.16	0.78
33:Y:18:LEU:O	33:Y:22:LEU:N	2.17	0.78
6:5:71:CYS:CA	6:5:117:LEU:CD1	2.62	0.77
9:A:1799:G:OP2	11:C:269:ARG:NH2	2.16	0.77
9:A:1509:A:O2'	9:A:1510:G:OP2	2.01	0.77
6:5:117:LEU:HD23	6:5:120:ALA:HA	1.65	0.77
9:A:2063:C:H2'	9:A:2064:C:C5'	2.15	0.77
6:5:35:VAL:HA	6:5:38:MET:SD	2.24	0.77
9:A:2611:C:H2'	9:A:2612:C:H6	1.47	0.77
12:D:184:ARG:NH1	24:P:6:GLN:OE1	2.17	0.77
9:A:2581:G:H2'	9:A:2581:G:N3	2.00	0.77
11:C:68:ARG:NH2	11:C:126:GLY:O	2.18	0.76
11:C:69:ASN:O	11:C:71:ASP:N	2.18	0.76
9:A:2580:U:C2'	9:A:2581:G:H5'	2.15	0.76
9:A:1187:G:OP1	26:R:85:LYS:NZ	2.19	0.75
6:5:131:THR:O	6:5:134:GLU:N	2.20	0.75
9:A:1342:A:O2'	9:A:1344:U:OP2	2.04	0.75
9:A:572:A:OP2	26:R:80:ARG:NH2	2.21	0.74
6:5:57:ASN:O	6:5:59:LEU:N	2.21	0.74
9:A:2592:G:N1	9:A:2603:G:C6	2.55	0.74
12:D:91:THR:O	12:D:93:GLY:N	2.21	0.74
5:4:11:CYS:SG	5:4:14:CYS:N	2.60	0.74
9:A:2707:U:O2	22:N:71:ARG:NH1	2.20	0.73
9:A:1998:A:OP2	12:D:141:ARG:NH2	2.21	0.73
9:A:2611:C:H2'	9:A:2612:C:C6	2.24	0.73
9:A:2331:G:O2'	31:W:39:GLN:O	2.04	0.73
18:J:43:GLU:O	18:J:45:THR:N	2.22	0.73
9:A:1799:G:O2'	11:C:179:GLU:OE2	2.07	0.72
15:G:22:VAL:HG12	15:G:36:LEU:CD1	2.19	0.72
9:A:2061:G:H4'	9:A:2061:G:OP1	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2579:C:H2'	9:A:2580:U:C5'	2.17	0.72
6:5:106:PHE:O	6:5:108:VAL:N	2.23	0.71
9:A:2060:A:O2'	9:A:2061:G:OP2	2.08	0.71
24:P:5:LYS:NZ	24:P:9:GLN:OE1	2.23	0.71
6:5:1:MET:SD	6:5:2:ALA:N	2.58	0.71
9:A:2063:C:C6	9:A:2064:C:C5	2.78	0.71
9:A:2599:G:C2'	9:A:2600:A:H5'	2.20	0.71
9:A:1993:U:H4'	12:D:133:THR:HG21	1.73	0.70
9:A:1805:A:N3	11:C:49:THR:OG1	2.24	0.70
8:7:76:A:C6	9:A:2451:A:C4'	2.74	0.70
9:A:161:A:H3'	9:A:162:U:H5"	1.72	0.70
5:4:2:LYS:NZ	9:A:2478:A:OP2	2.23	0.70
9:A:2353:G:H1'	31:W:30:VAL:HG12	1.72	0.70
9:A:2580:U:H2'	9:A:2581:G:C5'	2.20	0.70
9:A:971:G:OP2	9:A:974:G:N2	2.25	0.70
14:F:116:LEU:N	14:F:176:PHE:O	2.24	0.69
9:A:587:C:OP2	20:L:21:ARG:NH1	2.25	0.69
9:A:1783:A:N1	9:A:2587:A:H2'	2.07	0.69
9:A:2503:A:H3'	9:A:2503:A:OP2	1.92	0.69
9:A:2502:G:C5'	9:A:2503:A:H5"	2.22	0.69
21:M:66:ARG:NH1	21:M:104:GLU:OE1	2.26	0.69
34:Z:8:GLN:O	34:Z:10:ARG:N	2.25	0.69
9:A:2324:U:H3'	9:A:2325:G:H5"	1.74	0.68
6:5:26:VAL:O	6:5:27:VAL:HB	1.93	0.68
6:5:25:ALA:O	6:5:26:VAL:HG13	1.94	0.68
6:5:129:LEU:O	6:5:131:THR:N	2.26	0.68
9:A:2061:G:N7	9:A:2501:C:H1'	2.09	0.68
9:A:2582:G:H2'	9:A:2583:G:H5'	1.75	0.68
9:A:2592:G:C2	9:A:2603:G:C6	2.82	0.68
9:A:1820:U:OP1	11:C:176:ARG:NH2	2.27	0.68
9:A:1936:A:N6	9:A:1963:U:O2	2.26	0.68
17:I:100:ILE:HB	17:I:139:VAL:HA	1.75	0.68
9:A:2091:C:O2	32:X:33:HIS:NE2	2.26	0.68
6:5:24:SER:CB	6:5:116:GLU:HG2	2.24	0.68
9:A:301:G:OP2	29:U:81:ARG:NH1	2.26	0.68
12:D:149:ASN:OD1	12:D:150:GLN:N	2.26	0.68
20:L:93:ASN:O	20:L:95:LEU:N	2.27	0.67
10:B:73:A:C4	10:B:104:A:C2	2.82	0.67
9:A:2062:A:H62	36:A:9000:ERY:C27	2.05	0.67
18:J:4:PHE:N	18:J:44:TYR:OH	2.28	0.67
6:5:117:LEU:HD22	6:5:120:ALA:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:948:C:O2	9:A:984:A:O2'	2.12	0.67
19:K:76:VAL:HB	24:P:72:VAL:HG22	1.76	0.66
9:A:324:A:N6	9:A:338:G:O2'	2.27	0.66
19:K:18:ARG:HB2	19:K:45:GLU:HB2	1.77	0.66
20:L:93:ASN:OD1	20:L:94:THR:N	2.28	0.66
31:W:30:VAL:HG13	31:W:30:VAL:O	1.92	0.66
8:7:76:A:N6	9:A:2451:A:H4'	2.10	0.66
9:A:42:A:C2'	9:A:43:G:H5'	2.25	0.66
9:A:2142:A:H4'	9:A:2143:C:OP2	1.96	0.66
9:A:2063:C:C5	9:A:2064:C:C4	2.84	0.66
19:K:71:ARG:HB3	19:K:72:PRO:HD3	1.78	0.65
31:W:37:VAL:HG12	31:W:38:ARG:H	1.61	0.65
9:A:2582:G:C2'	9:A:2583:G:H5'	2.26	0.65
22:N:118:ARG:O	22:N:120:GLU:N	2.30	0.65
6:5:39:THR:HA	6:5:42:ARG:HD2	1.78	0.65
9:A:363:G:H2'	9:A:364:C:C6	2.32	0.65
8:7:76:A:N3	9:A:2451:A:H1'	2.12	0.65
9:A:2061:G:C2	9:A:2063:C:C4	2.84	0.65
9:A:2576:G:N3	9:A:2576:G:H3'	2.11	0.65
9:A:2503:A:H4'	9:A:2504:U:OP1	1.96	0.65
23:O:76:LYS:NZ	23:O:80:GLU:OE1	2.29	0.64
9:A:2604:U:O5'	9:A:2604:U:H6	1.80	0.64
11:C:43:ASN:OD1	11:C:44:ASN:N	2.30	0.64
9:A:1199:U:H5'	25:Q:4:LYS:HE3	1.79	0.64
13:E:58:LYS:NZ	13:E:70:SER:O	2.31	0.64
24:P:50:ARG:HG3	24:P:57:ALA:O	1.97	0.64
9:A:819:A:OP2	9:A:1187:G:N2	2.23	0.64
15:G:38:ASP:N	15:G:38:ASP:OD1	2.29	0.64
9:A:2063:C:C5	9:A:2064:C:H5	2.08	0.64
24:P:4:ILE:O	24:P:6:GLN:N	2.31	0.64
27:S:18:ARG:O	27:S:19:LEU:HB2	1.98	0.64
8:7:76:A:N1	9:A:2451:A:O4'	2.31	0.64
9:A:1482:G:H1'	9:A:1509:A:H61	1.62	0.63
10:B:87:U:H3'	10:B:88:C:H5'	1.80	0.63
29:U:73:ASN:ND2	29:U:80:ASP:OD2	2.31	0.63
8:7:75:C:O5'	8:7:75:C:H6	1.81	0.63
9:A:1417:C:HO2'	9:A:1587:G:HO2'	1.45	0.63
15:G:1:SER:O	15:G:3:VAL:N	2.31	0.63
18:J:44:TYR:HB2	25:Q:63:ARG:HB3	1.79	0.63
9:A:2502:G:C5'	9:A:2503:A:C5'	2.76	0.63
18:J:6:ALA:HB3	18:J:45:THR:HG21	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:42:ILE:HD11	22:N:98:LEU:HB3	1.79	0.63
9:A:861:A:N3	10:B:79:G:O2'	2.27	0.63
9:A:1813:G:H1'	11:C:49:THR:HG21	1.81	0.63
9:A:2608:G:O5'	9:A:2608:G:H8	1.82	0.63
9:A:2346:A:H3'	9:A:2347:C:C5'	2.29	0.63
31:W:35:ILE:O	31:W:37:VAL:N	2.31	0.63
17:I:108:ILE:O	17:I:111:THR:OG1	2.17	0.63
9:A:1385:A:H1'	9:A:1386:C:C6	2.34	0.63
31:W:9:THR:OG1	31:W:10:ARG:N	2.31	0.62
9:A:2062:A:O2'	9:A:2063:C:O5'	2.17	0.62
17:I:131:THR:O	17:I:134:SER:OG	2.16	0.62
9:A:923:G:H1'	31:W:23:LYS:HD3	1.81	0.62
17:I:73:PRO:O	17:I:112:LYS:NZ	2.31	0.62
29:U:15:GLY:O	29:U:17:ASP:N	2.32	0.62
9:A:42:A:H2'	9:A:43:G:H5'	1.80	0.62
9:A:163:C:O2'	9:A:164:C:O5'	2.17	0.62
24:P:50:ARG:CB	24:P:57:ALA:H	2.11	0.62
9:A:546:U:O2'	9:A:547:A:H4'	1.99	0.62
9:A:2063:C:C6	9:A:2064:C:H5	2.17	0.62
22:N:73:ASN:HA	22:N:76:VAL:HG12	1.81	0.61
9:A:856:G:H21	31:W:19:ARG:NH1	1.97	0.61
9:A:1248:G:N7	13:E:46:GLN:NE2	2.48	0.61
9:A:2603:G:C2	9:A:2604:U:C2	2.88	0.61
28:T:32:LEU:H	28:T:83:ALA:HB3	1.63	0.61
9:A:2060:A:O2'	13:E:63:LYS:NZ	2.32	0.61
6:5:29:ASP:HA	6:5:108:VAL:HG11	1.82	0.61
9:A:1567:G:H5'	11:C:57:HIS:CD2	2.35	0.61
22:N:98:LEU:O	22:N:112:TYR:N	2.34	0.61
6:5:26:VAL:HG21	6:5:115:GLY:N	2.06	0.61
9:A:1930:G:O2'	9:A:1968:G:O6	2.17	0.61
5:4:36:ARG:HG2	5:4:37:GLN:H	1.66	0.61
6:5:27:VAL:HG13	6:5:83:ALA:HB3	1.83	0.61
9:A:616:A:H4'	13:E:101:TYR:CE2	2.36	0.61
12:D:118:PHE:HD1	12:D:119:ALA:H	1.49	0.60
9:A:2502:G:H5"	9:A:2503:A:H5"	1.81	0.60
17:I:100:ILE:HG22	17:I:101:SER:N	2.15	0.60
9:A:2502:G:H5'	9:A:2503:A:C5'	2.31	0.60
9:A:276:U:O2'	9:A:278:A:N7	2.34	0.60
9:A:1338:G:O2'	28:T:18:GLU:OE1	2.20	0.60
9:A:2011:U:OP2	27:S:16:LYS:NZ	2.31	0.60
23:O:105:ALA:O	23:O:107:ALA:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:480:A:OP2	29:U:43:LYS:NZ	2.34	0.60
9:A:2581:G:HO2'	9:A:2610:C:H41	1.49	0.60
7:6:18:ASP:OD1	7:6:18:ASP:N	2.32	0.60
9:A:983:A:C6	9:A:984:A:C2	2.90	0.60
9:A:2579:C:C2'	9:A:2580:U:C5'	2.72	0.60
9:A:2595:G:N1	9:A:2599:G:C6	2.70	0.60
18:J:6:ALA:CB	18:J:45:THR:HG21	2.31	0.60
9:A:27:G:O2'	9:A:28:A:OP2	2.19	0.60
6:5:15:VAL:HG22	6:5:66:GLY:HA3	1.84	0.60
9:A:1262:A:OP2	27:S:99:ARG:NH2	2.35	0.60
9:A:2353:G:N3	31:W:30:VAL:CG1	2.65	0.60
9:A:2681:C:OP2	12:D:114:LYS:NZ	2.33	0.60
31:W:55:ASP:O	31:W:57:THR:N	2.34	0.60
9:A:635:C:OP2	20:L:126:ARG:NH1	2.35	0.59
9:A:2502:G:H5'	9:A:2503:A:H5"	1.82	0.59
11:C:16:VAL:N	11:C:203:VAL:HG12	2.18	0.59
23:O:89:ASP:HA	23:O:116:GLN:HB3	1.84	0.59
9:A:947:A:HO2'	9:A:984:A:H2	1.50	0.59
9:A:1803:A:O3'	11:C:256:THR:OG1	2.19	0.59
9:A:2592:G:N2	9:A:2603:G:C5	2.70	0.59
9:A:2800:A:H3'	9:A:2801:G:C5'	2.32	0.59
29:U:38:ILE:CG2	29:U:39:ASN:N	2.64	0.59
31:W:51:GLY:HA3	31:W:59:PHE:CE1	2.38	0.59
8:7:76:A:C4	9:A:2451:A:H1'	2.38	0.59
17:I:92:PRO:O	17:I:94:LYS:N	2.36	0.59
17:I:93:ASN:ND2	17:I:135:MET:O	2.36	0.59
24:P:63:ILE:HA	24:P:68:GLY:HA2	1.85	0.59
9:A:370:G:O2'	9:A:424:G:OP1	2.15	0.58
9:A:1076:C:H2'	9:A:1077:A:O4'	2.03	0.58
9:A:2063:C:C2'	9:A:2064:C:H5'	2.26	0.58
9:A:2780:G:OP2	18:J:120:ARG:NE	2.33	0.58
28:T:35:ALA:HB3	28:T:38:ALA:HB2	1.85	0.58
9:A:2581:G:HO2'	9:A:2610:C:H5	1.50	0.58
28:T:19:LYS:O	28:T:23:ALA:N	2.35	0.58
9:A:1131:G:OP1	18:J:82:GLY:HA2	2.02	0.58
25:Q:63:ARG:NH1	25:Q:95:ALA:O	2.35	0.58
6:5:62:ARG:NH2	9:A:1106:G:OP1	2.35	0.58
31:W:76:ARG:HH21	31:W:76:ARG:CG	2.16	0.58
5:4:2:LYS:HZ1	9:A:2478:A:P	2.27	0.58
9:A:784:G:O2'	9:A:785:G:OP2	2.15	0.58
25:Q:84:LYS:O	25:Q:86:SER:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:168:ASP:OD2	13:E:170:ARG:NH2	2.36	0.58
9:A:1076:C:H1'	17:I:93:ASN:HB3	1.86	0.58
28:T:54:GLU:HG3	28:T:88:LYS:HB2	1.86	0.58
31:W:51:GLY:HA3	31:W:59:PHE:CZ	2.38	0.58
9:A:2582:G:C2	9:A:2583:G:N7	2.71	0.58
6:5:45:GLY:HA2	6:5:49:GLY:HA2	1.85	0.57
9:A:2574:G:O2'	9:A:2575:C:H5'	2.04	0.57
9:A:1386:C:H2'	9:A:1387:A:C8	2.39	0.57
9:A:2517:C:C6	9:A:2542:A:N7	2.72	0.57
21:M:41:LEU:HD11	21:M:126:ILE:HD13	1.85	0.57
9:A:2061:G:C2	9:A:2063:C:N3	2.72	0.57
9:A:422:A:C2	9:A:423:A:C4	2.92	0.57
9:A:1936:A:H2	9:A:1943:U:C5	2.23	0.57
11:C:77:VAL:HG23	11:C:111:ALA:HA	1.86	0.57
25:Q:63:ARG:HH22	25:Q:95:ALA:C	2.08	0.57
25:Q:81:GLY:O	25:Q:85:ALA:N	2.37	0.57
9:A:2331:G:O2'	9:A:2336:A:N1	2.38	0.57
17:I:37:PHE:O	17:I:41:PHE:HB3	2.04	0.57
18:J:49:ASP:OD1	18:J:121:LYS:NZ	2.32	0.57
31:W:28:GLU:HB3	31:W:31:LEU:HD21	1.86	0.57
8:7:76:A:C2	9:A:2451:A:O4'	2.57	0.57
9:A:673:C:OP1	13:E:49:ARG:NH2	2.36	0.57
9:A:1654:A:O2'	12:D:118:PHE:CG	2.55	0.57
9:A:2063:C:C5	9:A:2064:C:N4	2.73	0.57
13:E:150:THR:HG21	13:E:153:LEU:HA	1.87	0.57
6:5:3:LEU:CD1	6:5:5:LEU:HG	2.35	0.56
9:A:1324:G:C4	9:A:1328:A:N6	2.73	0.56
9:A:1509:A:HO2'	9:A:1510:G:P	2.26	0.56
9:A:2583:G:N2	9:A:2584:U:C2	2.73	0.56
11:C:14:HIS:O	11:C:203:VAL:HG11	2.05	0.56
24:P:58:PHE:CD1	24:P:75:THR:HG22	2.40	0.56
31:W:39:GLN:HG2	31:W:41:GLY:H	1.69	0.56
9:A:2548:U:O2	19:K:23:LYS:NZ	2.37	0.56
17:I:100:ILE:HD11	17:I:137:LEU:HG	1.87	0.56
19:K:121:GLU:OE1	24:P:62:LYS:NZ	2.37	0.56
25:Q:105:PHE:O	25:Q:108:LEU:N	2.38	0.56
2:1:8:ILE:HD11	2:1:24:LYS:N	2.21	0.56
9:A:2574:G:H2'	9:A:2575:C:C5'	2.30	0.56
9:A:1773:A:N7	9:A:1829:A:H1'	2.20	0.56
32:X:32:LEU:O	32:X:33:HIS:ND1	2.39	0.56
9:A:2680:U:H5'	12:D:194:PRO:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Y:56:LEU:O	33:Y:58:ASN:N	2.39	0.56
6:5:58:THR:CG2	9:A:1107:G:H5"	2.36	0.56
6:5:132:TYR:CZ	7:6:23:ILE:HD11	2.40	0.56
9:A:2061:G:OP2	13:E:63:LYS:HE2	2.06	0.56
9:A:85:G:OP2	29:U:6:ARG:HG3	2.06	0.56
9:A:443:A:N7	13:E:40:ARG:HD3	2.21	0.56
9:A:1353:A:C8	9:A:1378:A:N6	2.73	0.56
18:J:81:ILE:HG13	18:J:82:GLY:N	2.21	0.56
24:P:50:ARG:HB3	24:P:57:ALA:N	2.17	0.56
9:A:100:U:H4'	9:A:101:A:O5'	2.06	0.55
9:A:2502:G:H5"	9:A:2503:A:C5'	2.36	0.55
9:A:2585:U:C4	9:A:2608:G:O6	2.59	0.55
9:A:2603:G:H2'	9:A:2604:U:C6	2.41	0.55
17:I:135:MET:HB3	17:I:137:LEU:HD22	1.88	0.55
28:T:59:ASN:O	28:T:83:ALA:O	2.24	0.55
6:5:64:VAL:O	6:5:68:PRO:HD2	2.06	0.55
9:A:1750:G:O2'	9:A:2860:A:N1	2.37	0.55
14:F:151:LEU:HD12	14:F:152:ASP:N	2.21	0.55
20:L:85:VAL:CG2	20:L:94:THR:HG22	2.36	0.55
31:W:18:LYS:HG3	31:W:19:ARG:N	2.21	0.55
6:5:129:LEU:C	6:5:131:THR:H	2.10	0.55
9:A:811:U:C4	20:L:21:ARG:NH2	2.74	0.55
6:5:43:LYS:HZ3	6:5:98:GLU:HB2	1.71	0.55
23:O:2:ASP:OD1	23:O:3:LYS:N	2.39	0.55
6:5:56:ARG:O	6:5:57:ASN:ND2	2.39	0.55
17:I:116:MET:SD	17:I:124:MET:HE2	2.47	0.55
18:J:17:VAL:HG23	18:J:139:VAL:HA	1.88	0.55
26:R:39:LEU:O	26:R:49:ILE:HG23	2.07	0.55
28:T:32:LEU:N	28:T:83:ALA:HB3	2.21	0.55
9:A:1019:U:H3	9:A:1142:A:H62	1.53	0.55
9:A:1397:U:OP2	9:A:1398:C:N4	2.34	0.55
12:D:118:PHE:O	12:D:120:GLY:N	2.36	0.55
9:A:1482:G:C6	9:A:1508:A:C2	2.94	0.55
9:A:2061:G:C4	9:A:2063:C:N4	2.75	0.55
9:A:2582:G:N2	9:A:2583:G:N9	2.55	0.55
9:A:283:G:C2	9:A:284:U:H1'	2.41	0.55
1:0:2:VAL:HG22	9:A:2015:A:C2	2.41	0.55
5:4:36:ARG:NH1	9:A:2742:G:OP1	2.38	0.55
9:A:2355:G:H4'	31:W:20:LEU:HD13	1.88	0.55
22:N:30:ARG:NH1	22:N:74:GLU:OE1	2.40	0.55
9:A:834:G:C6	9:A:835:C:C4	2.95	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2506:U:H6	9:A:2506:U:H3'	1.72	0.54
9:A:2757:A:N1	15:G:66:THR:HG21	2.21	0.54
12:D:107:VAL:CG2	12:D:203:VAL:HG23	2.38	0.54
6:5:81:LEU:HA	9:A:1107:G:H4'	1.88	0.54
9:A:1458:U:H4'	9:A:1459:G:O5'	2.07	0.54
9:A:2698:U:H2'	9:A:2699:C:H6	1.72	0.54
11:C:68:ARG:CD	11:C:103:ILE:HD11	2.37	0.54
25:Q:91:ARG:NH1	26:R:10:LYS:HB3	2.23	0.54
6:5:44:ALA:O	6:5:49:GLY:N	2.40	0.54
9:A:1715:G:N2	9:A:1744:A:OP2	2.36	0.54
9:A:1754:A:H4'	24:P:102:ARG:NH2	2.22	0.54
9:A:2576:G:HO2'	9:A:2577:A:P	2.30	0.54
19:K:107:LEU:O	19:K:109:SER:N	2.38	0.54
1:0:2:VAL:HG11	9:A:2016:U:H1'	1.89	0.54
6:5:129:LEU:HB3	6:5:130:PRO:HD2	1.89	0.54
9:A:396:G:OP2	32:X:9:LYS:NZ	2.40	0.54
9:A:674:G:H1'	13:E:69:ARG:HE	1.72	0.54
9:A:1786:A:H1'	9:A:1938:A:N6	2.22	0.54
9:A:2415:G:H4'	20:L:66:PHE:HB2	1.90	0.54
9:A:277:G:O2'	9:A:278:A:OP2	2.25	0.54
9:A:686:U:H2'	9:A:788:A:N1	2.21	0.54
9:A:877:A:C2	9:A:899:A:C2	2.95	0.54
9:A:1936:A:N6	9:A:1963:U:H3	2.05	0.54
9:A:2335:A:C6	9:A:2337:G:H1'	2.42	0.54
9:A:2533:U:OP1	9:A:2665:A:O2'	2.20	0.54
21:M:33:LEU:HD22	21:M:128:THR:HB	1.90	0.54
24:P:33:GLU:HB2	24:P:38:ARG:HH11	1.71	0.54
29:U:38:ILE:HG22	29:U:39:ASN:H	1.73	0.54
30:V:80:HIS:HD2	30:V:83:LYS:N	2.05	0.54
9:A:1824:G:N3	11:C:251:THR:HG21	2.21	0.54
15:G:84:LYS:HG3	15:G:132:LEU:H	1.73	0.54
24:P:50:ARG:CG	24:P:57:ALA:O	2.55	0.54
6:5:60:LEU:O	6:5:64:VAL:HB	2.08	0.54
9:A:163:C:O2'	9:A:164:C:P	2.65	0.54
12:D:12:THR:OG1	24:P:8:GLU:OE2	2.21	0.54
19:K:80:ASP:HB2	24:P:67:GLU:HG3	1.90	0.54
34:Z:5:LYS:H	34:Z:5:LYS:HD2	1.72	0.54
6:5:23:LEU:HG	6:5:24:SER:N	2.22	0.54
6:5:54:VAL:HA	6:5:84:TYR:O	2.07	0.54
6:5:58:THR:HB	6:5:82:ILE:HB	1.89	0.54
9:A:910:A:N6	9:A:2277:G:O2'	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1779:U:H5	9:A:1784:A:N7	2.06	0.54
9:A:2580:U:O2'	9:A:2581:G:H5'	2.08	0.54
20:L:77:ILE:CD1	20:L:108:ALA:HB1	2.38	0.54
24:P:4:ILE:HG22	24:P:5:LYS:H	1.72	0.54
25:Q:81:GLY:HA2	25:Q:116:LEU:CD1	2.38	0.54
28:T:50:LEU:C	28:T:52:GLU:H	2.11	0.54
9:A:84:A:P	29:U:5:ARG:NH2	2.81	0.54
9:A:411:G:OP2	9:A:2406:A:O2'	2.25	0.54
9:A:1772:A:N1	9:A:1980:G:C6	2.75	0.54
12:D:106:LYS:HB3	12:D:206:ALA:HB3	1.89	0.54
14:F:103:ILE:HG23	14:F:175:PRO:HD3	1.90	0.54
18:J:32:LEU:HD22	18:J:54:ILE:HD12	1.90	0.54
19:K:43:ILE:CD1	19:K:52:VAL:HB	2.37	0.54
25:Q:93:ILE:O	25:Q:96:ASP:N	2.39	0.54
26:R:49:ILE:HB	26:R:51:VAL:O	2.08	0.54
9:A:855:G:H1'	31:W:23:LYS:HE3	1.89	0.54
29:U:21:ARG:CZ	29:U:72:PHE:CE2	2.90	0.53
9:A:384:A:H2'	9:A:385:C:H5'	1.91	0.53
9:A:1187:G:H5"	26:R:83:TYR:CE2	2.44	0.53
31:W:46:ALA:HB3	31:W:80:SER:HB3	1.91	0.53
5:4:1:MET:N	9:A:2526:G:N3	2.57	0.53
9:A:2505:G:C2'	9:A:2506:U:H5"	2.38	0.53
9:A:189:G:O6	9:A:205:G:O2'	2.19	0.53
9:A:265:A:H4'	9:A:266:G:OP1	2.07	0.53
9:A:2586:U:O2	9:A:2586:U:H2'	2.07	0.53
12:D:120:GLY:HA2	12:D:162:ALA:CB	2.38	0.53
19:K:10:VAL:HG11	19:K:16:ALA:HB3	1.90	0.53
27:S:73:LYS:HB3	27:S:106:VAL:HB	1.90	0.53
17:I:98:GLY:HA3	17:I:137:LEU:HB3	1.90	0.53
25:Q:65:ASN:OD1	25:Q:69:ARG:NH2	2.42	0.53
26:R:49:ILE:HG22	26:R:54:VAL:HG13	1.89	0.53
9:A:954:G:OP2	21:M:16:ARG:NH2	2.42	0.53
15:G:84:LYS:HB3	15:G:132:LEU:O	2.09	0.53
18:J:39:LYS:HA	18:J:43:GLU:HG3	1.91	0.53
1:0:12:ARG:NH1	9:A:1263:U:OP1	2.41	0.53
6:5:4:ASN:O	6:5:6:GLN:N	2.41	0.53
6:5:25:ALA:HB3	6:5:85:SER:OG	2.09	0.53
9:A:630:G:N2	9:A:633:A:OP2	2.37	0.53
9:A:2425:A:H5"	9:A:2427:C:O4'	2.09	0.53
9:A:2505:G:HO2'	9:A:2506:U:H5"	1.70	0.53
28:T:50:LEU:HD12	28:T:50:LEU:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:273:G:N2	9:A:365:U:C2	2.77	0.53
9:A:1069:A:C4	9:A:1073:A:N7	2.77	0.53
9:A:1080:A:H1'	17:I:127:SER:HA	1.91	0.53
9:A:2053:G:H1	9:A:2616:C:H42	1.57	0.53
9:A:2547:A:H2'	9:A:2548:U:C6	2.43	0.53
24:P:50:ARG:CD	24:P:51:ASN:N	2.72	0.53
25:Q:63:ARG:HH12	25:Q:96:ASP:CA	2.22	0.53
9:A:1535:A:H4'	9:A:1536:C:OP2	2.08	0.53
9:A:2297:A:N1	9:A:2321:U:H5	2.07	0.53
23:O:31:THR:HG22	23:O:34:HIS:H	1.74	0.53
28:T:50:LEU:O	28:T:52:GLU:N	2.42	0.53
34:Z:48:ASN:O	34:Z:51:SER:OG	2.27	0.53
6:5:81:LEU:HD23	6:5:82:ILE:N	2.24	0.52
9:A:2092:U:H4'	9:A:2093:G:O5'	2.09	0.52
23:O:36:TYR:N	23:O:36:TYR:CD1	2.78	0.52
31:W:13:ARG:HG2	31:W:14:ASP:H	1.73	0.52
31:W:37:VAL:HG13	31:W:55:ASP:C	2.29	0.52
9:A:1069:A:C5	9:A:1073:A:N7	2.77	0.52
9:A:1738:G:O2'	9:A:1739:A:O5'	2.25	0.52
9:A:2582:G:H2'	9:A:2583:G:H8	1.74	0.52
25:Q:31:TYR:O	25:Q:34:ALA:N	2.42	0.52
28:T:89:GLU:O	28:T:91:GLN:N	2.41	0.52
31:W:37:VAL:HB	31:W:38:ARG:HH11	1.74	0.52
1:0:2:VAL:CG1	9:A:2016:U:H1'	2.40	0.52
8:7:76:A:C2	9:A:2451:A:C1'	2.92	0.52
8:7:76:A:C2	9:A:2451:A:H1'	2.45	0.52
9:A:2232:C:P	32:X:26:ARG:HH22	2.32	0.52
22:N:73:ASN:HA	22:N:76:VAL:CG1	2.39	0.52
9:A:1288:G:C4	9:A:1327:A:C2	2.98	0.52
19:K:70:ARG:HD3	19:K:76:VAL:HG22	1.90	0.52
6:5:43:LYS:NZ	6:5:98:GLU:HB2	2.24	0.52
6:5:118:ILE:HB	6:5:119:PRO:CD	2.40	0.52
9:A:1328:A:H2'	9:A:1330:C:C5	2.45	0.52
2:1:33:LEU:N	2:1:51:ALA:HB3	2.25	0.52
9:A:2211:A:O2'	9:A:2212:A:OP1	2.25	0.52
26:R:61:ALA:HB2	26:R:98:ILE:HA	1.92	0.52
28:T:44:LYS:HG3	28:T:55:VAL:HG11	1.90	0.52
29:U:35:VAL:HB	29:U:38:ILE:HG21	1.90	0.52
29:U:82:VAL:HG12	29:U:83:GLY:N	2.25	0.52
34:Z:6:ILE:O	34:Z:34:THR:HA	2.10	0.52
5:4:7:VAL:O	5:4:35:GLN:NE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:36:ASP:O	6:5:39:THR:OG1	2.26	0.52
9:A:2504:U:O5'	9:A:2504:U:H6	1.93	0.52
9:A:2507:C:O2	9:A:2507:C:H2'	2.08	0.52
18:J:39:LYS:HA	18:J:43:GLU:HB2	1.91	0.52
18:J:55:ILE:HD11	18:J:130:HIS:CG	2.44	0.52
9:A:38:A:O2'	13:E:43:THR:HA	2.09	0.52
9:A:974:G:H8	9:A:990:A:H62	1.58	0.52
9:A:2354:C:H4'	31:W:31:LEU:HD22	1.92	0.52
11:C:256:THR:OG1	11:C:256:THR:O	2.28	0.52
9:A:729:G:H2'	9:A:1775:U:H1'	1.91	0.51
9:A:1759:A:HO2'	9:A:2714:G:HO2'	1.47	0.51
9:A:2039:U:H2'	9:A:2040:G:C8	2.45	0.51
9:A:2134:A:HO2'	9:A:2135:A:H8	1.56	0.51
9:A:2313:C:H5"	14:F:87:LYS:HD3	1.92	0.51
11:C:255:LYS:O	11:C:257:ARG:N	2.43	0.51
12:D:151:THR:HG22	12:D:152:PRO:HD3	1.92	0.51
15:G:83:THR:HA	15:G:84:LYS:CE	2.39	0.51
19:K:13:ASN:O	19:K:15:GLY:N	2.43	0.51
21:M:53:MET:HE3	21:M:63:ILE:HD13	1.92	0.51
24:P:33:GLU:CD	24:P:34:GLY:N	2.63	0.51
31:W:8:SER:O	31:W:9:THR:HG22	2.10	0.51
6:5:3:LEU:HD12	6:5:5:LEU:H	1.76	0.51
9:A:2061:G:C2	9:A:2063:C:N4	2.78	0.51
9:A:2604:U:H2'	9:A:2605:U:C6	2.45	0.51
9:A:2387:U:O2'	31:W:38:ARG:NH2	2.43	0.51
9:A:2803:G:H2'	9:A:2804:U:C6	2.45	0.51
20:L:91:ASP:OD1	20:L:92:LEU:N	2.43	0.51
21:M:73:ILE:HG21	21:M:91:TYR:CZ	2.45	0.51
15:G:96:ALA:HB3	15:G:103:ASN:HB2	1.92	0.51
30:V:44:HIS:HE1	30:V:86:LEU:H	1.59	0.51
30:V:51:GLN:OE1	30:V:57:TYR:OH	2.28	0.51
6:5:94:ARG:O	6:5:97:LYS:N	2.43	0.51
9:A:1300:G:H4'	9:A:1301:A:H5'	1.92	0.51
9:A:1797:G:O2'	11:C:256:THR:CG2	2.59	0.51
9:A:2062:A:N6	36:A:9000:ERY:C27	2.54	0.51
13:E:148:ILE:HA	13:E:187:VAL:HB	1.93	0.51
14:F:132:ARG:O	14:F:133:GLU:HB3	2.10	0.51
16:H:41:LYS:HA	16:H:44:ILE:HG12	1.93	0.51
17:I:36:GLU:HB3	17:I:66:PHE:CE1	2.46	0.51
25:Q:94:LEU:C	25:Q:96:ASP:H	2.14	0.51
9:A:1816:C:C5	11:C:61:TYR:CE2	2.98	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:W:16:GLU:O	31:W:17:ALA:HB3	2.10	0.51
3:2:27:GLY:O	3:2:30:VAL:HB	2.11	0.51
6:5:25:ALA:O	6:5:116:GLU:OE1	2.28	0.51
12:D:91:THR:O	12:D:91:THR:OG1	2.28	0.51
25:Q:94:LEU:C	25:Q:96:ASP:N	2.64	0.51
28:T:69:ARG:CG	28:T:70:HIS:H	2.23	0.51
30:V:9:ARG:NH2	30:V:12:GLN:HA	2.26	0.51
9:A:26:G:C6	9:A:27:G:N1	2.79	0.51
9:A:2063:C:C2'	9:A:2064:C:C5'	2.88	0.51
9:A:460:A:C2	9:A:470:A:C4	2.99	0.51
9:A:565:C:H2'	9:A:566:U:O4'	2.11	0.51
21:M:8:LYS:HE3	21:M:9:PHE:CE2	2.45	0.51
34:Z:41:PRO:HA	34:Z:44:ARG:HB3	1.93	0.51
9:A:27:G:N2	9:A:512:G:H1'	2.26	0.51
9:A:84:A:N1	9:A:98:G:O2'	2.30	0.51
9:A:489:G:N7	27:S:49:LYS:NZ	2.58	0.51
9:A:748:G:P	27:S:88:ARG:NH2	2.83	0.51
9:A:1322:A:OP1	27:S:11:ARG:NE	2.38	0.51
18:J:81:ILE:CG1	18:J:82:GLY:N	2.74	0.51
5:4:3:VAL:HG23	5:4:4:ARG:H	1.74	0.50
9:A:1394:U:H4'	9:A:1603:A:H4'	1.92	0.50
9:A:1533:C:C2	9:A:1534:U:C4	2.99	0.50
9:A:2314:A:OP1	14:F:87:LYS:NZ	2.44	0.50
15:G:16:VAL:HG21	15:G:44:HIS:CD2	2.46	0.50
19:K:9:ASN:O	19:K:83:ALA:HA	2.11	0.50
20:L:81:ASP:O	20:L:83:ALA:N	2.41	0.50
25:Q:91:ARG:HE	25:Q:93:ILE:CG2	2.25	0.50
9:A:391:A:C6	9:A:411:G:C2	3.00	0.50
9:A:1533:C:H2'	9:A:1534:U:C6	2.46	0.50
15:G:30:GLY:O	15:G:32:LEU:N	2.38	0.50
27:S:86:MET:HB2	27:S:96:ILE:HG21	1.92	0.50
28:T:29:THR:OG1	28:T:86:THR:N	2.43	0.50
31:W:76:ARG:HH21	31:W:76:ARG:HG2	1.76	0.50
9:A:945:A:C5	9:A:2448:A:C2	2.98	0.50
9:A:1778:U:H2'	9:A:1784:A:N6	2.27	0.50
14:F:71:LYS:HD3	14:F:72:SER:N	2.26	0.50
3:2:34:ARG:NH1	3:2:41:ARG:O	2.45	0.50
9:A:1179:G:H2'	9:A:1180:U:O4'	2.12	0.50
9:A:2074:U:H2'	9:A:2075:U:C6	2.46	0.50
12:D:148:GLN:OE1	12:D:148:GLN:N	2.45	0.50
9:A:139:U:O2'	28:T:1:MET:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:322:A:H5'	9:A:340:A:H1'	1.94	0.50
18:J:44:TYR:O	18:J:45:THR:HB	2.11	0.50
21:M:35:ALA:O	21:M:36:VAL:HB	2.11	0.50
26:R:39:LEU:HA	26:R:49:ILE:HG21	1.92	0.50
9:A:1203:U:O2'	20:L:4:ASN:OD1	2.28	0.50
9:A:1654:A:H2'	9:A:1655:A:H8	1.76	0.50
9:A:1753:G:OP1	24:P:92:ARG:NE	2.38	0.50
9:A:2094:A:C2	9:A:2196:C:C2	2.99	0.50
9:A:2329:U:H2'	9:A:2330:G:C8	2.47	0.50
9:A:2352:A:C6	31:W:30:VAL:HG11	2.47	0.50
22:N:52:ILE:HB	22:N:94:TYR:CD2	2.46	0.50
9:A:2576:G:N3	9:A:2576:G:C3'	2.75	0.50
19:K:19:VAL:CG1	19:K:41:ILE:HG12	2.40	0.50
33:Y:8:GLU:O	33:Y:12:GLU:HB2	2.12	0.50
34:Z:26:LEU:O	34:Z:37:ARG:NH1	2.44	0.50
9:A:118:A:N3	9:A:178:G:H1'	2.27	0.50
9:A:504:A:HO2'	9:A:505:A:P	2.28	0.50
9:A:654:A:H3'	9:A:654:A:N3	2.26	0.50
9:A:1437:C:H2'	9:A:1438:U:C6	2.46	0.50
9:A:1475:G:O2'	9:A:1514:G:O6	2.30	0.50
9:A:2601:C:O2'	9:A:2602:A:O5'	2.26	0.50
12:D:62:LYS:HB2	12:D:63:PRO:HD3	1.93	0.50
12:D:193:VAL:HG21	12:D:201:LEU:HD21	1.93	0.50
34:Z:30:ARG:HB3	34:Z:30:ARG:HH11	1.76	0.50
9:A:221:A:N1	9:A:265:A:O2'	2.45	0.50
9:A:1808:A:O2'	32:X:2:ARG:NH1	2.45	0.50
9:A:747:U:O2'	27:S:88:ARG:NH2	2.45	0.49
9:A:2061:G:O6	9:A:2501:C:O2	2.30	0.49
21:M:20:LEU:HD22	21:M:20:LEU:N	2.26	0.49
2:1:4:ILE:HG23	2:1:5:ARG:H	1.76	0.49
4:3:30:HIS:HD2	9:A:2421:G:N7	2.10	0.49
6:5:4:ASN:C	6:5:6:GLN:N	2.66	0.49
9:A:1869:G:H3'	9:A:1870:C:H5"	1.94	0.49
17:I:109:ALA:HB2	17:I:128:ILE:HG13	1.93	0.49
6:5:138:ARG:NH2	7:6:26:MET:HA	2.27	0.49
9:A:748:G:OP1	27:S:88:ARG:NH2	2.45	0.49
9:A:2571:U:O2'	12:D:151:THR:CG2	2.60	0.49
9:A:2604:U:H2'	9:A:2605:U:H6	1.75	0.49
12:D:151:THR:CG2	12:D:152:PRO:HD3	2.43	0.49
22:N:96:ARG:NH2	22:N:114:GLU:OE1	2.44	0.49
23:O:51:ALA:HB3	23:O:78:VAL:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:W:9:THR:HG23	31:W:10:ARG:HD3	1.94	0.49
6:5:95:LEU:HD22	6:5:95:LEU:H	1.77	0.49
9:A:1614:A:N1	27:S:93:ALA:HB2	2.27	0.49
18:J:21:THR:HG22	18:J:22:GLY:N	2.27	0.49
28:T:54:GLU:CG	28:T:88:LYS:HB2	2.42	0.49
32:X:70:LEU:O	32:X:75:GLU:N	2.45	0.49
9:A:2228:G:H22	32:X:33:HIS:HE2	1.61	0.49
9:A:2330:G:C2	9:A:2386:A:C2	3.01	0.49
17:I:123:ALA:HA	17:I:126:ARG:CZ	2.43	0.49
9:A:250:G:C6	9:A:251:A:C6	3.01	0.49
9:A:443:A:C5	13:E:40:ARG:HD3	2.47	0.49
9:A:1199:U:H5'	25:Q:4:LYS:CE	2.42	0.49
9:A:2109:U:H2'	9:A:2110:G:H5'	1.94	0.49
17:I:48:ILE:HG13	17:I:49:GLU:H	1.77	0.49
27:S:20:VAL:HG11	27:S:44:ALA:HA	1.93	0.49
9:A:2755:C:HO2'	9:A:2756:U:H6	1.61	0.49
17:I:87:SER:OG	17:I:88:GLY:N	2.43	0.49
25:Q:63:ARG:NH1	25:Q:96:ASP:HA	2.27	0.49
6:5:51:TYR:C	6:5:51:TYR:CD1	2.86	0.49
6:5:68:PRO:HA	6:5:72:LEU:HD11	1.94	0.49
9:A:107:G:H2'	9:A:108:G:H8	1.78	0.49
9:A:564:C:O2	9:A:578:G:N2	2.46	0.49
9:A:1567:G:H2'	11:C:84:PRO:HG3	1.95	0.49
9:A:1844:C:O3'	11:C:255:LYS:NZ	2.43	0.49
9:A:2609:U:H3'	9:A:2610:C:H5'	1.95	0.49
9:A:2867:G:O2'	9:A:2868:A:OP2	2.28	0.49
13:E:112:LEU:HD13	13:E:186:VAL:HG11	1.94	0.49
14:F:5:ASP:OD1	14:F:8:LYS:NZ	2.46	0.49
6:5:55:VAL:HG13	9:A:1084:A:H5'	1.93	0.49
9:A:223:A:C5	9:A:422:A:C8	3.00	0.49
9:A:2580:U:C2'	9:A:2581:G:C5'	2.86	0.49
15:G:84:LYS:HG3	15:G:132:LEU:N	2.28	0.49
28:T:34:VAL:O	28:T:34:VAL:CG2	2.61	0.49
4:3:51:LYS:NZ	9:A:938:G:OP2	2.33	0.49
9:A:308:G:O2'	9:A:329:G:N2	2.46	0.49
9:A:1022:G:C5	9:A:1140:C:C4	3.00	0.49
9:A:1474:U:H2'	9:A:1475:G:H5'	1.95	0.49
9:A:1730:C:OP1	9:A:1730:C:H4'	2.12	0.49
9:A:1778:U:H2'	9:A:1784:A:H62	1.78	0.49
9:A:2211:A:O2'	9:A:2212:A:P	2.70	0.49
9:A:2483:C:N3	21:M:123:LYS:NZ	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2701:U:H3'	9:A:2702:G:C5'	2.42	0.49
21:M:106:ASP:O	21:M:108:VAL:N	2.44	0.49
22:N:12:ARG:CZ	22:N:20:MET:HE1	2.43	0.49
27:S:13:SER:O	27:S:14:ALA:CB	2.60	0.49
6:5:4:ASN:C	6:5:6:GLN:H	2.16	0.48
9:A:1327:A:N6	9:A:1328:A:C2	2.81	0.48
9:A:1485:U:H2'	9:A:1486:U:C6	2.48	0.48
9:A:1607:C:H4'	9:A:1608:A:O5'	2.13	0.48
9:A:2063:C:C4	9:A:2064:C:C4	3.01	0.48
9:A:2393:U:H5'	20:L:60:ARG:O	2.13	0.48
12:D:174:SER:OG	12:D:175:LEU:N	2.46	0.48
16:H:9:VAL:O	16:H:13:GLY:N	2.46	0.48
27:S:24:ILE:HG22	27:S:71:VAL:HG11	1.95	0.48
1:0:2:VAL:CG2	9:A:2015:A:C2	2.96	0.48
9:A:2016:U:H2'	9:A:2017:U:C6	2.48	0.48
15:G:73:SER:O	15:G:77:GLY:N	2.45	0.48
6:5:71:CYS:CA	6:5:117:LEU:HD13	2.31	0.48
9:A:2600:A:C2'	9:A:2601:C:C5'	2.86	0.48
14:F:79:ARG:HB3	14:F:82:TYR:CE1	2.48	0.48
17:I:14:ALA:HB3	17:I:51:GLY:H	1.79	0.48
18:J:43:GLU:O	18:J:45:THR:HG22	2.13	0.48
20:L:19:LEU:HB2	20:L:27:LEU:HB3	1.94	0.48
24:P:91:VAL:O	24:P:92:ARG:HG2	2.12	0.48
29:U:85:ARG:HD3	29:U:86:PHE:N	2.28	0.48
11:C:265:PHE:N	11:C:265:PHE:CD1	2.82	0.48
14:F:79:ARG:HB3	14:F:82:TYR:CZ	2.48	0.48
21:M:34:LYS:HD2	21:M:131:VAL:HG11	1.95	0.48
9:A:580:U:H2'	9:A:581:C:H6	1.79	0.48
9:A:856:G:H21	31:W:19:ARG:HH12	1.58	0.48
9:A:856:G:O2'	31:W:22:VAL:HG23	2.14	0.48
9:A:1348:C:H2'	9:A:1349:C:H5'	1.96	0.48
9:A:2580:U:H6	9:A:2580:U:O5'	1.96	0.48
9:A:2747:G:O2'	15:G:66:THR:HG22	2.14	0.48
32:X:39:VAL:HG22	32:X:44:ARG:O	2.14	0.48
6:5:77:VAL:O	6:5:79:PRO:HD2	2.13	0.48
9:A:391:A:C5	9:A:411:G:C2	3.02	0.48
9:A:923:G:H1'	31:W:23:LYS:CD	2.43	0.48
9:A:1022:G:C6	9:A:1140:C:C4	3.01	0.48
9:A:1135:C:N4	9:A:1139:G:C6	2.82	0.48
9:A:1760:C:H2'	9:A:1761:C:O4'	2.14	0.48
9:A:2800:A:H3'	9:A:2801:G:H5"	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:225:ASN:HB3	11:C:226:PRO:HD2	1.96	0.48
12:D:68:PHE:C	12:D:73:VAL:HG12	2.33	0.48
13:E:164:LEU:HB3	13:E:167:VAL:CG1	2.44	0.48
21:M:1:MET:O	21:M:2:LEU:CB	2.62	0.48
31:W:18:LYS:HA	31:W:36:ILE:HG13	1.95	0.48
32:X:70:LEU:O	32:X:74:GLY:N	2.46	0.48
34:Z:38:GLU:O	34:Z:43:ILE:HG12	2.13	0.48
6:5:58:THR:HG23	9:A:1107:G:H5"	1.94	0.48
9:A:301:G:H1'	9:A:302:C:C6	2.48	0.48
9:A:528:A:C2	9:A:2043:C:H4'	2.49	0.48
9:A:973:A:P	26:R:81:LYS:HZ3	2.35	0.48
9:A:995:C:O2	18:J:3:THR:HG23	2.13	0.48
9:A:1277:G:C5'	22:N:20:MET:HE2	2.44	0.48
9:A:1996:C:OP1	19:K:31:ARG:NE	2.46	0.48
9:A:2230:G:O3'	32:X:29:LEU:HD23	2.14	0.48
9:A:2678:C:H2'	9:A:2679:A:O4'	2.14	0.48
14:F:110:ILE:O	14:F:112:ASP:N	2.46	0.48
32:X:67:LEU:HD23	32:X:70:LEU:HD12	1.96	0.48
2:1:20:TYR:HH	9:A:2347:C:HO2'	1.59	0.48
3:2:10:LEU:HD23	9:A:770:G:H5"	1.96	0.48
9:A:11:C:C3'	9:A:12:U:H5'	2.44	0.48
9:A:1738:G:HO2'	9:A:1739:A:P	2.37	0.48
9:A:2355:G:H4'	31:W:20:LEU:CD1	2.44	0.48
13:E:32:VAL:HG23	13:E:178:VAL:HG12	1.95	0.48
18:J:32:LEU:CD2	18:J:54:ILE:HD12	2.44	0.48
24:P:19:PHE:N	24:P:19:PHE:CD1	2.82	0.48
31:W:49:ASN:ND2	31:W:49:ASN:C	2.66	0.48
9:A:996:A:H4'	25:Q:91:ARG:NE	2.29	0.48
9:A:1069:A:C1'	9:A:1073:A:H62	2.26	0.48
9:A:1327:A:H2'	9:A:1328:A:O4'	2.14	0.48
14:F:10:GLU:O	14:F:12:VAL:N	2.44	0.48
15:G:22:VAL:HG23	15:G:22:VAL:O	2.14	0.48
15:G:23:ILE:HG21	15:G:71:LEU:HD11	1.95	0.48
26:R:49:ILE:HD12	26:R:52:PRO:HA	1.95	0.48
31:W:18:LYS:CG	31:W:19:ARG:N	2.77	0.48
9:A:749:A:C6	9:A:1618:A:C2	3.01	0.48
9:A:995:C:N4	18:J:2:LYS:HB3	2.29	0.48
9:A:1799:G:C5	11:C:175:LEU:HD23	2.49	0.48
12:D:148:GLN:HB2	12:D:152:PRO:HG2	1.96	0.48
15:G:15:ASP:O	15:G:16:VAL:HG13	2.12	0.48
15:G:104:LEU:HB2	15:G:112:VAL:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:J:44:TYR:CD1	25:Q:63:ARG:HG2	2.49	0.48
31:W:44:PHE:HD1	31:W:45:HIS:CE1	2.31	0.48
6:5:110:ALA:HB1	6:5:113:PHE:CZ	2.49	0.47
9:A:479:A:C2	9:A:480:A:C4	3.01	0.47
9:A:983:A:N6	9:A:984:A:C2	2.82	0.47
9:A:1417:C:N3	9:A:1581:G:N2	2.60	0.47
9:A:2062:A:H61	36:A:9000:ERY:H273	1.70	0.47
9:A:2592:G:C6	9:A:2603:G:O6	2.67	0.47
15:G:118:ALA:O	15:G:120:ILE:N	2.41	0.47
17:I:60:VAL:HG22	17:I:66:PHE:HB3	1.95	0.47
24:P:105:LYS:HA	24:P:108:ARG:HD2	1.95	0.47
9:A:1814:G:C6	9:A:1815:A:N6	2.82	0.47
11:C:232:GLY:H	11:C:241:LYS:HE3	1.79	0.47
14:F:134:GLN:O	14:F:136:ILE:N	2.47	0.47
27:S:24:ILE:HD11	27:S:36:LEU:HD13	1.96	0.47
27:S:63:GLY:O	27:S:64:ALA:CB	2.62	0.47
31:W:23:LYS:HE2	31:W:24:ARG:H	1.78	0.47
14:F:64:PRO:HA	14:F:88:VAL:HG22	1.95	0.47
17:I:100:ILE:HD13	17:I:137:LEU:HD12	1.96	0.47
18:J:84:ILE:HG23	18:J:84:ILE:O	2.15	0.47
19:K:72:PRO:O	19:K:74:GLY:N	2.43	0.47
26:R:68:ARG:HD3	26:R:92:TRP:CZ2	2.49	0.47
31:W:47:GLY:H	31:W:80:SER:HB3	1.80	0.47
6:5:23:LEU:H	6:5:87:GLU:HB2	1.79	0.47
6:5:110:ALA:HB1	6:5:113:PHE:CE1	2.49	0.47
9:A:983:A:N6	9:A:984:A:N1	2.62	0.47
9:A:2406:A:C2	20:L:69:ARG:NH2	2.82	0.47
9:A:2862:G:C5	9:A:2863:C:C5	3.02	0.47
14:F:69:ALA:N	14:F:82:TYR:O	2.47	0.47
31:W:42:THR:HG22	31:W:43:LYS:HZ2	1.80	0.47
31:W:63:ASP:OD1	31:W:63:ASP:N	2.35	0.47
32:X:39:VAL:HG21	32:X:42:GLU:HB2	1.96	0.47
2:1:16:THR:HG21	2:1:41:VAL:HG13	1.97	0.47
9:A:587:C:P	20:L:21:ARG:NH1	2.88	0.47
25:Q:91:ARG:HH21	25:Q:93:ILE:HD13	1.80	0.47
31:W:49:ASN:HA	31:W:61:LYS:HB2	1.94	0.47
5:4:6:SER:HB2	9:A:1031:G:H4'	1.95	0.47
6:5:15:VAL:HG21	6:5:66:GLY:HA2	1.96	0.47
6:5:123:ILE:HG12	6:5:124:ASP:N	2.30	0.47
6:5:127:ALA:O	6:5:129:LEU:N	2.48	0.47
9:A:451:U:C2	9:A:453:A:N7	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:478:A:C6	9:A:480:A:C6	3.03	0.47
9:A:2346:A:H3'	9:A:2347:C:H5"	1.95	0.47
19:K:24:VAL:HG13	19:K:33:ALA:HB2	1.95	0.47
20:L:82:LEU:CD1	20:L:116:VAL:HG23	2.44	0.47
33:Y:56:LEU:O	33:Y:57:LEU:HB3	2.14	0.47
6:5:39:THR:HA	6:5:42:ARG:CD	2.43	0.47
6:5:60:LEU:HD23	6:5:78:GLY:HA3	1.97	0.47
6:5:88:HIS:CB	6:5:89:PRO:HD3	2.44	0.47
6:5:100:ALA:HB2	6:5:125:ARG:HE	1.79	0.47
9:A:419:U:H2'	9:A:420:C:C6	2.50	0.47
9:A:725:G:C6	9:A:726:G:N1	2.82	0.47
9:A:1090:A:C2	9:A:1102:C:H1'	2.50	0.47
9:A:1417:C:O2'	9:A:1587:G:O2'	2.19	0.47
9:A:1474:U:C2'	9:A:1475:G:H5'	2.44	0.47
9:A:2061:G:N2	9:A:2063:C:N3	2.63	0.47
9:A:2425:A:C5'	9:A:2427:C:O4'	2.62	0.47
11:C:246:PRO:HG2	11:C:247:TRP:CZ3	2.50	0.47
17:I:89:SER:OG	17:I:135:MET:SD	2.68	0.47
17:I:135:MET:HB3	17:I:137:LEU:CD2	2.43	0.47
26:R:64:VAL:HG21	26:R:97:LYS:HB2	1.97	0.47
28:T:61:LEU:C	28:T:61:LEU:HD12	2.35	0.47
31:W:39:GLN:HG2	31:W:40:ARG:N	2.28	0.47
33:Y:1:MET:H3	33:Y:2:LYS:HD2	1.79	0.47
6:5:15:VAL:HG22	6:5:66:GLY:CA	2.44	0.47
9:A:523:C:H5"	9:A:540:C:O2'	2.15	0.47
9:A:947:A:O2'	9:A:984:A:H2	1.98	0.47
9:A:1478:G:C2	9:A:1479:G:N7	2.83	0.47
9:A:1614:A:N6	27:S:92:ARG:O	2.43	0.47
9:A:2210:U:H4'	9:A:2211:A:H5'	1.97	0.47
9:A:2902:C:C2'	9:A:2903:U:O5'	2.63	0.47
36:A:9000:ERY:H8	36:A:9000:ERY:H321	1.58	0.47
10:B:55:U:O3'	14:F:23:SER:OG	2.21	0.47
17:I:40:ALA:O	17:I:43:ALA:HB3	2.14	0.47
18:J:36:LEU:O	18:J:121:LYS:NZ	2.39	0.47
24:P:50:ARG:HG2	24:P:57:ALA:N	2.30	0.47
31:W:9:THR:HG23	31:W:10:ARG:N	2.30	0.47
31:W:60:ALA:HA	31:W:81:ILE:HD12	1.97	0.47
1:0:9:ARG:NH2	9:A:517:C:OP2	2.48	0.47
6:5:51:TYR:HD1	6:5:52:MET:N	2.12	0.47
9:A:1161:C:H1'	26:R:8:GLY:O	2.15	0.47
9:A:1198:U:O3'	25:Q:4:LYS:HE3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2063:C:H5	9:A:2064:C:H41	1.63	0.47
9:A:2609:U:C3'	9:A:2610:C:H5'	2.44	0.47
9:A:2839:G:N2	9:A:2880:C:C4	2.82	0.47
14:F:131:VAL:HG22	14:F:151:LEU:H	1.80	0.47
31:W:28:GLU:O	31:W:30:VAL:N	2.48	0.47
31:W:30:VAL:HG23	31:W:60:ALA:O	2.15	0.47
6:5:54:VAL:HG22	6:5:83:ALA:HB1	1.97	0.47
9:A:479:A:H4'	9:A:480:A:OP1	2.15	0.47
9:A:1079:C:O2	17:I:130:GLY:HA3	2.15	0.47
9:A:1088:A:HO2'	9:A:1089:A:P	2.37	0.47
21:M:46:ILE:HD13	21:M:47:GLU:N	2.30	0.47
9:A:657:U:H2'	9:A:658:U:C6	2.50	0.46
9:A:1817:G:H2'	9:A:1818:U:H5'	1.97	0.46
11:C:38:LYS:NZ	11:C:57:HIS:O	2.39	0.46
12:D:169:ARG:O	12:D:170:VAL:HG13	2.15	0.46
15:G:112:VAL:HG23	15:G:113:ASP:N	2.28	0.46
17:I:14:ALA:HB1	17:I:45:THR:HG23	1.97	0.46
20:L:23:ILE:HD12	26:R:84:ARG:CZ	2.45	0.46
22:N:103:ARG:HD3	22:N:110:MET:HE3	1.97	0.46
26:R:68:ARG:HD3	26:R:92:TRP:CE2	2.50	0.46
28:T:69:ARG:CD	28:T:70:HIS:H	2.28	0.46
9:A:747:U:C2'	27:S:88:ARG:NH2	2.78	0.46
9:A:1219:U:OP2	25:Q:18:LYS:NZ	2.46	0.46
9:A:1392:A:N6	9:A:1393:A:N6	2.63	0.46
9:A:1509:A:C4	9:A:1510:G:C8	3.04	0.46
13:E:44:ARG:HH21	13:E:44:ARG:HG3	1.80	0.46
16:H:8:LYS:O	16:H:9:VAL:HB	2.15	0.46
19:K:24:VAL:CG1	19:K:30:ARG:HD3	2.45	0.46
20:L:68:SER:O	20:L:69:ARG:HB3	2.15	0.46
25:Q:63:ARG:HH22	25:Q:96:ASP:N	2.12	0.46
9:A:1378:A:O2'	9:A:1380:G:N7	2.27	0.46
9:A:2318:G:C6	9:A:2319:G:C6	3.03	0.46
9:A:2365:G:H4'	31:W:59:PHE:CZ	2.51	0.46
9:A:2889:C:N4	9:A:2890:G:C6	2.83	0.46
14:F:39:VAL:HG13	14:F:40:GLY:N	2.31	0.46
15:G:123:GLU:HG2	15:G:124:CYS:N	2.30	0.46
16:H:21:VAL:CG2	16:H:25:TYR:CD2	2.98	0.46
18:J:37:ARG:HA	18:J:118:MET:CE	2.45	0.46
19:K:98:ARG:HA	19:K:118:LEU:HD23	1.97	0.46
21:M:22:GLN:O	21:M:24:THR:N	2.48	0.46
28:T:54:GLU:N	28:T:54:GLU:OE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:W:72:GLY:N	31:W:73:PRO:CD	2.78	0.46
6:5:68:PRO:HA	6:5:72:LEU:CG	2.46	0.46
9:A:2335:A:C5	9:A:2337:G:C4	3.02	0.46
9:A:2583:G:N2	9:A:2584:U:O2	2.48	0.46
15:G:23:ILE:HD12	15:G:23:ILE:H	1.81	0.46
17:I:19:PRO:CG	17:I:23:VAL:HG23	2.45	0.46
19:K:30:ARG:NH1	19:K:32:TYR:O	2.45	0.46
20:L:85:VAL:HG22	20:L:94:THR:HG22	1.97	0.46
25:Q:4:LYS:NZ	25:Q:7:VAL:CG1	2.79	0.46
26:R:49:ILE:HG22	26:R:53:PHE:C	2.36	0.46
1:0:42:ILE:H	1:0:42:ILE:HD12	1.80	0.46
9:A:2436:G:C2	9:A:2437:G:C8	3.04	0.46
9:A:2698:U:H2'	9:A:2699:C:C6	2.51	0.46
11:C:67:LYS:HG2	11:C:150:GLY:HA2	1.97	0.46
13:E:119:ILE:HG13	13:E:119:ILE:O	2.16	0.46
16:H:31:VAL:HB	16:H:32:PRO:CD	2.46	0.46
17:I:120:ASP:O	17:I:123:ALA:N	2.46	0.46
20:L:19:LEU:HD23	20:L:19:LEU:C	2.35	0.46
25:Q:91:ARG:HH21	25:Q:93:ILE:HG21	1.81	0.46
6:5:136:ILE:HG13	6:5:139:LEU:HD12	1.98	0.46
9:A:747:U:H2'	27:S:88:ARG:NH2	2.30	0.46
9:A:1313:U:H2'	9:A:1610:A:C2	2.51	0.46
9:A:1567:G:C2'	11:C:84:PRO:HG3	2.46	0.46
9:A:1569:A:N6	9:A:1570:A:C6	2.84	0.46
9:A:1838:C:H4'	9:A:1839:G:C8	2.51	0.46
9:A:2581:G:H4'	9:A:2582:G:C8	2.51	0.46
10:B:29:A:H2'	10:B:30:C:C6	2.50	0.46
10:B:37:C:C5	10:B:38:C:C4	3.04	0.46
11:C:75:ALA:HB2	11:C:95:TYR:HA	1.97	0.46
12:D:1:MET:HG2	12:D:205:PRO:HG3	1.98	0.46
14:F:30:VAL:CG1	14:F:96:TRP:CH2	2.99	0.46
9:A:1939:U:O2	9:A:1967:C:H4'	2.15	0.46
9:A:2701:U:H3'	9:A:2702:G:H5"	1.96	0.46
9:A:2897:U:H2'	9:A:2898:U:C6	2.51	0.46
17:I:57:VAL:HG23	17:I:71:LYS:CE	2.46	0.46
23:O:79:ALA:O	23:O:82:ALA:N	2.49	0.46
26:R:66:HIS:CG	26:R:94:THR:HG22	2.49	0.46
29:U:73:ASN:HA	29:U:95:PHE:CE2	2.51	0.46
31:W:9:THR:CG2	31:W:10:ARG:HD3	2.44	0.46
9:A:2024:G:C4	9:A:2040:G:N2	2.84	0.46
9:A:2793:C:H2'	9:A:2794:C:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:93:VAL:HG12	11:C:94:LEU:N	2.31	0.46
14:F:147:ARG:HG3	14:F:148:VAL:N	2.30	0.46
17:I:24:GLY:O	17:I:27:LEU:HG	2.16	0.46
17:I:61:TYR:N	17:I:61:TYR:CD1	2.82	0.46
24:P:50:ARG:CB	24:P:57:ALA:N	2.78	0.46
28:T:29:THR:HB	28:T:86:THR:HG22	1.98	0.46
28:T:29:THR:CB	28:T:86:THR:H	2.29	0.46
2:1:4:ILE:HD11	2:1:27:ARG:HB2	1.97	0.46
9:A:247:G:H4'	9:A:386:G:C5	2.51	0.46
9:A:593:U:H2'	9:A:594:U:C6	2.51	0.46
9:A:751:A:C6	9:A:789:A:C5	3.04	0.46
9:A:959:A:H62	21:M:82:MET:CE	2.28	0.46
14:F:62:GLN:NE2	14:F:89:THR:O	2.47	0.46
15:G:163:TYR:O	15:G:164:ALA:HB2	2.16	0.46
17:I:100:ILE:CG2	17:I:101:SER:N	2.79	0.46
19:K:61:VAL:HG22	19:K:87:LEU:HD11	1.98	0.46
20:L:132:ARG:HG3	20:L:142:ILE:HD12	1.98	0.46
24:P:58:PHE:CE1	24:P:75:THR:HG22	2.51	0.46
24:P:72:VAL:HG23	24:P:72:VAL:O	2.15	0.46
31:W:19:ARG:CZ	31:W:22:VAL:HB	2.46	0.46
12:D:193:VAL:HB	12:D:194:PRO:HD2	1.98	0.46
14:F:113:PHE:HE1	14:F:116:LEU:HD13	1.81	0.46
6:5:63:ALA:HB3	6:5:84:TYR:CE2	2.52	0.45
6:5:71:CYS:CA	6:5:117:LEU:HD11	2.43	0.45
8:7:76:A:C6	9:A:2451:A:O4'	2.69	0.45
9:A:281:C:H2'	9:A:282:A:C8	2.51	0.45
9:A:1057:A:C6	9:A:1086:A:C2	3.04	0.45
9:A:1060:U:H3	9:A:1088:A:H2	1.64	0.45
9:A:1936:A:N6	9:A:1963:U:C2	2.84	0.45
18:J:12:LYS:O	18:J:13:ARG:HB2	2.15	0.45
18:J:44:TYR:O	18:J:45:THR:CB	2.64	0.45
19:K:13:ASN:O	19:K:14:SER:OG	2.29	0.45
1:0:3:GLN:HA	9:A:2615:U:C2	2.51	0.45
9:A:11:C:H2'	9:A:12:U:H5'	1.98	0.45
9:A:33:C:O2	9:A:447:A:N6	2.50	0.45
9:A:118:A:C8	9:A:119:A:C8	3.04	0.45
9:A:597:G:C2	9:A:661:A:C2	3.04	0.45
9:A:833:A:OP2	20:L:39:LYS:NZ	2.45	0.45
9:A:923:G:N3	31:W:23:LYS:HD2	2.31	0.45
9:A:1171:G:C6	9:A:1172:C:C4	3.04	0.45
9:A:1248:G:C5	13:E:46:GLN:NE2	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1593:A:H2'	9:A:1594:U:O4'	2.17	0.45
9:A:1662:U:O2	9:A:2687:U:H4'	2.17	0.45
11:C:24:HIS:NE2	11:C:79:ARG:NH2	2.65	0.45
17:I:137:LEU:HD23	17:I:137:LEU:H	1.81	0.45
4:3:21:PHE:O	4:3:22:LYS:O	2.33	0.45
9:A:141:G:N1	28:T:1:MET:O	2.44	0.45
9:A:271:G:H4'	9:A:272:A:OP1	2.17	0.45
9:A:1783:A:N1	9:A:2587:A:C4	2.85	0.45
10:B:51:G:OP2	23:O:64:TYR:HD2	1.98	0.45
19:K:80:ASP:CB	24:P:67:GLU:HG3	2.47	0.45
19:K:98:ARG:HA	19:K:118:LEU:CD2	2.47	0.45
22:N:70:THR:HB	22:N:75:ILE:CD1	2.46	0.45
23:O:15:ARG:NE	23:O:93:ASP:OD2	2.44	0.45
27:S:1:MET:O	27:S:108:SER:HB2	2.16	0.45
30:V:80:HIS:HD2	30:V:83:LYS:H	1.62	0.45
31:W:39:GLN:HG3	31:W:42:THR:H	1.81	0.45
1:0:8:THR:HG21	9:A:2021:C:P	2.56	0.45
4:3:3:ILE:HG21	4:3:62:PRO:HG3	1.98	0.45
4:3:12:ARG:HD3	20:L:61:LEU:O	2.16	0.45
5:4:36:ARG:O	5:4:37:GLN:C	2.55	0.45
9:A:1150:C:H2'	9:A:1151:A:O5'	2.17	0.45
9:A:2144:G:H3'	9:A:2144:G:N3	2.31	0.45
9:A:2262:U:H4'	9:A:2328:A:C2	2.52	0.45
9:A:2852:G:C6	9:A:2853:C:N3	2.84	0.45
9:A:2862:G:C6	9:A:2863:C:C4	3.04	0.45
12:D:70:LYS:O	12:D:71:ALA:HB3	2.17	0.45
18:J:12:LYS:O	18:J:13:ARG:CB	2.64	0.45
19:K:99:ILE:HG21	19:K:119:ALA:HB2	1.98	0.45
30:V:80:HIS:CD2	30:V:83:LYS:HB2	2.52	0.45
2:1:33:LEU:N	2:1:51:ALA:CB	2.80	0.45
5:4:8:LYS:NZ	9:A:2467:C:OP1	2.48	0.45
9:A:85:G:OP1	29:U:6:ARG:N	2.49	0.45
9:A:799:G:C6	9:A:800:A:C6	3.05	0.45
9:A:2108:A:C2'	9:A:2109:U:O5'	2.65	0.45
9:A:2326:C:C6	9:A:2326:C:H3'	2.52	0.45
9:A:2326:C:H4'	9:A:2327:A:OP1	2.16	0.45
9:A:2581:G:N3	9:A:2581:G:C2'	2.75	0.45
9:A:2649:C:H2'	9:A:2650:U:C6	2.50	0.45
9:A:2758:A:H2'	9:A:2759:G:H5'	1.99	0.45
10:B:11:C:O2'	10:B:15:A:N6	2.50	0.45
13:E:154:ASP:OD1	13:E:154:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:14:SER:OG	16:H:17:ASP:CG	2.55	0.45
18:J:55:ILE:HD11	18:J:130:HIS:CD2	2.51	0.45
25:Q:91:ARG:HH12	26:R:10:LYS:HB3	1.82	0.45
27:S:18:ARG:HG3	27:S:76:VAL:HG13	1.98	0.45
1:0:42:ILE:HD11	22:N:98:LEU:CB	2.46	0.45
2:1:4:ILE:HG23	2:1:5:ARG:N	2.32	0.45
4:3:38:LYS:NZ	9:A:2365:G:N7	2.52	0.45
6:5:48:ALA:HB3	6:5:51:TYR:HB3	1.98	0.45
6:5:71:CYS:HA	6:5:117:LEU:HD11	1.96	0.45
9:A:2478:A:H2'	9:A:2479:U:H5'	1.98	0.45
9:A:2592:G:C2	9:A:2603:G:C5	3.05	0.45
9:A:2740:A:C6	9:A:2764:A:C8	3.04	0.45
24:P:21:PRO:HD3	24:P:49:ILE:HD12	1.98	0.45
25:Q:4:LYS:NZ	25:Q:7:VAL:HG11	2.31	0.45
2:1:6:GLU:OE1	2:1:52:LYS:CE	2.64	0.45
6:5:110:ALA:O	6:5:113:PHE:N	2.46	0.45
9:A:855:G:H21	31:W:23:LYS:HG2	1.82	0.45
9:A:1141:U:H4'	9:A:1142:A:O4'	2.17	0.45
9:A:1428:C:C5	9:A:1569:A:H5"	2.52	0.45
9:A:2058:A:C5	9:A:2059:A:N6	2.85	0.45
13:E:187:VAL:O	13:E:188:MET:HB3	2.16	0.45
16:H:40:THR:C	16:H:42:LYS:H	2.19	0.45
17:I:125:THR:O	17:I:128:ILE:N	2.48	0.45
22:N:33:ILE:CD1	22:N:118:ARG:NE	2.80	0.45
24:P:91:VAL:HG11	24:P:96:LEU:HD21	1.98	0.45
30:V:80:HIS:CD2	30:V:82:TYR:H	2.35	0.45
34:Z:3:THR:HA	34:Z:37:ARG:O	2.16	0.45
9:A:728:G:H4'	11:C:12:ARG:HD3	1.98	0.45
9:A:996:A:H4'	25:Q:91:ARG:CD	2.47	0.45
12:D:86:GLU:CD	12:D:86:GLU:N	2.69	0.45
14:F:127:TYR:O	14:F:128:SER:CB	2.65	0.45
2:1:8:ILE:HG21	2:1:51:ALA:HA	1.98	0.45
6:5:125:ARG:CZ	6:5:125:ARG:HA	2.46	0.45
9:A:2405:G:O2'	9:A:2406:A:OP1	2.26	0.45
9:A:2407:A:C2	9:A:2408:U:C2	3.05	0.45
11:C:163:ILE:HG23	11:C:171:VAL:CG1	2.47	0.45
22:N:103:ARG:CZ	22:N:110:MET:CE	2.95	0.45
23:O:43:ASN:O	23:O:45:SER:N	2.50	0.45
24:P:102:ARG:O	24:P:103:THR:HG22	2.17	0.45
25:Q:91:ARG:HH11	26:R:11:GLN:H	1.64	0.45
5:4:6:SER:HB2	9:A:1031:G:C4'	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:129:LEU:CB	6:5:130:PRO:HD2	2.47	0.45
9:A:2564:A:C2	9:A:2647:U:H4'	2.52	0.45
12:D:73:VAL:HG23	12:D:74:GLU:H	1.82	0.45
14:F:107:VAL:HG11	14:F:116:LEU:HD21	1.99	0.45
14:F:128:SER:HA	14:F:154:THR:HA	1.99	0.45
18:J:30:THR:HG22	18:J:31:GLU:N	2.32	0.45
25:Q:7:VAL:HG13	25:Q:8:ILE:N	2.32	0.45
31:W:17:ALA:O	31:W:18:LYS:CB	2.64	0.45
9:A:627:A:C6	9:A:637:A:C8	3.04	0.44
9:A:973:A:O4'	9:A:1188:U:C6	2.70	0.44
9:A:980:A:C4	9:A:1136:G:O4'	2.70	0.44
9:A:2043:C:OP1	9:A:2777:G:O2'	2.24	0.44
9:A:2283:C:H5"	9:A:2389:G:O2'	2.18	0.44
10:B:51:G:H5"	23:O:64:TYR:CD2	2.52	0.44
12:D:121:THR:O	12:D:122:VAL:HB	2.17	0.44
15:G:83:THR:C	15:G:84:LYS:HD3	2.37	0.44
16:H:8:LYS:O	16:H:13:GLY:HA2	2.16	0.44
19:K:118:LEU:O	19:K:119:ALA:HB3	2.17	0.44
21:M:102:LEU:N	21:M:102:LEU:HD12	2.32	0.44
9:A:646:U:H3'	9:A:647:G:H5"	1.99	0.44
9:A:1181:U:H2'	9:A:1182:G:C8	2.53	0.44
9:A:1387:A:H5'	9:A:1469:A:H1'	2.00	0.44
9:A:2307:G:N2	9:A:2311:A:C8	2.85	0.44
12:D:44:GLY:HA3	12:D:45:TYR:HD1	1.82	0.44
17:I:109:ALA:CB	17:I:128:ILE:HG13	2.48	0.44
28:T:40:LYS:HG2	28:T:58:VAL:HG22	1.99	0.44
29:U:53:GLN:N	29:U:54:PRO:CD	2.80	0.44
31:W:37:VAL:HG11	31:W:55:ASP:HB2	1.99	0.44
34:Z:15:ARG:HG2	34:Z:15:ARG:HH11	1.82	0.44
6:5:15:VAL:CG2	6:5:66:GLY:HA2	2.47	0.44
6:5:139:LEU:O	6:5:142:THR:OG1	2.26	0.44
9:A:81:G:O2'	9:A:295:G:O2'	2.26	0.44
9:A:315:G:H2'	9:A:316:C:C6	2.52	0.44
9:A:750:A:OP1	9:A:1615:C:N4	2.40	0.44
9:A:792:A:C6	9:A:2440:C:C6	3.05	0.44
9:A:819:A:C4	9:A:1189:A:C2	3.05	0.44
9:A:1443:U:H2'	9:A:1444:G:C8	2.53	0.44
9:A:1686:C:C2	9:A:1703:G:C2	3.05	0.44
9:A:1936:A:C2	9:A:1943:U:C5	3.03	0.44
12:D:3:GLY:HA3	12:D:204:LYS:HG2	1.99	0.44
14:F:72:SER:HB2	14:F:80:GLN:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:J:80:HIS:O	18:J:82:GLY:N	2.50	0.44
29:U:6:ARG:O	29:U:24:VAL:HB	2.17	0.44
6:5:100:ALA:HB3	6:5:125:ARG:HD2	1.98	0.44
9:A:277:G:H2'	9:A:361:G:O6	2.17	0.44
9:A:635:C:O2'	9:A:639:U:OP1	2.34	0.44
9:A:818:G:H5'	9:A:839:U:OP1	2.18	0.44
9:A:1867:G:C5	9:A:1868:C:C5	3.06	0.44
9:A:2344:U:H4'	9:A:2345:G:OP1	2.17	0.44
9:A:2683:C:O2	19:K:70:ARG:NH2	2.38	0.44
15:G:24:THR:HG23	15:G:34:ARG:HG2	1.99	0.44
15:G:60:GLY:O	15:G:61:TRP:HB2	2.17	0.44
17:I:100:ILE:HD11	17:I:137:LEU:CG	2.48	0.44
25:Q:103:VAL:HG23	25:Q:104:ALA:N	2.32	0.44
31:W:19:ARG:NH1	31:W:22:VAL:HG21	2.33	0.44
1:0:3:GLN:NE2	9:A:2016:U:O2	2.46	0.44
9:A:666:A:H4'	20:L:48:ARG:HD2	1.99	0.44
9:A:994:C:H1'	26:R:10:LYS:CE	2.47	0.44
9:A:1045:C:C3'	9:A:1046:A:H5'	2.48	0.44
9:A:1482:G:H1'	9:A:1509:A:N6	2.30	0.44
9:A:1523:U:O2'	9:A:1524:G:H5'	2.18	0.44
9:A:2108:A:H2'	9:A:2109:U:O5'	2.17	0.44
9:A:2276:G:P	21:M:83:GLY:O	2.76	0.44
9:A:2283:C:C2	9:A:2389:G:C2	3.06	0.44
9:A:2582:G:C2	9:A:2583:G:N9	2.86	0.44
9:A:2584:U:H5"	9:A:2584:U:H6	1.82	0.44
9:A:2745:C:C4	9:A:2746:U:C4	3.05	0.44
9:A:2747:G:O6	9:A:2755:C:H5"	2.18	0.44
9:A:2846:G:H2'	9:A:2847:U:O4'	2.17	0.44
13:E:147:LEU:HB3	13:E:186:VAL:HG23	1.99	0.44
15:G:104:LEU:HB2	15:G:112:VAL:CG2	2.47	0.44
31:W:19:ARG:C	31:W:19:ARG:CD	2.85	0.44
34:Z:5:LYS:HD2	34:Z:5:LYS:N	2.32	0.44
6:5:51:TYR:CE1	6:5:52:MET:HG2	2.53	0.44
9:A:336:C:N3	9:A:337:C:C5	2.86	0.44
9:A:820:A:H2'	9:A:821:A:O4'	2.16	0.44
9:A:1197:G:H2'	9:A:1198:U:H6	1.83	0.44
9:A:2577:A:H8	9:A:2577:A:OP2	1.99	0.44
9:A:2582:G:C2	9:A:2583:G:C5	3.06	0.44
9:A:2788:C:H2'	9:A:2789:C:C6	2.53	0.44
9:A:2902:C:H2'	9:A:2903:U:O5'	2.18	0.44
14:F:94:ARG:HH11	14:F:94:ARG:CG	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:I:46:ASP:HA	17:I:50:LYS:HD2	2.00	0.44
19:K:10:VAL:HG21	19:K:17:ARG:H	1.81	0.44
27:S:66:ILE:HD13	27:S:67:ASP:N	2.33	0.44
3:2:12:ARG:HH11	3:2:44:VAL:HG11	1.82	0.44
4:3:31:ILE:O	4:3:31:ILE:HG13	2.17	0.44
9:A:61:C:H2'	9:A:62:U:H5'	2.00	0.44
9:A:278:A:N1	9:A:362:A:C8	2.85	0.44
9:A:855:G:H21	31:W:23:LYS:CG	2.31	0.44
9:A:979:A:H2'	9:A:982:C:H42	1.82	0.44
9:A:1340:U:H4'	9:A:1341:G:OP2	2.17	0.44
9:A:1542:U:H2'	9:A:1543:G:O4'	2.16	0.44
9:A:1737:G:H5"	9:A:1738:G:OP2	2.17	0.44
9:A:1779:U:C5	9:A:1784:A:N7	2.86	0.44
9:A:2577:A:OP2	9:A:2577:A:C8	2.70	0.44
10:B:78:A:H2'	10:B:79:G:O4'	2.18	0.44
11:C:24:HIS:CE1	11:C:79:ARG:HH21	2.36	0.44
17:I:40:ALA:O	17:I:68:PHE:CZ	2.71	0.44
18:J:44:TYR:HA	25:Q:59:LEU:CD2	2.48	0.44
28:T:48:GLN:O	28:T:52:GLU:HA	2.17	0.44
31:W:17:ALA:O	31:W:18:LYS:HB2	2.18	0.44
9:A:132:G:C2'	9:A:133:U:H5'	2.48	0.44
9:A:201:C:OP1	32:X:17:ARG:NH1	2.51	0.44
9:A:222:A:N6	9:A:231:A:C2	2.86	0.44
9:A:948:C:H1'	9:A:984:A:O2'	2.18	0.44
9:A:1232:G:C5	9:A:1233:C:C5	3.06	0.44
9:A:2103:C:H2'	9:A:2104:C:C5'	2.47	0.44
12:D:69:ALA:HA	12:D:73:VAL:CG1	2.47	0.44
21:M:13:HIS:O	21:M:14:LYS:CB	2.66	0.44
22:N:20:MET:HE1	22:N:40:LYS:HE2	2.00	0.44
22:N:38:LEU:HB3	22:N:39:PRO:CD	2.48	0.44
2:1:8:ILE:CD1	2:1:24:LYS:HG2	2.48	0.44
9:A:288:U:H2'	9:A:289:G:C8	2.52	0.44
9:A:2661:G:C6	9:A:2662:A:C2	3.06	0.44
10:B:78:A:C2	10:B:99:A:C4	3.06	0.44
13:E:44:ARG:HH21	13:E:44:ARG:CG	2.31	0.44
15:G:35:THR:HG22	15:G:36:LEU:N	2.33	0.44
18:J:44:TYR:O	18:J:44:TYR:CD2	2.71	0.44
28:T:69:ARG:CG	28:T:70:HIS:N	2.81	0.44
30:V:29:ILE:HD13	30:V:30:ILE:N	2.33	0.44
31:W:18:LYS:N	31:W:36:ILE:HG13	2.33	0.44
9:A:720:U:H2'	9:A:721:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:980:A:C6	9:A:981:A:N1	2.86	0.43
9:A:1071:G:H1'	9:A:1089:A:C5	2.53	0.43
9:A:2335:A:N6	9:A:2337:G:H1'	2.33	0.43
9:A:2423:U:H5'	9:A:2423:U:H6	1.83	0.43
9:A:2603:G:C2'	9:A:2604:U:H5'	2.47	0.43
9:A:2657:A:C2	9:A:2665:A:C4	3.06	0.43
11:C:76:VAL:HG22	11:C:76:VAL:O	2.17	0.43
18:J:44:TYR:HD1	25:Q:63:ARG:HG2	1.81	0.43
20:L:112:LEU:HD23	20:L:114:GLY:H	1.83	0.43
31:W:19:ARG:HA	31:W:34:SER:HA	2.00	0.43
33:Y:45:GLN:O	33:Y:46:VAL:HB	2.17	0.43
6:5:3:LEU:HB2	6:5:4:ASN:H	1.68	0.43
9:A:1439:A:C2	9:A:1553:A:C4	3.06	0.43
9:A:1584:U:H2'	9:A:1585:C:H5'	2.00	0.43
9:A:1786:A:N6	9:A:2606:C:O4'	2.46	0.43
9:A:1857:G:C2	9:A:1884:G:N3	2.86	0.43
11:C:265:PHE:N	11:C:265:PHE:HD1	2.15	0.43
18:J:4:PHE:O	18:J:44:TYR:OH	2.34	0.43
18:J:110:PRO:HB2	18:J:111:LYS:HG3	2.00	0.43
20:L:2:ARG:HA	20:L:5:THR:CG2	2.48	0.43
25:Q:91:ARG:HH11	26:R:11:GLN:N	2.16	0.43
4:3:31:ILE:O	4:3:31:ILE:CG1	2.66	0.43
6:5:17:GLU:OE1	6:5:53:ARG:NH1	2.51	0.43
6:5:71:CYS:HB3	6:5:74:ASP:OD2	2.18	0.43
7:6:13:ALA:HB1	7:6:17:MET:CE	2.49	0.43
9:A:545:U:H6	9:A:545:U:O5'	2.02	0.43
9:A:581:C:H2'	9:A:582:A:C8	2.53	0.43
9:A:936:A:H2'	9:A:937:C:C6	2.54	0.43
9:A:1252:G:C2	25:Q:32:ARG:HG2	2.52	0.43
9:A:2031:A:C6	9:A:2498:C:H1'	2.53	0.43
9:A:2180:U:C2	9:A:2181:U:C5	3.06	0.43
9:A:2517:C:C5	9:A:2542:A:C5	3.06	0.43
9:A:2595:G:C6	9:A:2599:G:O6	2.72	0.43
11:C:109:LEU:HD23	11:C:110:LYS:H	1.83	0.43
12:D:45:TYR:N	12:D:45:TYR:CD1	2.86	0.43
15:G:36:LEU:N	15:G:36:LEU:HD22	2.33	0.43
19:K:47:ILE:HG13	19:K:48:PRO:HD2	2.00	0.43
20:L:111:ILE:N	20:L:111:ILE:HD12	2.33	0.43
31:W:24:ARG:HD3	31:W:65:LYS:CD	2.48	0.43
6:5:17:GLU:HA	6:5:88:HIS:CE1	2.54	0.43
9:A:172:A:H2'	9:A:173:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:684:G:C2	9:A:794:A:C2	3.06	0.43
9:A:822:G:H2'	9:A:823:C:H6	1.83	0.43
9:A:1914:C:H2'	9:A:1915:U:O4'	2.18	0.43
9:A:2134:A:O2'	9:A:2135:A:O4'	2.36	0.43
10:B:27:C:C5	10:B:28:C:C5	3.06	0.43
12:D:133:THR:HG23	12:D:134:HIS:N	2.33	0.43
13:E:158:PHE:HD2	13:E:159:LEU:HD12	1.83	0.43
13:E:160:ALA:O	13:E:161:ALA:HB3	2.18	0.43
14:F:134:GLN:OE1	14:F:149:ARG:HB3	2.18	0.43
15:G:123:GLU:HG2	15:G:125:PRO:HD3	2.00	0.43
17:I:82:ALA:HB1	17:I:108:ILE:HG21	2.00	0.43
25:Q:4:LYS:HZ3	25:Q:7:VAL:CG1	2.32	0.43
26:R:64:VAL:O	26:R:65:ALA:HB3	2.18	0.43
26:R:74:ILE:HB	26:R:87:GLN:O	2.18	0.43
6:5:71:CYS:SG	6:5:117:LEU:HD12	2.58	0.43
9:A:1171:G:N2	9:A:1179:G:C4	2.86	0.43
12:D:124:ARG:HA	12:D:165:MET:SD	2.58	0.43
22:N:70:THR:HB	22:N:75:ILE:HD11	2.01	0.43
31:W:49:ASN:ND2	31:W:50:VAL:N	2.67	0.43
2:1:5:ARG:CZ	2:1:24:LYS:HA	2.49	0.43
6:5:54:VAL:O	6:5:55:VAL:C	2.57	0.43
9:A:247:G:N7	9:A:249:C:C2	2.86	0.43
9:A:959:A:H62	21:M:82:MET:HE1	1.84	0.43
9:A:2582:G:N3	9:A:2582:G:H2'	2.34	0.43
18:J:11:VAL:HG11	18:J:50:THR:HA	2.01	0.43
19:K:35:VAL:HG12	19:K:36:GLY:N	2.34	0.43
20:L:2:ARG:HA	20:L:5:THR:HG21	2.01	0.43
25:Q:94:LEU:CD1	26:R:13:ARG:HB2	2.49	0.43
29:U:73:ASN:O	29:U:74:ALA:HB3	2.17	0.43
31:W:24:ARG:HD3	31:W:65:LYS:HG2	2.00	0.43
33:Y:21:LEU:HA	33:Y:25:GLN:HB3	2.01	0.43
2:1:7:LYS:NZ	9:A:2421:G:P	2.92	0.43
6:5:87:GLU:OE2	6:5:95:LEU:HD23	2.18	0.43
9:A:323:C:OP1	9:A:338:G:N2	2.51	0.43
9:A:545:U:H2'	9:A:546:U:O3'	2.18	0.43
9:A:580:U:O3'	25:Q:30:VAL:HG13	2.18	0.43
9:A:744:U:H2'	9:A:745:G:O4'	2.19	0.43
9:A:1485:U:H2'	9:A:1486:U:H6	1.82	0.43
9:A:1536:C:H1'	9:A:1537:G:N2	2.34	0.43
9:A:1956:U:H2'	9:A:1957:C:H5'	2.01	0.43
9:A:2204:G:OP2	11:C:146:LYS:NZ	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:90:C:H6	10:B:90:C:H5"	1.83	0.43
14:F:103:ILE:HG21	14:F:173:ASP:HB2	2.01	0.43
19:K:3:GLN:HG3	19:K:4:GLU:N	2.34	0.43
20:L:122:VAL:CG1	20:L:142:ILE:HG12	2.47	0.43
21:M:26:VAL:HB	21:M:133:LYS:HA	2.00	0.43
25:Q:60:TRP:CE2	25:Q:93:ILE:HB	2.54	0.43
28:T:29:THR:HB	28:T:86:THR:HA	2.01	0.43
34:Z:15:ARG:HD3	34:Z:53:MET:SD	2.59	0.43
4:3:22:LYS:HA	4:3:47:ALA:O	2.19	0.43
9:A:274:C:H2'	9:A:275:C:O4'	2.19	0.43
9:A:479:A:N3	9:A:481:G:H5"	2.34	0.43
9:A:645:C:O2	9:A:645:C:O2'	2.35	0.43
9:A:975:A:C5	9:A:990:A:N7	2.86	0.43
9:A:994:C:O2'	9:A:996:A:OP1	2.25	0.43
9:A:1003:G:N2	9:A:1004:U:C2	2.86	0.43
9:A:1188:U:H4'	26:R:81:LYS:O	2.19	0.43
9:A:1378:A:C4	9:A:1380:G:N7	2.87	0.43
9:A:1441:G:H2'	9:A:1442:U:C6	2.53	0.43
9:A:1494:A:C2	9:A:1495:A:C4	3.06	0.43
9:A:2094:A:P	16:H:22:LYS:HD2	2.59	0.43
9:A:2353:G:N3	31:W:30:VAL:HG12	2.32	0.43
9:A:2576:G:N3	9:A:2576:G:C5'	2.76	0.43
9:A:2601:C:HO2'	9:A:2602:A:P	2.41	0.43
13:E:187:VAL:O	13:E:188:MET:CB	2.67	0.43
16:H:8:LYS:O	16:H:9:VAL:CB	2.66	0.43
17:I:45:THR:O	17:I:48:ILE:HG13	2.18	0.43
22:N:117:ASP:O	22:N:118:ARG:C	2.57	0.43
32:X:67:LEU:HD22	32:X:77:TYR:CE1	2.53	0.43
33:Y:31:GLN:HG2	33:Y:36:GLN:HB2	2.01	0.43
9:A:570:G:C4	9:A:2030:A:N7	2.87	0.43
9:A:764:A:C6	9:A:781:A:C2	3.06	0.43
9:A:1509:A:O2'	9:A:1510:G:P	2.76	0.43
9:A:2682:A:C8	12:D:11:MET:HG3	2.53	0.43
18:J:60:ASP:N	18:J:60:ASP:OD1	2.52	0.43
25:Q:20:ALA:HA	25:Q:23:TYR:CE2	2.54	0.43
29:U:35:VAL:O	29:U:38:ILE:HB	2.19	0.43
31:W:36:ILE:HG22	31:W:36:ILE:O	2.18	0.43
31:W:44:PHE:O	31:W:78:PHE:HA	2.19	0.43
33:Y:56:LEU:HD22	33:Y:56:LEU:H	1.84	0.43
9:A:476:G:H4'	9:A:502:A:N1	2.33	0.43
9:A:528:A:P	18:J:116:ARG:HH21	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:742:A:H2'	9:A:743:A:C8	2.53	0.43
9:A:1096:A:H2'	9:A:1097:U:H5"	2.01	0.43
9:A:1223:G:P	26:R:68:ARG:HH11	2.41	0.43
9:A:1476:U:C5	9:A:1514:G:C2	3.07	0.43
9:A:2070:A:H2'	9:A:2071:A:O4'	2.19	0.43
9:A:2507:C:C2	9:A:2508:G:C8	3.07	0.43
1:0:42:ILE:HG22	1:0:43:THR:O	2.19	0.42
9:A:1281:G:C2	9:A:1290:C:C2	3.07	0.42
9:A:1338:G:O2'	9:A:1393:A:N1	2.44	0.42
9:A:2516:A:N6	9:A:2517:C:N4	2.67	0.42
9:A:2611:C:C3'	9:A:2611:C:C6	3.02	0.42
10:B:72:G:N2	10:B:103:U:C5	2.87	0.42
11:C:180:MET:O	11:C:267:VAL:N	2.42	0.42
12:D:110:THR:HG23	12:D:171:THR:HG22	2.00	0.42
18:J:88:THR:HG22	18:J:91:GLU:CG	2.49	0.42
19:K:13:ASN:O	19:K:14:SER:CB	2.67	0.42
22:N:8:ARG:HB3	22:N:10:LEU:CD2	2.48	0.42
23:O:41:ALA:O	23:O:44:GLY:N	2.41	0.42
28:T:69:ARG:HG3	28:T:70:HIS:H	1.83	0.42
28:T:76:ARG:HG3	28:T:77:ARG:N	2.34	0.42
30:V:72:VAL:HG12	30:V:93:ARG:HA	2.01	0.42
6:5:67:THR:C	6:5:69:PHE:N	2.73	0.42
9:A:226:A:C6	9:A:227:A:C6	3.07	0.42
9:A:348:A:C5	9:A:349:U:C5	3.07	0.42
9:A:580:U:H2'	9:A:581:C:C6	2.54	0.42
9:A:833:A:OP1	20:L:39:LYS:HE3	2.19	0.42
9:A:1747:U:H2'	9:A:1748:C:C6	2.55	0.42
9:A:2823:A:C5	9:A:2824:C:C5	3.07	0.42
12:D:118:PHE:HZ	22:N:1:MET:HB2	1.85	0.42
17:I:93:ASN:HB2	17:I:135:MET:SD	2.59	0.42
25:Q:86:SER:O	26:R:51:VAL:HA	2.18	0.42
26:R:5:PHE:HB3	26:R:59:ILE:HD12	2.01	0.42
27:S:59:GLU:HA	27:S:64:ALA:CB	2.50	0.42
33:Y:14:LEU:HA	33:Y:17:GLU:HB3	2.01	0.42
6:5:67:THR:CG2	6:5:72:LEU:HA	2.49	0.42
6:5:142:THR:OG1	6:5:143:MET:N	2.52	0.42
9:A:864:G:OP2	21:M:22:GLN:NE2	2.52	0.42
9:A:1094:U:N3	9:A:1097:U:OP2	2.51	0.42
9:A:1224:U:H4'	26:R:88:GLY:O	2.18	0.42
9:A:2047:C:O2'	9:A:2048:G:H5'	2.19	0.42
9:A:2748:A:H1'	15:G:66:THR:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:89:U:H3'	10:B:90:C:C5'	2.49	0.42
13:E:52:VAL:HG11	13:E:81:GLY:HA3	2.01	0.42
15:G:39:ALA:HB2	15:G:57:TYR:CD2	2.54	0.42
25:Q:27:ARG:HA	25:Q:33:VAL:HG12	2.00	0.42
30:V:75:GLN:HB2	30:V:92:VAL:CG2	2.48	0.42
9:A:726:G:O2'	9:A:727:A:OP2	2.37	0.42
9:A:959:A:N6	21:M:82:MET:CE	2.82	0.42
9:A:1112:G:C5	9:A:1113:U:C5	3.07	0.42
9:A:1312:U:H4'	9:A:1313:U:O5'	2.20	0.42
9:A:1681:G:N2	9:A:1763:G:OP2	2.45	0.42
9:A:2287:A:C8	9:A:2289:G:C8	3.08	0.42
12:D:149:ASN:CG	12:D:150:GLN:H	2.21	0.42
13:E:188:MET:HE3	13:E:196:VAL:HG21	2.01	0.42
14:F:111:ARG:NE	14:F:111:ARG:HA	2.34	0.42
22:N:79:LEU:O	22:N:80:PHE:HB2	2.19	0.42
32:X:52:ALA:O	32:X:53:LYS:CB	2.67	0.42
6:5:108:VAL:CG1	6:5:109:LYS:N	2.82	0.42
7:6:15:SER:OG	7:6:16:VAL:N	2.53	0.42
9:A:146:A:H2'	9:A:147:C:C6	2.54	0.42
9:A:479:A:C2	9:A:480:A:C5	3.08	0.42
9:A:573:U:O2'	9:A:574:A:H3'	2.19	0.42
9:A:846:U:HO2'	9:A:847:U:P	2.41	0.42
9:A:966:G:C6	9:A:967:U:C4	3.07	0.42
9:A:1204:A:C2	9:A:1240:U:N3	2.87	0.42
9:A:1239:G:H2'	9:A:1240:U:O4'	2.19	0.42
9:A:1814:G:C6	9:A:1815:A:C6	3.08	0.42
9:A:1937:A:N7	9:A:1939:U:H2'	2.35	0.42
9:A:2526:G:C5	9:A:2527:C:C5	3.08	0.42
14:F:134:GLN:HG2	14:F:135:ILE:N	2.34	0.42
17:I:91:LYS:HB2	17:I:95:ASP:HB2	2.00	0.42
22:N:24:MET:HE2	22:N:44:LEU:HD22	2.02	0.42
29:U:10:VAL:HG12	29:U:71:ILE:HA	2.01	0.42
31:W:37:VAL:HB	31:W:38:ARG:NH1	2.34	0.42
2:1:18:HIS:CE1	2:1:40:PRO:HD3	2.54	0.42
6:5:47:GLU:HG2	6:5:95:LEU:HD21	2.00	0.42
9:A:945:A:C4	9:A:2448:A:C2	3.07	0.42
9:A:1638:C:H4'	9:A:2710:C:O2	2.18	0.42
9:A:2039:U:H2'	9:A:2040:G:H8	1.82	0.42
9:A:2274:A:C5	9:A:2276:G:C8	3.07	0.42
9:A:2557:G:H2'	9:A:2558:C:C6	2.54	0.42
9:A:2582:G:C4	9:A:2583:G:N7	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2637:U:C2'	9:A:2638:G:H5'	2.50	0.42
9:A:2727:A:C6	9:A:2728:U:O4	2.73	0.42
12:D:120:GLY:HA2	12:D:162:ALA:HA	2.00	0.42
14:F:94:ARG:HH11	14:F:94:ARG:HB2	1.84	0.42
18:J:43:GLU:O	18:J:44:TYR:C	2.58	0.42
18:J:64:VAL:HG13	18:J:65:THR:N	2.35	0.42
21:M:8:LYS:CE	21:M:9:PHE:CE2	3.02	0.42
24:P:92:ARG:O	24:P:92:ARG:CG	2.68	0.42
25:Q:6:GLY:HA2	25:Q:9:ALA:HB3	2.02	0.42
26:R:16:GLU:HA	26:R:98:ILE:HG22	2.01	0.42
26:R:74:ILE:HD12	26:R:74:ILE:N	2.34	0.42
29:U:38:ILE:HG23	29:U:39:ASN:N	2.33	0.42
9:A:19:A:H2'	9:A:20:C:O4'	2.20	0.42
9:A:126:A:C6	9:A:127:A:N1	2.88	0.42
9:A:356:G:C6	9:A:357:C:C4	3.07	0.42
9:A:372:G:C4	32:X:60:LYS:HE2	2.54	0.42
9:A:996:A:C5	9:A:1160:G:C2	3.08	0.42
9:A:1179:G:C6	9:A:1180:U:C4	3.08	0.42
9:A:2062:A:O2'	9:A:2063:C:C6	2.70	0.42
9:A:2661:G:H2'	9:A:2662:A:O4'	2.20	0.42
9:A:2821:A:C2	9:A:2822:G:C4	3.08	0.42
10:B:106:G:H2'	10:B:107:G:O4'	2.19	0.42
11:C:16:VAL:N	11:C:203:VAL:CG1	2.82	0.42
17:I:20:SER:HB3	17:I:21:PRO:HD3	2.02	0.42
25:Q:91:ARG:HE	25:Q:93:ILE:HG23	1.85	0.42
27:S:96:ILE:O	27:S:96:ILE:HG13	2.20	0.42
6:5:3:LEU:HD12	6:5:5:LEU:N	2.35	0.42
9:A:636:G:OP2	20:L:109:LYS:NZ	2.45	0.42
9:A:1084:A:C6	9:A:1085:A:C6	3.08	0.42
9:A:1171:G:H1	9:A:1178:C:H42	1.66	0.42
9:A:1183:U:H2'	9:A:1184:U:C6	2.55	0.42
9:A:1238:G:O2'	9:A:1239:G:H5'	2.19	0.42
9:A:1465:G:H2'	9:A:1466:U:O4'	2.19	0.42
9:A:2071:A:H2'	9:A:2072:C:C6	2.54	0.42
9:A:2543:G:C6	9:A:2544:G:C6	3.08	0.42
9:A:2585:U:C5	9:A:2608:G:O6	2.73	0.42
9:A:2611:C:H5'	36:A:9000:ERY:H301	2.01	0.42
10:B:16:G:C5	10:B:69:G:C2	3.07	0.42
11:C:203:VAL:O	11:C:205:GLY:N	2.53	0.42
12:D:24:VAL:HA	12:D:191:GLY:H	1.85	0.42
13:E:42:GLY:O	13:E:43:THR:OG1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:77:ILE:HD13	20:L:108:ALA:HB1	2.02	0.42
23:O:14:ALA:O	23:O:17:LYS:N	2.52	0.42
6:5:22:ALA:N	6:5:87:GLU:O	2.53	0.42
6:5:88:HIS:CB	6:5:89:PRO:CD	2.97	0.42
9:A:803:U:C4	9:A:804:A:N7	2.88	0.42
9:A:1026:G:H2'	9:A:1027:A:C8	2.55	0.42
9:A:1268:A:H2'	9:A:1269:A:O4'	2.20	0.42
9:A:1789:A:H2'	9:A:1790:C:O4'	2.20	0.42
9:A:2506:U:C3'	9:A:2506:U:C6	3.02	0.42
9:A:2803:G:H2'	9:A:2804:U:H6	1.84	0.42
17:I:9:LYS:HB3	17:I:71:LYS:NZ	2.34	0.42
18:J:4:PHE:CD2	18:J:44:TYR:CE2	3.08	0.42
18:J:38:GLY:O	18:J:43:GLU:HB2	2.19	0.42
21:M:53:MET:CE	21:M:63:ILE:HG21	2.50	0.42
23:O:31:THR:HG22	23:O:34:HIS:N	2.33	0.42
24:P:58:PHE:HD1	24:P:75:THR:HG22	1.83	0.42
9:A:653:U:H5	9:A:654:A:C2	2.38	0.42
9:A:2352:A:N1	31:W:30:VAL:HG21	2.35	0.42
9:A:2796:U:C4	9:A:2798:U:C5	3.08	0.42
12:D:35:THR:N	12:D:49:GLN:O	2.41	0.42
14:F:107:VAL:HG13	14:F:110:ILE:HD12	2.02	0.42
18:J:81:ILE:CG1	18:J:82:GLY:H	2.33	0.42
19:K:71:ARG:HB3	19:K:72:PRO:CD	2.49	0.42
20:L:40:SER:O	20:L:41:ARG:CB	2.67	0.42
23:O:75:GLY:HA3	23:O:109:ALA:HB3	2.00	0.42
29:U:84:PHE:O	29:U:85:ARG:HB3	2.19	0.42
31:W:39:GLN:HG2	31:W:41:GLY:N	2.34	0.42
6:5:33:VAL:HB	6:5:36:ASP:OD1	2.20	0.41
9:A:75:G:H4'	33:Y:48:ARG:NH2	2.35	0.41
9:A:528:A:H2	9:A:2043:C:H5'	1.85	0.41
9:A:1194:A:C2'	9:A:1195:G:O5'	2.68	0.41
9:A:1298:C:C2	9:A:1643:G:N2	2.88	0.41
9:A:1414:C:O2	9:A:1588:G:N2	2.44	0.41
9:A:1486:U:H2'	9:A:1487:U:C6	2.55	0.41
9:A:1607:C:H42	9:A:1622:G:P	2.43	0.41
9:A:1770:G:C6	9:A:1983:G:C6	3.07	0.41
9:A:2636:C:O2'	12:D:45:TYR:OH	2.25	0.41
9:A:2755:C:O2'	9:A:2756:U:H2'	2.19	0.41
9:A:2869:G:C6	9:A:2870:C:C4	3.09	0.41
11:C:16:VAL:HB	11:C:203:VAL:HG12	2.02	0.41
14:F:28:PRO:HB2	14:F:168:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:U:98:ASN:ND2	29:U:100:GLU:OE1	2.53	0.41
34:Z:4:ILE:HD13	34:Z:44:ARG:NH1	2.34	0.41
9:A:45:G:H5'	9:A:46:G:H5'	2.02	0.41
9:A:485:C:C2	9:A:496:G:N2	2.88	0.41
9:A:518:G:H2'	9:A:519:U:C6	2.54	0.41
9:A:866:A:N7	9:A:914:G:C6	2.89	0.41
9:A:1591:A:H2'	9:A:1592:C:C6	2.55	0.41
9:A:1936:A:C2	9:A:1943:U:H5	2.38	0.41
9:A:1945:G:C6	9:A:1946:U:C4	3.09	0.41
9:A:2609:U:C3'	9:A:2610:C:C5'	2.98	0.41
9:A:2676:C:P	19:K:31:ARG:HH12	2.44	0.41
13:E:12:LEU:HD12	13:E:193:VAL:HG11	2.01	0.41
13:E:129:PRO:HG3	13:E:156:ASN:OD1	2.21	0.41
13:E:134:LEU:CD2	13:E:161:ALA:HB2	2.50	0.41
31:W:60:ALA:CB	31:W:81:ILE:CD1	2.98	0.41
34:Z:13:ILE:HG22	34:Z:14:GLY:N	2.34	0.41
6:5:131:THR:HA	6:5:134:GLU:CG	2.50	0.41
9:A:685:A:C2	9:A:689:A:C6	3.08	0.41
9:A:1019:U:H3	9:A:1142:A:N6	2.17	0.41
9:A:1669:A:O2'	9:A:2549:G:OP1	2.36	0.41
9:A:1817:G:C2'	9:A:1818:U:H5'	2.51	0.41
9:A:2058:A:C6	9:A:2059:A:N6	2.88	0.41
9:A:2341:G:H2'	9:A:2342:C:C6	2.55	0.41
11:C:16:VAL:H	11:C:203:VAL:HG12	1.84	0.41
15:G:26:LYS:CG	15:G:27:GLY:N	2.83	0.41
28:T:34:VAL:O	28:T:34:VAL:HG22	2.20	0.41
28:T:70:HIS:HB3	28:T:73:ARG:O	2.19	0.41
31:W:24:ARG:HH11	31:W:65:LYS:HG2	1.85	0.41
6:5:51:TYR:CD1	6:5:52:MET:HG2	2.55	0.41
9:A:109:C:H4'	9:A:348:A:H4'	2.02	0.41
9:A:527:C:H4'	9:A:528:A:O5'	2.21	0.41
9:A:1747:U:H2'	9:A:1748:C:H6	1.85	0.41
9:A:1843:C:O2'	11:C:253:GLY:O	2.29	0.41
9:A:2201:G:C6	9:A:2202:U:C4	3.08	0.41
9:A:2259:U:H1'	9:A:2427:C:C2	2.56	0.41
9:A:2478:A:C2'	9:A:2479:U:H5'	2.51	0.41
9:A:2685:G:H1	9:A:2724:U:H3	1.68	0.41
11:C:77:VAL:HG23	11:C:77:VAL:O	2.20	0.41
15:G:31:GLU:O	15:G:33:THR:N	2.52	0.41
22:N:8:ARG:HB3	22:N:10:LEU:HD22	2.01	0.41
25:Q:4:LYS:HZ3	25:Q:7:VAL:HG11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Q:82:LEU:HD12	25:Q:112:ALA:HB2	2.02	0.41
1:0:42:ILE:HD12	22:N:99:LYS:O	2.20	0.41
6:5:108:VAL:HG12	6:5:109:LYS:N	2.35	0.41
9:A:179:C:C2	9:A:180:G:C8	3.08	0.41
9:A:1674:G:N2	9:A:1677:A:N1	2.69	0.41
9:A:2063:C:N4	9:A:2064:C:N4	2.69	0.41
9:A:2580:U:C5	9:A:2581:G:C6	3.08	0.41
9:A:2618:G:C6	9:A:2619:C:C4	3.09	0.41
13:E:79:ARG:HG2	13:E:80:SER:N	2.35	0.41
14:F:151:LEU:CD1	14:F:153:ILE:HG23	2.51	0.41
17:I:52:LEU:HB3	17:I:53:PRO:HD2	2.03	0.41
17:I:74:PRO:HG2	17:I:77:VAL:HB	2.01	0.41
18:J:4:PHE:HB3	18:J:44:TYR:CE2	2.55	0.41
18:J:65:THR:HG22	18:J:68:LYS:NZ	2.36	0.41
26:R:61:ALA:HB1	26:R:98:ILE:H	1.84	0.41
27:S:63:GLY:O	27:S:64:ALA:HB3	2.21	0.41
6:5:106:PHE:CG	6:5:107:GLU:N	2.87	0.41
9:A:608:A:C8	9:A:621:A:N6	2.89	0.41
9:A:1020:A:C2	9:A:1141:U:C2	3.09	0.41
9:A:1381:G:H1’	9:A:1571:A:N1	2.36	0.41
9:A:1494:A:C6	9:A:1495:A:C5	3.08	0.41
9:A:1587:G:C4	9:A:1588:G:C8	3.09	0.41
9:A:1647:U:P	9:A:1647:U:H3’	2.60	0.41
9:A:1691:C:C4	9:A:1692:U:C4	3.08	0.41
9:A:1722:A:C2	9:A:1739:A:N3	2.89	0.41
9:A:1843:C:H5’	11:C:250:GLN:NE2	2.36	0.41
9:A:2063:C:H41	9:A:2064:C:N4	2.18	0.41
12:D:46:ARG:HB3	12:D:46:ARG:CZ	2.50	0.41
14:F:10:GLU:HG2	14:F:13:LYS:HD3	2.02	0.41
14:F:169:LEU:O	14:F:174:PHE:HB2	2.21	0.41
16:H:39:ALA:HB1	16:H:44:ILE:HG22	2.01	0.41
19:K:15:GLY:O	19:K:46:ALA:HA	2.20	0.41
20:L:29:LYS:HG2	20:L:30:THR:N	2.36	0.41
21:M:63:ILE:HG22	21:M:64:TRP:N	2.36	0.41
24:P:92:ARG:HH11	24:P:92:ARG:HB2	1.85	0.41
27:S:69:LEU:HG	27:S:107:VAL:HG22	2.03	0.41
27:S:88:ARG:HD2	27:S:94:ASP:OD2	2.20	0.41
30:V:6:ALA:HB1	30:V:40:ILE:CG2	2.50	0.41
31:W:19:ARG:HG2	31:W:19:ARG:HH21	1.86	0.41
9:A:58:G:N2	9:A:70:G:C4	2.89	0.41
9:A:301:G:H2’	9:A:334:C:H2’	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:996:A:C6	9:A:1160:G:C2	3.08	0.41
9:A:1069:A:C2'	9:A:1070:A:OP2	2.68	0.41
9:A:1301:A:N3	9:A:1301:A:H2'	2.35	0.41
9:A:1392:A:C6	9:A:1393:A:C6	3.09	0.41
9:A:1494:A:C6	9:A:1495:A:C6	3.08	0.41
9:A:1868:C:O2	9:A:1873:G:N2	2.44	0.41
9:A:2298:A:C6	9:A:2321:U:C4	3.09	0.41
9:A:2409:G:H2'	9:A:2410:G:O4'	2.20	0.41
13:E:109:LEU:O	13:E:112:LEU:N	2.54	0.41
18:J:35:ARG:HG2	18:J:40:HIS:HD2	1.85	0.41
18:J:88:THR:HG23	18:J:91:GLU:H	1.86	0.41
22:N:24:MET:CE	22:N:36:THR:HG21	2.51	0.41
22:N:87:PHE:O	22:N:89:SER:N	2.54	0.41
23:O:49:VAL:HG12	23:O:50:ALA:N	2.35	0.41
34:Z:2:LYS:CB	34:Z:39:ASP:HB3	2.51	0.41
6:5:131:THR:HA	6:5:134:GLU:HG3	2.03	0.41
9:A:535:G:C6	9:A:559:G:C6	3.09	0.41
9:A:1069:A:N3	9:A:1073:A:C6	2.88	0.41
9:A:1403:A:C2	9:A:1404:C:C2	3.09	0.41
9:A:1509:A:H1'	9:A:1510:G:O5'	2.20	0.41
9:A:1714:U:H5'	9:A:1715:G:H5'	2.02	0.41
9:A:2070:A:C2	9:A:2071:A:C4	3.09	0.41
9:A:2180:U:N3	9:A:2181:U:C5	2.89	0.41
9:A:2601:C:C2	9:A:2603:G:N7	2.89	0.41
9:A:2682:A:C8	12:D:11:MET:CG	3.04	0.41
17:I:104:GLN:O	17:I:105:LEU:CB	2.69	0.41
22:N:51:LEU:HD21	22:N:70:THR:CG2	2.51	0.41
24:P:50:ARG:CD	24:P:56:SER:HB3	2.51	0.41
26:R:38:VAL:O	26:R:53:PHE:HA	2.20	0.41
27:S:18:ARG:HG3	27:S:76:VAL:CG1	2.50	0.41
33:Y:12:GLU:O	33:Y:15:ASN:HB2	2.21	0.41
1:0:12:ARG:HD2	1:0:16:ARG:NH2	2.36	0.41
5:4:32:LYS:HD3	9:A:2478:A:H5'	2.02	0.41
6:5:47:GLU:CG	6:5:95:LEU:HD21	2.51	0.41
6:5:59:LEU:HD23	6:5:62:ARG:HE	1.85	0.41
9:A:138:U:H5'	9:A:139:U:C5'	2.51	0.41
9:A:307:G:N2	9:A:310:A:C8	2.89	0.41
9:A:659:G:H4'	13:E:95:LYS:HD3	2.02	0.41
9:A:749:A:C5	9:A:1618:A:C2	3.09	0.41
9:A:1063:G:H2'	9:A:1064:C:O4'	2.20	0.41
9:A:1068:G:H3'	9:A:1069:A:H5"	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1078:U:H5”	9:A:1079:C:OP1	2.20	0.41
9:A:1378:A:H4’	9:A:1379:U:OP1	2.20	0.41
9:A:2017:U:H5”	9:A:2018:G:P	2.61	0.41
9:A:2038:G:H2’	9:A:2039:U:O4’	2.21	0.41
9:A:2103:C:N4	9:A:2186:G:H1	2.19	0.41
9:A:2145:C:N3	9:A:2146:C:N3	2.69	0.41
9:A:2674:G:H4’	19:K:30:ARG:HG3	2.02	0.41
10:B:114:C:H1’	23:O:47:VAL:HG11	2.03	0.41
11:C:143:VAL:HB	11:C:153:LEU:HB2	2.02	0.41
13:E:187:VAL:HG12	13:E:188:MET:N	2.36	0.41
14:F:46:LYS:H	14:F:46:LYS:HD3	1.86	0.41
14:F:112:ASP:N	14:F:112:ASP:OD1	2.54	0.41
15:G:68:ARG:HH21	15:G:72:ASN:ND2	2.19	0.41
17:I:52:LEU:HB3	17:I:53:PRO:CD	2.51	0.41
19:K:71:ARG:O	19:K:72:PRO:O	2.39	0.41
22:N:12:ARG:HB3	22:N:16:HIS:HB3	2.01	0.41
23:O:75:GLY:HA3	23:O:106:LEU:HA	2.03	0.41
26:R:80:ARG:O	26:R:81:LYS:HD3	2.20	0.41
29:U:98:ASN:O	29:U:99:SER:C	2.59	0.41
31:W:19:ARG:NH2	31:W:22:VAL:CG2	2.83	0.41
33:Y:2:LYS:HD2	33:Y:2:LYS:N	2.36	0.41
6:5:88:HIS:HB3	6:5:89:PRO:HD3	2.03	0.41
9:A:301:G:C6	9:A:317:G:C6	3.09	0.41
9:A:629:G:H4’	9:A:650:C:O2	2.21	0.41
9:A:2845:U:H5”	24:P:51:ASN:O	2.20	0.41
12:D:104:VAL:HG12	12:D:106:LYS:H	1.86	0.41
14:F:148:VAL:HG23	14:F:149:ARG:N	2.36	0.41
15:G:19:ASN:O	15:G:22:VAL:HG22	2.21	0.41
16:H:24:GLY:O	16:H:28:ASN:HB2	2.21	0.41
19:K:19:VAL:HG13	19:K:41:ILE:HG12	2.02	0.41
21:M:12:MET:HE3	21:M:71:LYS:HG3	2.03	0.41
25:Q:46:TYR:CZ	25:Q:50:ARG:NH2	2.89	0.41
31:W:22:VAL:O	31:W:23:LYS:HG3	2.21	0.41
6:5:23:LEU:HD22	6:5:92:ALA:O	2.21	0.40
6:5:111:ALA:C	6:5:113:PHE:N	2.75	0.40
9:A:176:A:N7	9:A:177:G:C6	2.89	0.40
9:A:635:C:P	20:L:126:ARG:HH11	2.44	0.40
9:A:783:A:C8	9:A:784:G:H4’	2.56	0.40
9:A:996:A:C5	9:A:1160:G:N2	2.89	0.40
9:A:2868:A:C2	9:A:2869:G:C4	3.09	0.40
11:C:158:GLY:H	11:C:194:VAL:HG22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:184:GLU:O	11:C:185:ALA:HB3	2.20	0.40
12:D:46:ARG:HH21	12:D:86:GLU:H	1.69	0.40
17:I:19:PRO:HG2	17:I:24:GLY:H	1.86	0.40
23:O:7:ARG:HA	23:O:10:ARG:NH2	2.36	0.40
24:P:30:TRP:CE3	24:P:39:LEU:HD12	2.56	0.40
31:W:39:GLN:OE1	31:W:43:LYS:HB2	2.21	0.40
31:W:67:LYS:O	31:W:68:PHE:HB2	2.20	0.40
9:A:84:A:P	29:U:5:ARG:HH22	2.42	0.40
9:A:580:U:O3'	25:Q:30:VAL:CG1	2.70	0.40
9:A:1579:A:H2'	9:A:1580:A:C8	2.56	0.40
9:A:1613:G:O6	9:A:1617:C:H2'	2.21	0.40
9:A:1905:C:N4	9:A:1930:G:C2	2.89	0.40
9:A:2766:A:N3	9:A:2766:A:H2'	2.36	0.40
11:C:172:THR:HG22	11:C:182:LYS:HG2	2.02	0.40
12:D:68:PHE:CE2	12:D:75:ALA:HB1	2.56	0.40
21:M:64:TRP:HZ3	21:M:106:ASP:HB2	1.86	0.40
32:X:67:LEU:HD22	32:X:77:TYR:CZ	2.57	0.40
3:2:9:VAL:HG13	9:A:1309:G:OP1	2.21	0.40
5:4:38:GLY:OXT	9:A:1124:G:H1'	2.21	0.40
9:A:230:G:N2	9:A:231:A:C4	2.90	0.40
9:A:364:C:H2'	9:A:365:U:H6	1.87	0.40
9:A:544:C:N4	9:A:548:G:OP1	2.45	0.40
9:A:811:U:H2'	20:L:21:ARG:HA	2.04	0.40
9:A:1773:A:N7	9:A:1829:A:C1'	2.85	0.40
9:A:2347:C:H2'	9:A:2348:U:C6	2.56	0.40
10:B:77:U:OP1	30:V:21:ARG:NH1	2.54	0.40
11:C:254:LYS:O	11:C:256:THR:N	2.51	0.40
14:F:148:VAL:HG23	14:F:149:ARG:H	1.87	0.40
15:G:10:VAL:HG22	15:G:47:ASN:C	2.41	0.40
17:I:100:ILE:CD1	17:I:137:LEU:HD12	2.51	0.40
20:L:127:VAL:HG11	20:L:142:ILE:HG21	2.03	0.40
29:U:82:VAL:HG13	29:U:93:ARG:HB3	2.03	0.40
1:0:33:SER:OG	1:0:35:GLU:HG3	2.21	0.40
2:1:35:LEU:HD22	2:1:35:LEU:N	2.37	0.40
4:3:30:HIS:ND1	4:3:31:ILE:HG23	2.37	0.40
6:5:91:ALA:C	6:5:93:ALA:N	2.66	0.40
9:A:136:G:H1	9:A:143:C:H42	1.69	0.40
9:A:347:A:C2	9:A:348:A:C4	3.09	0.40
9:A:669:G:N3	9:A:669:G:C2'	2.83	0.40
9:A:1096:A:N6	9:A:1097:U:C4	2.89	0.40
9:A:1149:G:H2'	9:A:1150:C:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1365:A:OP1	32:X:2:ARG:NE	2.48	0.40
9:A:1967:C:H2'	9:A:1968:G:H5'	2.03	0.40
9:A:2318:G:C5	9:A:2319:G:C6	3.10	0.40
9:A:2469:A:C6	9:A:2482:A:C8	3.10	0.40
9:A:2555:U:C5	9:A:2556:C:C2	3.09	0.40
36:A:9000:ERY:H343	36:A:9000:ERY:O13	2.21	0.40
12:D:106:LYS:HB3	12:D:206:ALA:CB	2.52	0.40
14:F:111:ARG:HA	14:F:111:ARG:CZ	2.51	0.40
15:G:137:LYS:HA	15:G:140:ILE:HG22	2.02	0.40
17:I:11:GLN:OE1	17:I:11:GLN:N	2.43	0.40
19:K:39:ILE:HD12	19:K:41:ILE:HD11	2.02	0.40
6:5:34:THR:O	6:5:38:MET:HG3	2.22	0.40
6:5:132:TYR:HE1	7:6:19:VAL:HG13	1.85	0.40
9:A:45:G:C5'	9:A:46:G:H5'	2.51	0.40
9:A:528:A:H2	9:A:2043:C:C5'	2.34	0.40
9:A:841:G:C2	9:A:938:G:C2	3.10	0.40
9:A:1847:A:H4'	9:A:1848:A:OP2	2.21	0.40
9:A:1864:U:O3'	9:A:2409:G:N2	2.54	0.40
9:A:2134:A:H2'	9:A:2135:A:H8	1.85	0.40
9:A:2514:U:H2'	9:A:2515:C:C6	2.57	0.40
9:A:2537:U:C4	9:A:2538:C:N4	2.89	0.40
9:A:2681:C:C2	9:A:2724:U:O4	2.74	0.40
9:A:2684:U:C4	9:A:2685:G:N7	2.90	0.40
11:C:115:ILE:HG22	11:C:116:GLN:N	2.36	0.40
12:D:88:GLU:O	12:D:89:GLU:HG3	2.21	0.40
13:E:178:VAL:HG23	13:E:179:SER:N	2.36	0.40
14:F:114:ARG:N	14:F:114:ARG:HD2	2.37	0.40
17:I:14:ALA:HB1	17:I:45:THR:CG2	2.52	0.40
18:J:26:GLY:HA2	18:J:29:ALA:HB3	2.02	0.40
19:K:76:VAL:HG12	19:K:77:ILE:N	2.37	0.40
29:U:12:VAL:HG21	29:U:38:ILE:CD1	2.52	0.40
31:W:19:ARG:HG2	31:W:19:ARG:NH2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	0	54/57 (95%)	43 (80%)	7 (13%)	4 (7%)	1 16
2	1	48/55 (87%)	42 (88%)	3 (6%)	3 (6%)	1 19
3	2	44/46 (96%)	41 (93%)	3 (7%)	0	100 100
4	3	62/65 (95%)	53 (86%)	7 (11%)	2 (3%)	4 32
5	4	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	1 14
6	5	146/165 (88%)	77 (53%)	40 (27%)	29 (20%)	0 2
7	6	28/121 (23%)	20 (71%)	7 (25%)	1 (4%)	3 29
11	C	269/273 (98%)	211 (78%)	43 (16%)	15 (6%)	2 21
12	D	207/209 (99%)	163 (79%)	30 (14%)	14 (7%)	1 18
13	E	199/201 (99%)	162 (81%)	27 (14%)	10 (5%)	2 23
14	F	175/179 (98%)	141 (81%)	30 (17%)	4 (2%)	6 38
15	G	174/177 (98%)	127 (73%)	30 (17%)	17 (10%)	0 10
16	H	48/149 (32%)	29 (60%)	14 (29%)	5 (10%)	0 9
17	I	139/142 (98%)	97 (70%)	33 (24%)	9 (6%)	1 19
18	J	140/142 (99%)	113 (81%)	18 (13%)	9 (6%)	1 19
19	K	120/123 (98%)	95 (79%)	15 (12%)	10 (8%)	1 14
20	L	141/144 (98%)	104 (74%)	32 (23%)	5 (4%)	3 30
21	M	134/136 (98%)	107 (80%)	16 (12%)	11 (8%)	1 14
22	N	118/127 (93%)	101 (86%)	16 (14%)	1 (1%)	19 57
23	O	114/117 (97%)	95 (83%)	18 (16%)	1 (1%)	17 54
24	P	112/115 (97%)	86 (77%)	17 (15%)	9 (8%)	1 15
25	Q	115/118 (98%)	99 (86%)	12 (10%)	4 (4%)	3 30
26	R	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	4 33
27	S	108/110 (98%)	94 (87%)	9 (8%)	5 (5%)	2 25
28	T	91/100 (91%)	57 (63%)	24 (26%)	10 (11%)	0 8
29	U	100/104 (96%)	74 (74%)	16 (16%)	10 (10%)	0 10
30	V	92/94 (98%)	81 (88%)	11 (12%)	0	100 100
31	W	77/85 (91%)	39 (51%)	22 (29%)	16 (21%)	0 2
32	X	75/78 (96%)	64 (85%)	8 (11%)	3 (4%)	3 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
33	Y	61/63 (97%)	39 (64%)	18 (30%)	4 (7%)	1 19
34	Z	56/59 (95%)	46 (82%)	8 (14%)	2 (4%)	3 29
35	a	1/19 (5%)	1 (100%)	0	0	100 100
All	All	3385/3714 (91%)	2613 (77%)	553 (16%)	219 (6%)	2 19

All (219) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	23	ALA
4	3	22	LYS
5	4	8	LYS
6	5	27	VAL
6	5	48	ALA
6	5	54	VAL
6	5	55	VAL
6	5	58	THR
6	5	69	PHE
6	5	93	ALA
6	5	107	GLU
6	5	108	VAL
6	5	120	ALA
6	5	124	ASP
6	5	130	PRO
11	C	70	LYS
11	C	104	LEU
11	C	121	ALA
11	C	140	VAL
12	D	43	ASP
12	D	73	VAL
12	D	170	VAL
13	E	79	ARG
14	F	111	ARG
15	G	2	ARG
15	G	16	VAL
15	G	28	LYS
15	G	31	GLU
15	G	84	LYS
15	G	164	ALA
15	G	168	VAL
16	H	3	VAL
18	J	13	ARG

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Mol	Chain	Res	Type
18	J	21	THR
18	J	44	TYR
18	J	45	THR
18	J	81	ILE
18	J	125	TYR
20	L	66	PHE
21	M	14	LYS
21	M	77	PRO
22	N	119	SER
24	P	50	ARG
24	P	51	ASN
24	P	93	LYS
27	S	3	THR
27	S	14	ALA
27	S	64	ALA
28	T	27	SER
28	T	29	THR
28	T	40	LYS
29	U	6	ARG
29	U	87	GLU
29	U	92	VAL
29	U	98	ASN
29	U	99	SER
31	W	9	THR
31	W	18	LYS
31	W	29	SER
31	W	36	ILE
31	W	56	HIS
34	Z	9	THR
1	0	35	GLU
2	1	4	ILE
2	1	50	GLU
6	5	3	LEU
6	5	33	VAL
6	5	88	HIS
6	5	92	ALA
6	5	116	GLU
6	5	119	PRO
11	C	37	SER
11	C	77	VAL
11	C	238	ASN
11	C	256	THR

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Mol	Chain	Res	Type
12	D	92	VAL
12	D	99	GLU
12	D	107	VAL
12	D	118	PHE
14	F	135	ILE
14	F	176	PHE
15	G	169	ARG
16	H	9	VAL
16	H	16	GLY
17	I	20	SER
17	I	79	LEU
18	J	111	LYS
19	K	35	VAL
19	K	71	ARG
20	L	111	ILE
21	M	2	LEU
21	M	36	VAL
21	M	56	ALA
26	R	65	ALA
27	S	19	LEU
27	S	96	ILE
28	T	36	LYS
28	T	49	LYS
29	U	51	LEU
31	W	14	ASP
31	W	47	GLY
31	W	50	VAL
31	W	74	LYS
33	Y	37	LEU
2	1	51	ALA
5	4	4	ARG
6	5	5	LEU
6	5	78	GLY
6	5	118	ILE
7	6	14	MET
11	C	110	LYS
12	D	95	SER
12	D	109	VAL
12	D	192	ALA
13	E	7	ASP
13	E	70	SER
13	E	123	LYS

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Mol	Chain	Res	Type
15	G	32	LEU
15	G	117	PRO
15	G	170	THR
16	H	10	ALA
17	I	11	GLN
18	J	74	TYR
19	K	13	ASN
19	K	46	ALA
19	K	93	GLN
21	M	69	PRO
23	O	3	LYS
24	P	113	LEU
26	R	98	ILE
29	U	85	ARG
29	U	101	THR
31	W	34	SER
32	X	17	ARG
32	X	34	SER
34	Z	34	THR
1	0	54	ILE
5	4	16	ILE
6	5	89	PRO
11	C	59	GLN
11	C	197	ALA
12	D	169	ARG
12	D	175	LEU
14	F	132	ARG
15	G	33	THR
15	G	173	ALA
17	I	64	ARG
19	K	119	ALA
20	L	29	LYS
21	M	23	GLY
21	M	134	THR
24	P	4	ILE
24	P	92	ARG
24	P	103	THR
25	Q	87	VAL
25	Q	88	GLU
25	Q	95	ALA
28	T	28	ASN
28	T	51	PHE

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Mol	Chain	Res	Type
28	T	55	VAL
31	W	37	VAL
32	X	76	LYS
33	Y	7	ARG
6	5	36	ASP
6	5	72	LEU
6	5	128	THR
11	C	64	VAL
11	C	120	ASP
11	C	196	ASN
12	D	183	GLU
13	E	46	GLN
13	E	96	VAL
15	G	97	VAL
15	G	163	TYR
15	G	166	GLU
17	I	12	VAL
17	I	71	LYS
18	J	65	THR
19	K	49	ARG
19	K	108	ARG
20	L	5	THR
20	L	41	ARG
21	M	35	ALA
21	M	73	ILE
24	P	34	GLY
25	Q	85	ALA
28	T	86	THR
28	T	89	GLU
29	U	88	ASP
31	W	46	ALA
31	W	76	ARG
33	Y	9	LYS
6	5	59	LEU
6	5	94	ARG
6	5	102	ALA
13	E	83	VAL
13	E	153	LEU
15	G	118	ALA
16	H	14	SER
17	I	93	ASN
19	K	6	THR

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Mol	Chain	Res	Type
19	K	50	GLY
21	M	13	HIS
26	R	40	MET
29	U	16	LYS
31	W	10	ARG
31	W	78	PHE
24	P	63	ILE
31	W	41	GLY
6	5	32	GLY
13	E	148	ILE
33	Y	62	GLY
4	3	6	VAL
11	C	232	GLY
12	D	122	VAL
17	I	22	PRO
17	I	88	GLY
1	0	24	VAL
13	E	71	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	47/48 (98%)	46 (98%)	1 (2%)	53 73
2	1	45/49 (92%)	42 (93%)	3 (7%)	16 46
3	2	38/38 (100%)	35 (92%)	3 (8%)	12 41
4	3	51/52 (98%)	46 (90%)	5 (10%)	8 31
5	4	34/34 (100%)	31 (91%)	3 (9%)	10 37
6	5	112/123 (91%)	93 (83%)	19 (17%)	2 14
7	6	26/85 (31%)	22 (85%)	4 (15%)	2 17
11	C	216/218 (99%)	202 (94%)	14 (6%)	17 46
12	D	164/164 (100%)	151 (92%)	13 (8%)	12 41
13	E	165/165 (100%)	146 (88%)	19 (12%)	5 26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	F	148/150 (99%)	138 (93%)	10 (7%)	16 45
15	G	137/138 (99%)	122 (89%)	15 (11%)	6 28
16	H	40/114 (35%)	39 (98%)	1 (2%)	47 69
17	I	109/110 (99%)	105 (96%)	4 (4%)	34 60
18	J	116/116 (100%)	100 (86%)	16 (14%)	3 21
19	K	103/104 (99%)	92 (89%)	11 (11%)	6 29
20	L	102/103 (99%)	95 (93%)	7 (7%)	15 45
21	M	109/109 (100%)	93 (85%)	16 (15%)	3 19
22	N	100/103 (97%)	93 (93%)	7 (7%)	15 44
23	O	86/87 (99%)	78 (91%)	8 (9%)	9 34
24	P	99/100 (99%)	91 (92%)	8 (8%)	11 40
25	Q	89/90 (99%)	81 (91%)	8 (9%)	9 36
26	R	84/84 (100%)	78 (93%)	6 (7%)	14 44
27	S	93/93 (100%)	84 (90%)	9 (10%)	8 32
28	T	80/84 (95%)	77 (96%)	3 (4%)	33 59
29	U	83/85 (98%)	76 (92%)	7 (8%)	11 39
30	V	78/78 (100%)	75 (96%)	3 (4%)	33 59
31	W	59/63 (94%)	53 (90%)	6 (10%)	7 30
32	X	67/68 (98%)	61 (91%)	6 (9%)	9 36
33	Y	55/55 (100%)	52 (94%)	3 (6%)	21 51
34	Z	48/49 (98%)	40 (83%)	8 (17%)	2 15
35	a	4/18 (22%)	4 (100%)	0	100 100
All	All	2787/2977 (94%)	2541 (91%)	246 (9%)	13 37

All (246) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	24	VAL
2	1	8	ILE
2	1	35	LEU
2	1	47	ILE
3	2	8	SER
3	2	9	VAL
3	2	24	THR

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Mol	Chain	Res	Type
4	3	7	ARG
4	3	30	HIS
4	3	31	ILE
4	3	49	VAL
4	3	56	LEU
5	4	4	ARG
5	4	15	LYS
5	4	27	CYS
6	5	1	MET
6	5	3	LEU
6	5	26	VAL
6	5	42	ARG
6	5	51	TYR
6	5	54	VAL
6	5	59	LEU
6	5	65	GLU
6	5	69	PHE
6	5	70	GLU
6	5	96	PHE
6	5	106	PHE
6	5	107	GLU
6	5	116	GLU
6	5	121	SER
6	5	125	ARG
6	5	130	PRO
6	5	132	TYR
6	5	143	MET
7	6	17	MET
7	6	18	ASP
7	6	24	SER
7	6	26	MET
11	C	51	ARG
11	C	57	HIS
11	C	109	LEU
11	C	117	SER
11	C	124	LYS
11	C	129	LEU
11	C	142	ASN
11	C	155	ARG
11	C	166	ARG
11	C	176	ARG
11	C	194	VAL

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Mol	Chain	Res	Type
11	C	212	TRP
11	C	251	THR
11	C	270	ARG
12	D	33	ARG
12	D	37	VAL
12	D	97	SER
12	D	103	ASP
12	D	107	VAL
12	D	118	PHE
12	D	124	ARG
12	D	170	VAL
12	D	171	THR
12	D	177	VAL
12	D	183	GLU
12	D	201	LEU
12	D	203	VAL
13	E	5	LEU
13	E	12	LEU
13	E	21	ARG
13	E	40	ARG
13	E	44	ARG
13	E	65	THR
13	E	69	ARG
13	E	70	SER
13	E	78	TRP
13	E	88	ARG
13	E	109	LEU
13	E	113	VAL
13	E	118	LEU
13	E	120	VAL
13	E	126	VAL
13	E	131	THR
13	E	149	ILE
13	E	167	VAL
13	E	171	ASP
14	F	9	ASP
14	F	16	MET
14	F	34	THR
14	F	41	GLU
14	F	46	LYS
14	F	90	LEU
14	F	94	ARG

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Mol	Chain	Res	Type
14	F	111	ARG
14	F	114	ARG
14	F	154	THR
15	G	3	VAL
15	G	16	VAL
15	G	44	HIS
15	G	68	ARG
15	G	84	LYS
15	G	94	ARG
15	G	103	ASN
15	G	110	HIS
15	G	121	THR
15	G	126	THR
15	G	131	VAL
15	G	132	LEU
15	G	151	ARG
15	G	170	THR
15	G	176	LYS
16	H	3	VAL
17	I	23	VAL
17	I	63	ASP
17	I	102	ARG
17	I	137	LEU
18	J	2	LYS
18	J	17	VAL
18	J	24	THR
18	J	30	THR
18	J	36	LEU
18	J	40	HIS
18	J	54	ILE
18	J	55	ILE
18	J	65	THR
18	J	72	LYS
18	J	73	VAL
18	J	95	ARG
18	J	103	ILE
18	J	129	GLU
18	J	131	ASN
18	J	140	LEU
19	K	3	GLN
19	K	8	LEU
19	K	13	ASN

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Mol	Chain	Res	Type
19	K	18	ARG
19	K	21	CYS
19	K	23	LYS
19	K	41	ILE
19	K	54	LYS
19	K	73	ASP
19	K	93	GLN
19	K	105	ARG
20	L	5	THR
20	L	19	LEU
20	L	82	LEU
20	L	91	ASP
20	L	100	ILE
20	L	121	THR
20	L	144	GLU
21	M	12	MET
21	M	13	HIS
21	M	31	PHE
21	M	33	LEU
21	M	46	ILE
21	M	53	MET
21	M	70	ASP
21	M	72	PRO
21	M	81	ARG
21	M	88	ASN
21	M	95	LEU
21	M	96	ILE
21	M	97	GLN
21	M	100	LYS
21	M	110	GLU
21	M	134	THR
22	N	6	SER
22	N	8	ARG
22	N	33	ILE
22	N	65	LEU
22	N	69	ARG
22	N	70	THR
22	N	71	ARG
23	O	18	LEU
23	O	31	THR
23	O	33	ARG
23	O	36	TYR

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Mol	Chain	Res	Type
23	O	38	GLN
23	O	47	VAL
23	O	106	LEU
23	O	115	LEU
24	P	16	VAL
24	P	19	PHE
24	P	62	LYS
24	P	83	ILE
24	P	85	VAL
24	P	92	ARG
24	P	95	LYS
24	P	103	THR
25	Q	16	ILE
25	Q	40	LYS
25	Q	50	ARG
25	Q	59	LEU
25	Q	63	ARG
25	Q	88	GLU
25	Q	93	ILE
25	Q	97	ILE
26	R	4	VAL
26	R	29	THR
26	R	38	VAL
26	R	46	GLU
26	R	48	LYS
26	R	63	VAL
27	S	3	THR
27	S	4	ILE
27	S	7	HIS
27	S	36	LEU
27	S	45	VAL
27	S	66	ILE
27	S	76	VAL
27	S	96	ILE
27	S	101	SER
28	T	32	LEU
28	T	43	ILE
28	T	58	VAL
29	U	6	ARG
29	U	26	ASN
29	U	30	SER
29	U	38	ILE

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Mol	Chain	Res	Type
29	U	61	GLU
29	U	86	PHE
29	U	92	VAL
30	V	29	ILE
30	V	61	LEU
30	V	87	GLN
31	W	19	ARG
31	W	23	LYS
31	W	25	PHE
31	W	30	VAL
31	W	49	ASN
31	W	63	ASP
32	X	19	HIS
32	X	24	THR
32	X	26	ARG
32	X	29	LEU
32	X	34	SER
32	X	77	TYR
33	Y	10	SER
33	Y	16	THR
33	Y	57	LEU
34	Z	2	LYS
34	Z	9	THR
34	Z	15	ARG
34	Z	23	LEU
34	Z	30	ARG
34	Z	31	ILE
34	Z	37	ARG
34	Z	40	THR

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

Mol	Chain	Res	Type
4	3	30	HIS
14	F	26	GLN
27	S	15	GLN
30	V	44	HIS
30	V	80	HIS
33	Y	41	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	B	117/118 (99%)	17 (14%)	0
8	7	1/3 (33%)	0	0
9	A	2850/2903 (98%)	466 (16%)	43 (1%)
All	All	2968/3024 (98%)	483 (16%)	43 (1%)

All (483) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	A	10	A
9	A	12	U
9	A	15	G
9	A	34	U
9	A	35	G
9	A	42	A
9	A	43	G
9	A	45	G
9	A	46	G
9	A	51	G
9	A	61	C
9	A	71	A
9	A	74	A
9	A	75	G
9	A	80	G
9	A	82	U
9	A	84	A
9	A	96	C
9	A	101	A
9	A	118	A
9	A	119	A
9	A	120	U
9	A	131	A
9	A	135	U
9	A	136	G
9	A	137	U
9	A	138	U
9	A	139	U
9	A	140	C
9	A	141	G
9	A	142	A
9	A	144	A
9	A	149	A
9	A	162	U
9	A	163	C

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Mol	Chain	Res	Type
9	A	164	C
9	A	181	A
9	A	188	G
9	A	196	A
9	A	199	A
9	A	215	G
9	A	216	A
9	A	222	A
9	A	226	A
9	A	230	G
9	A	248	G
9	A	255	A
9	A	264	C
9	A	265	A
9	A	266	G
9	A	267	C
9	A	272	A
9	A	273	G
9	A	276	U
9	A	277	G
9	A	278	A
9	A	281	C
9	A	285	G
9	A	302	C
9	A	311	A
9	A	329	G
9	A	330	A
9	A	346	A
9	A	347	A
9	A	353	C
9	A	355	U
9	A	361	G
9	A	362	A
9	A	371	A
9	A	372	G
9	A	382	A
9	A	383	C
9	A	386	G
9	A	388	G
9	A	396	G
9	A	404	A
9	A	405	U

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Mol	Chain	Res	Type
9	A	411	G
9	A	412	A
9	A	424	G
9	A	451	U
9	A	455	C
9	A	481	G
9	A	491	G
9	A	503	A
9	A	504	A
9	A	505	A
9	A	509	C
9	A	528	A
9	A	531	C
9	A	532	A
9	A	533	G
9	A	538	A
9	A	543	G
9	A	544	C
9	A	546	U
9	A	547	A
9	A	548	G
9	A	549	G
9	A	563	A
9	A	573	U
9	A	575	A
9	A	586	A
9	A	603	A
9	A	604	G
9	A	613	A
9	A	614	A
9	A	615	U
9	A	627	A
9	A	631	A
9	A	637	A
9	A	645	C
9	A	646	U
9	A	647	G
9	A	648	G
9	A	654	A
9	A	655	A
9	A	656	G
9	A	686	U

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Mol	Chain	Res	Type
9	A	714	U
9	A	715	A
9	A	730	A
9	A	738	G
9	A	747	U
9	A	775	G
9	A	776	G
9	A	782	A
9	A	784	G
9	A	785	G
9	A	805	G
9	A	812	C
9	A	819	A
9	A	827	U
9	A	828	U
9	A	845	A
9	A	846	U
9	A	847	U
9	A	859	G
9	A	878	A
9	A	883	G
9	A	884	U
9	A	896	A
9	A	897	C
9	A	910	A
9	A	914	G
9	A	915	C
9	A	932	U
9	A	941	A
9	A	946	C
9	A	961	C
9	A	974	G
9	A	983	A
9	A	985	C
9	A	995	C
9	A	996	A
9	A	1003	G
9	A	1012	U
9	A	1013	C
9	A	1021	A
9	A	1022	G
9	A	1023	U

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Mol	Chain	Res	Type
9	A	1025	G
9	A	1026	G
9	A	1033	U
9	A	1045	C
9	A	1046	A
9	A	1047	G
9	A	1051	G
9	A	1053	C
9	A	1059	G
9	A	1060	U
9	A	1061	U
9	A	1062	G
9	A	1067	A
9	A	1069	A
9	A	1070	A
9	A	1072	C
9	A	1074	G
9	A	1078	U
9	A	1083	U
9	A	1084	A
9	A	1088	A
9	A	1089	A
9	A	1090	A
9	A	1091	G
9	A	1097	U
9	A	1098	A
9	A	1110	G
9	A	1111	A
9	A	1112	G
9	A	1129	A
9	A	1132	U
9	A	1133	A
9	A	1135	C
9	A	1136	G
9	A	1139	G
9	A	1142	A
9	A	1151	A
9	A	1155	A
9	A	1169	A
9	A	1170	C
9	A	1172	C
9	A	1174	U

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Mol	Chain	Res	Type
9	A	1175	A
9	A	1176	U
9	A	1180	U
9	A	1186	G
9	A	1238	G
9	A	1248	G
9	A	1250	G
9	A	1253	A
9	A	1256	G
9	A	1266	G
9	A	1268	A
9	A	1271	G
9	A	1272	A
9	A	1273	U
9	A	1281	G
9	A	1300	G
9	A	1301	A
9	A	1313	U
9	A	1317	G
9	A	1352	U
9	A	1365	A
9	A	1368	G
9	A	1378	A
9	A	1379	U
9	A	1383	A
9	A	1395	A
9	A	1415	U
9	A	1416	G
9	A	1419	A
9	A	1420	A
9	A	1428	C
9	A	1435	G
9	A	1452	G
9	A	1459	G
9	A	1482	G
9	A	1493	C
9	A	1504	A
9	A	1508	A
9	A	1510	G
9	A	1515	A
9	A	1524	G
9	A	1533	C

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Mol	Chain	Res	Type
9	A	1534	U
9	A	1535	A
9	A	1536	C
9	A	1566	A
9	A	1569	A
9	A	1578	U
9	A	1583	A
9	A	1584	U
9	A	1585	C
9	A	1607	C
9	A	1608	A
9	A	1610	A
9	A	1613	G
9	A	1627	G
9	A	1647	U
9	A	1648	U
9	A	1649	G
9	A	1652	A
9	A	1653	G
9	A	1674	G
9	A	1714	U
9	A	1715	G
9	A	1723	G
9	A	1729	U
9	A	1730	C
9	A	1737	G
9	A	1738	G
9	A	1739	A
9	A	1744	A
9	A	1758	U
9	A	1764	C
9	A	1773	A
9	A	1776	G
9	A	1791	A
9	A	1800	C
9	A	1801	A
9	A	1802	A
9	A	1808	A
9	A	1811	G
9	A	1816	C
9	A	1829	A
9	A	1833	C

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Mol	Chain	Res	Type
9	A	1847	A
9	A	1848	A
9	A	1858	A
9	A	1869	G
9	A	1870	C
9	A	1871	A
9	A	1872	A
9	A	1873	G
9	A	1884	G
9	A	1906	G
9	A	1913	A
9	A	1914	C
9	A	1927	A
9	A	1929	G
9	A	1930	G
9	A	1937	A
9	A	1938	A
9	A	1955	U
9	A	1960	A
9	A	1966	A
9	A	1967	C
9	A	1970	A
9	A	1971	U
9	A	1972	G
9	A	1991	U
9	A	1993	U
9	A	1997	C
9	A	2017	U
9	A	2020	A
9	A	2022	U
9	A	2023	C
9	A	2031	A
9	A	2033	A
9	A	2043	C
9	A	2055	C
9	A	2056	G
9	A	2060	A
9	A	2061	G
9	A	2063	C
9	A	2064	C
9	A	2069	G
9	A	2072	C

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Mol	Chain	Res	Type
9	A	2093	G
9	A	2104	C
9	A	2106	U
9	A	2107	G
9	A	2108	A
9	A	2109	U
9	A	2110	G
9	A	2134	A
9	A	2135	A
9	A	2137	U
9	A	2138	G
9	A	2139	U
9	A	2140	G
9	A	2142	A
9	A	2143	C
9	A	2144	G
9	A	2145	C
9	A	2146	C
9	A	2147	A
9	A	2148	G
9	A	2149	U
9	A	2150	C
9	A	2151	U
9	A	2153	C
9	A	2154	A
9	A	2155	U
9	A	2156	G
9	A	2157	G
9	A	2180	U
9	A	2183	A
9	A	2185	U
9	A	2194	U
9	A	2198	A
9	A	2199	A
9	A	2204	G
9	A	2211	A
9	A	2212	A
9	A	2214	C
9	A	2225	A
9	A	2226	C
9	A	2238	G
9	A	2239	G

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Mol	Chain	Res	Type
9	A	2250	G
9	A	2268	A
9	A	2278	A
9	A	2283	C
9	A	2284	A
9	A	2286	G
9	A	2287	A
9	A	2305	U
9	A	2308	G
9	A	2311	A
9	A	2322	A
9	A	2325	G
9	A	2327	A
9	A	2333	A
9	A	2336	A
9	A	2347	C
9	A	2354	C
9	A	2361	G
9	A	2383	G
9	A	2385	C
9	A	2402	U
9	A	2403	C
9	A	2406	A
9	A	2423	U
9	A	2424	C
9	A	2425	A
9	A	2429	G
9	A	2430	A
9	A	2435	A
9	A	2441	U
9	A	2448	A
9	A	2470	G
9	A	2476	A
9	A	2491	U
9	A	2502	G
9	A	2503	A
9	A	2504	U
9	A	2505	G
9	A	2506	U
9	A	2508	G
9	A	2518	A
9	A	2529	G

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Mol	Chain	Res	Type
9	A	2554	U
9	A	2556	C
9	A	2566	A
9	A	2567	G
9	A	2572	A
9	A	2573	C
9	A	2575	C
9	A	2576	G
9	A	2577	A
9	A	2583	G
9	A	2585	U
9	A	2586	U
9	A	2587	A
9	A	2601	C
9	A	2602	A
9	A	2608	G
9	A	2609	U
9	A	2610	C
9	A	2611	C
9	A	2613	U
9	A	2629	U
9	A	2663	G
9	A	2671	G
9	A	2681	C
9	A	2682	A
9	A	2689	U
9	A	2690	U
9	A	2714	G
9	A	2716	C
9	A	2726	A
9	A	2733	A
9	A	2744	G
9	A	2748	A
9	A	2757	A
9	A	2760	C
9	A	2765	A
9	A	2778	A
9	A	2791	G
9	A	2798	U
9	A	2800	A
9	A	2801	G
9	A	2818	U

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Mol	Chain	Res	Type
9	A	2820	A
9	A	2821	A
9	A	2861	U
9	A	2867	G
9	A	2873	A
9	A	2874	C
9	A	2883	A
9	A	2884	U
9	A	2885	G
9	A	2891	U
9	A	2903	U
10	B	3	C
10	B	15	A
10	B	16	G
10	B	21	G
10	B	30	C
10	B	35	C
10	B	42	C
10	B	44	G
10	B	45	A
10	B	56	G
10	B	84	G
10	B	87	U
10	B	88	C
10	B	89	U
10	B	90	C
10	B	99	A
10	B	109	A

All (43) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A	119	A
9	A	271	G
9	A	277	G
9	A	301	G
9	A	403	U
9	A	404	A
9	A	503	A
9	A	527	C
9	A	613	A
9	A	655	A

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Mol	Chain	Res	Type
9	A	784	G
9	A	827	U
9	A	846	U
9	A	882	G
9	A	931	U
9	A	1020	A
9	A	1025	G
9	A	1069	A
9	A	1088	A
9	A	1110	G
9	A	1247	A
9	A	1378	A
9	A	1458	U
9	A	1509	A
9	A	1535	A
9	A	1626	A
9	A	1738	G
9	A	1757	A
9	A	1847	A
9	A	1870	C
9	A	1939	U
9	A	2108	A
9	A	2142	A
9	A	2211	A
9	A	2286	G
9	A	2326	C
9	A	2423	U
9	A	2503	A
9	A	2576	G
9	A	2601	C
9	A	2756	U
9	A	2873	A
9	A	2902	C

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)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	ERY	A	9000	-	53,53,53	0.79	1 (1%)	82,82,82	1.66	19 (23%)

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
36	ERY	A	9000	-	-	7/72/107/107	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A	9000	ERY	C6-C5	2.32	1.59	1.55

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	A	9000	ERY	C25-C24-C23	-5.02	102.73	109.97
36	A	9000	ERY	O7-C5-C6	-4.80	100.47	106.39
36	A	9000	ERY	O2-C1-O1	-3.59	117.24	123.94
36	A	9000	ERY	C3-C2-C1	-3.46	102.94	110.01
36	A	9000	ERY	C27-C26-C25	-3.15	108.46	113.40
36	A	9000	ERY	C32-C6-C7	-2.90	106.19	111.09
36	A	9000	ERY	O3-C14-C15	-2.72	104.31	109.01
36	A	9000	ERY	O6-C17-C18	-2.63	104.78	109.39
36	A	9000	ERY	O3-C3-C4	-2.52	105.19	108.22
36	A	9000	ERY	O3-C3-C2	-2.50	106.78	111.14
36	A	9000	ERY	C19-C16-C17	2.42	116.20	111.24
36	A	9000	ERY	O11-C9-C8	-2.34	116.93	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	A	9000	ERY	C32-C6-C5	2.31	114.17	110.12
36	A	9000	ERY	O2-C13-C12	-2.25	103.62	107.29
36	A	9000	ERY	C16-C17-C18	-2.18	107.80	111.14
36	A	9000	ERY	C6-C7-C8	-2.15	110.78	115.38
36	A	9000	ERY	C8-C9-C10	2.12	122.79	119.10
36	A	9000	ERY	C15-C16-C17	-2.03	104.03	107.67
36	A	9000	ERY	C33-C8-C7	2.02	113.52	109.81

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	A	9000	ERY	C15-C16-O5-C20
36	A	9000	ERY	C19-C16-O5-C20
36	A	9000	ERY	C10-C11-C12-O13
36	A	9000	ERY	C25-C24-N1-C28
36	A	9000	ERY	C4-C5-C6-C32
36	A	9000	ERY	C17-C16-O5-C20
36	A	9000	ERY	O2-C13-C36-C37

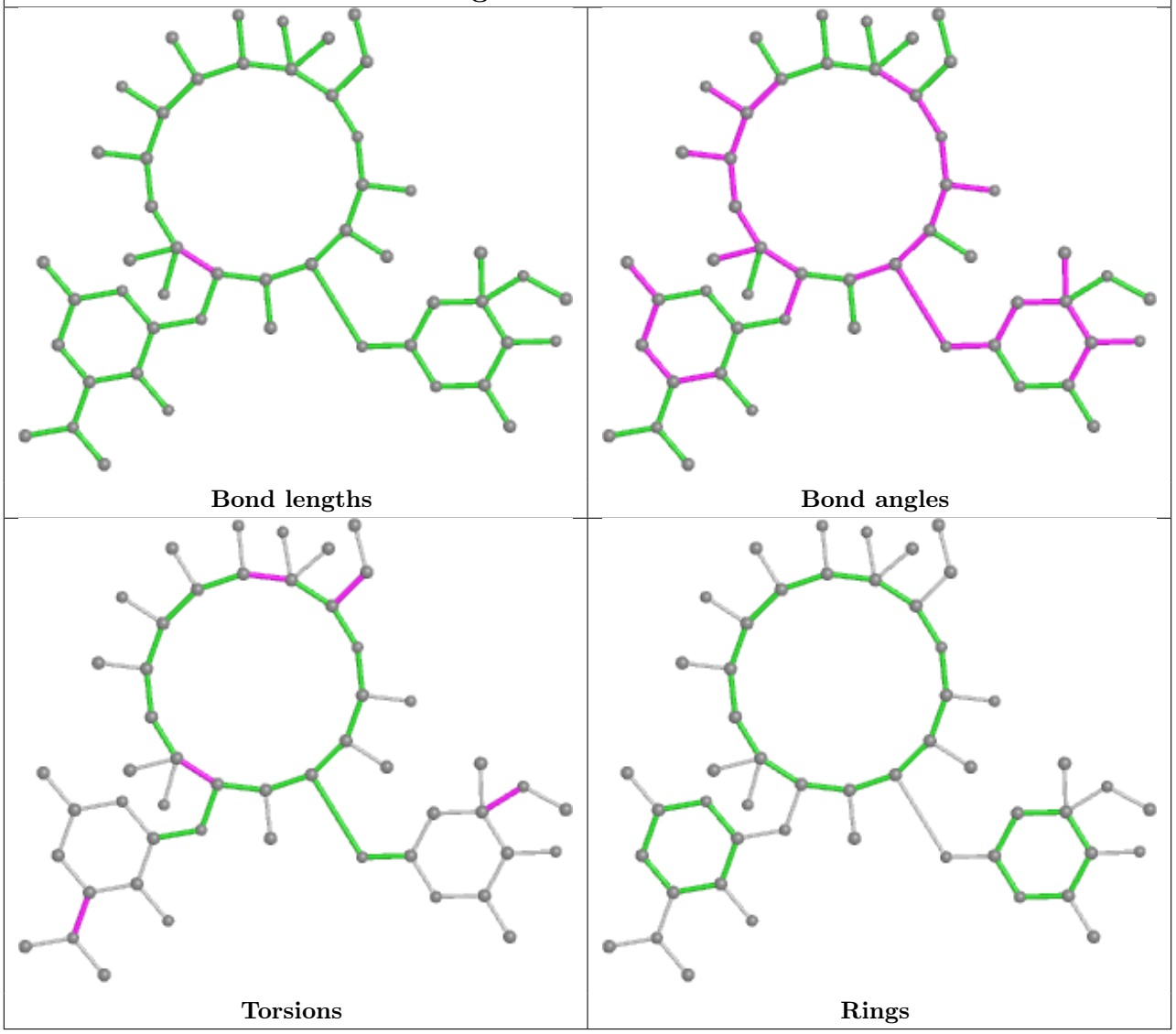
There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	A	9000	ERY	8	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.

Ligand ERY A 9000



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

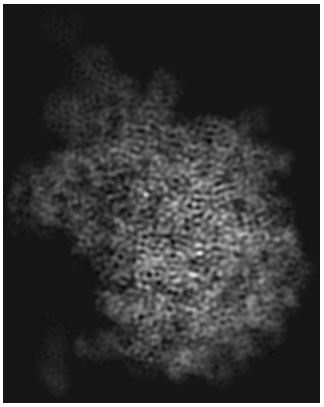
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6057. These allow visual inspection of the internal detail of the map and identification of artifacts.

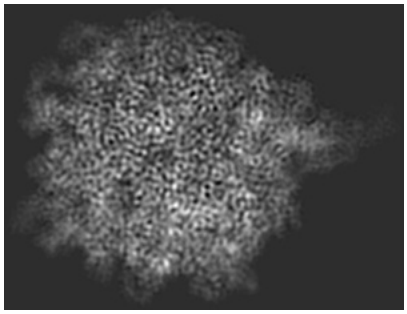
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

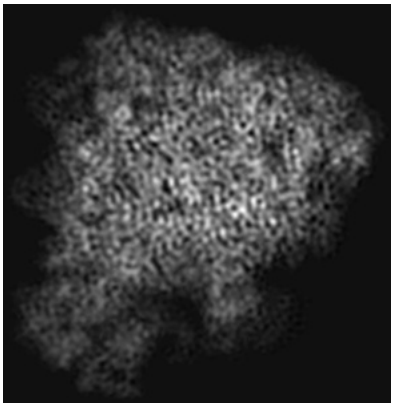
6.1.1 Primary map



X



Y

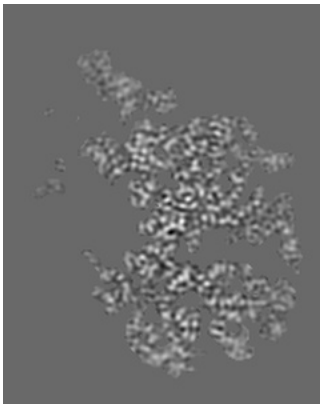


Z

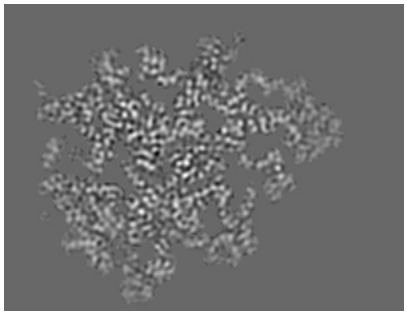
The images above show the map projected in three orthogonal directions.

6.2 Central slices

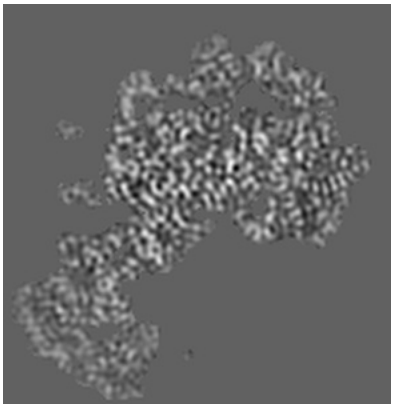
6.2.1 Primary map



X Index: 88



Y Index: 91

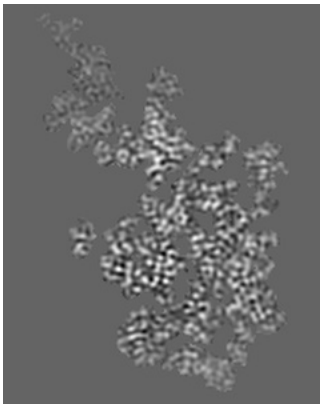


Z Index: 115

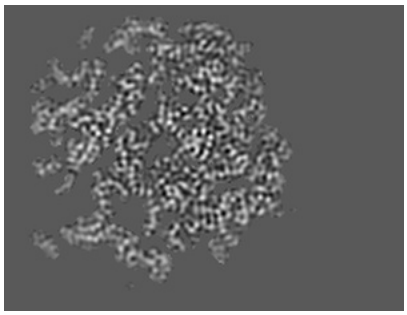
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

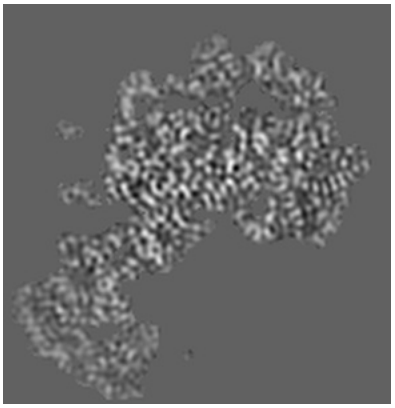
6.3.1 Primary map



X Index: 109



Y Index: 110

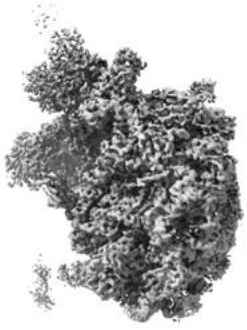


Z Index: 115

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.003. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

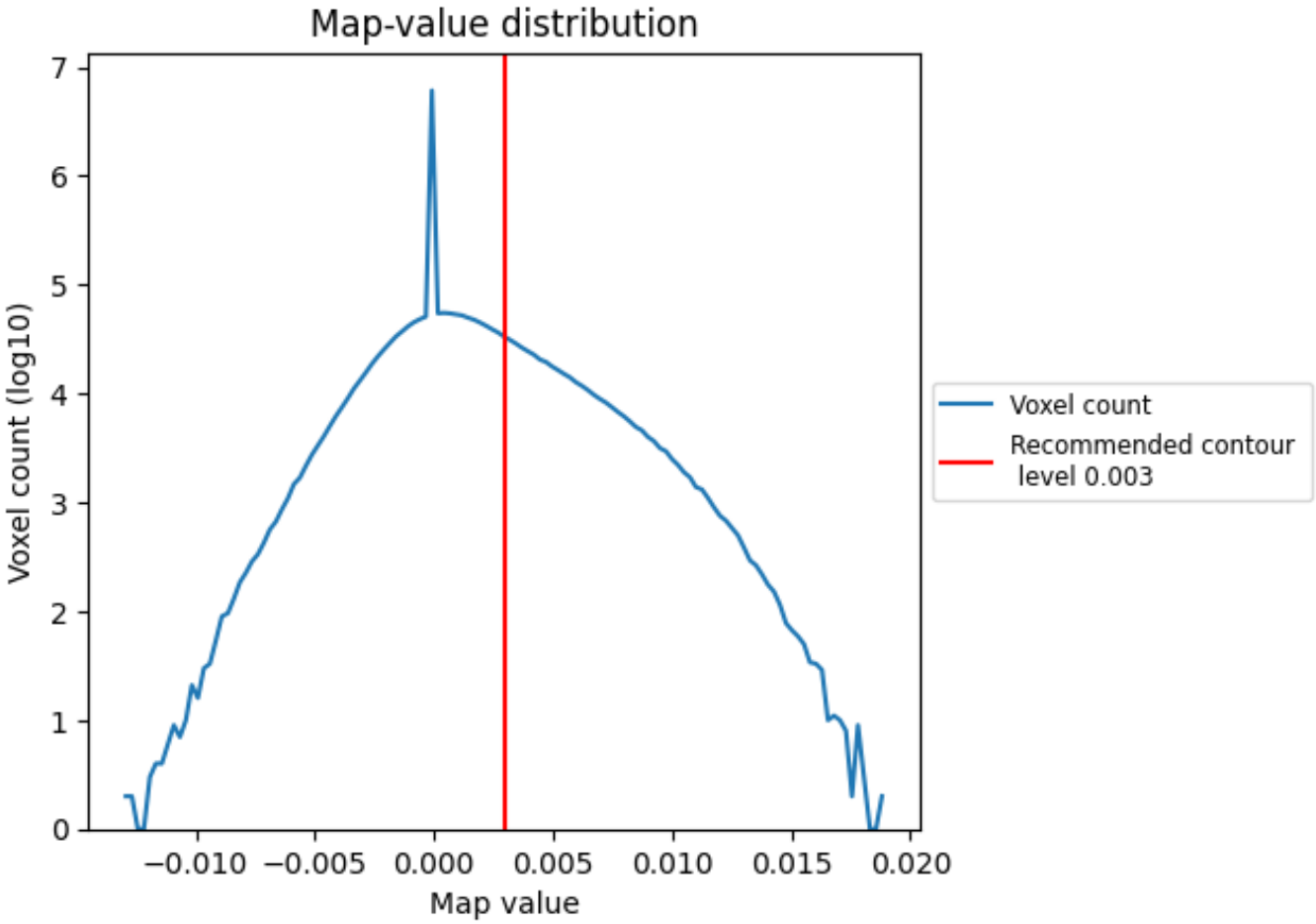
6.5 Mask visualisation (i)

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

7 Map analysis

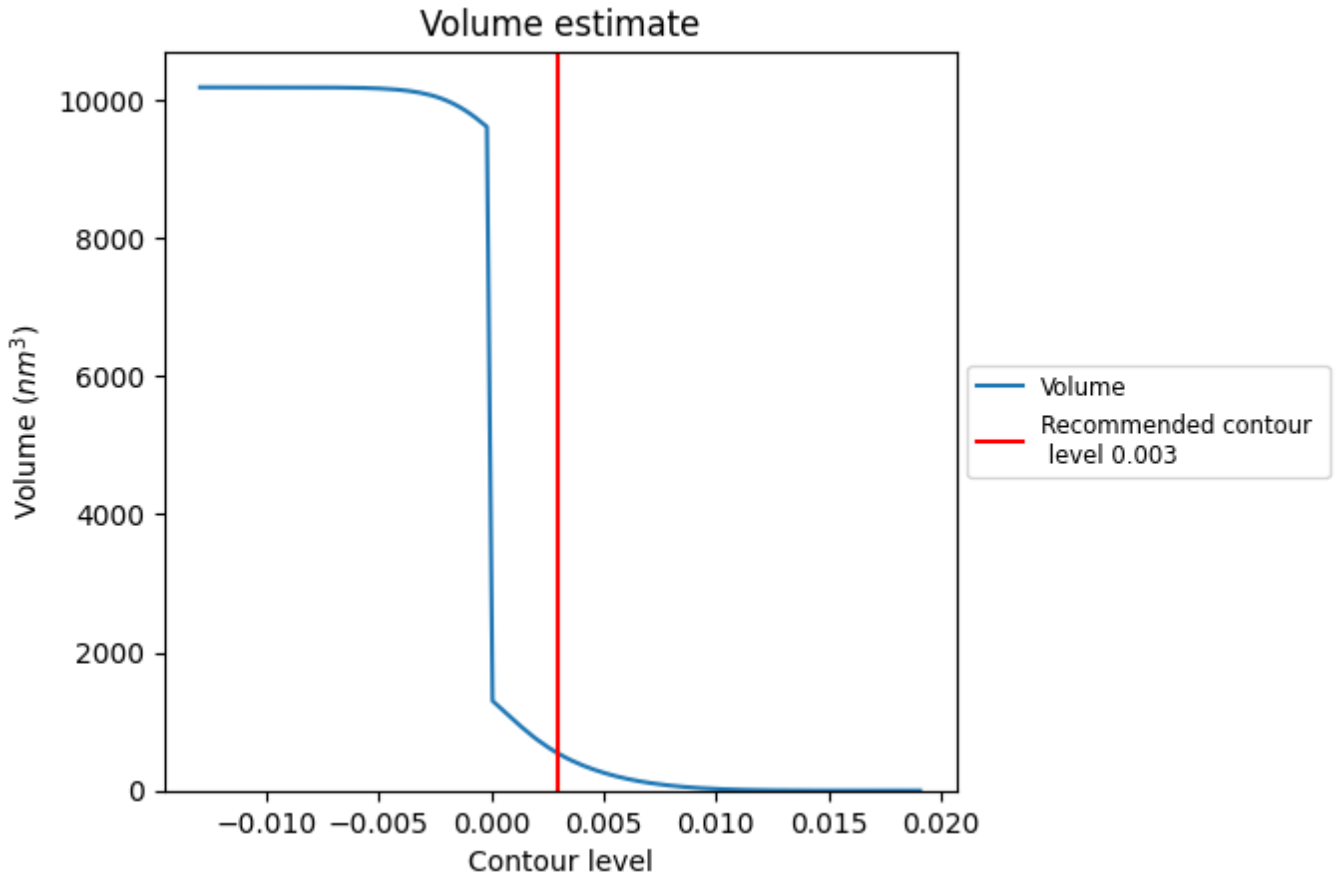
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

7.2 Volume estimate



The volume at the recommended contour level is 534 nm^3; this corresponds to an approximate mass of 483 kDa.

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

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

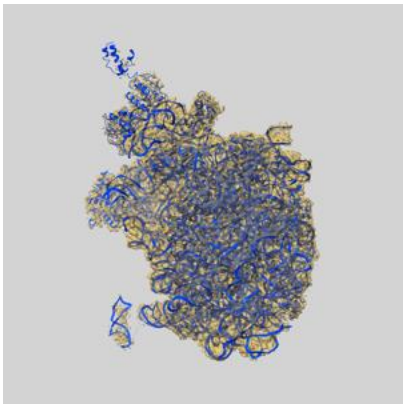
8 Fourier-Shell correlation (i)

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

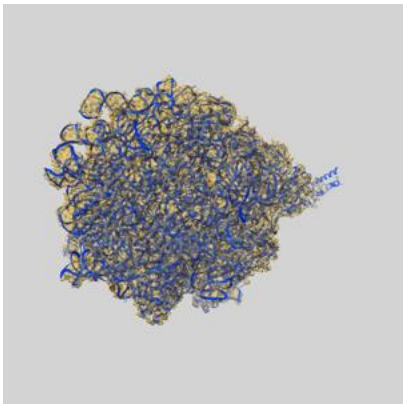
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6057 and PDB model 3J7Z. Per-residue inclusion information can be found in section 3 on page 11.

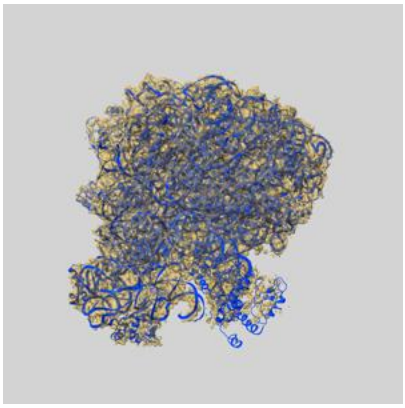
9.1 Map-model overlay



X



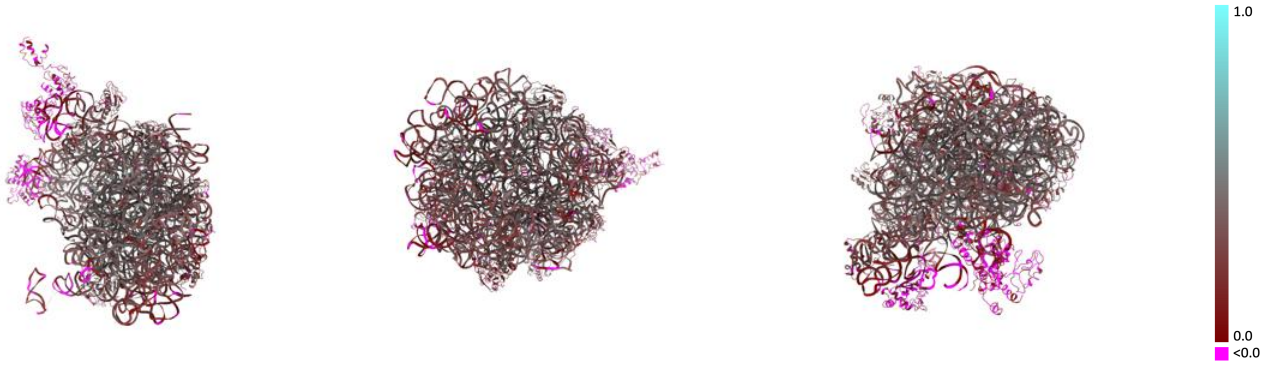
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.003 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

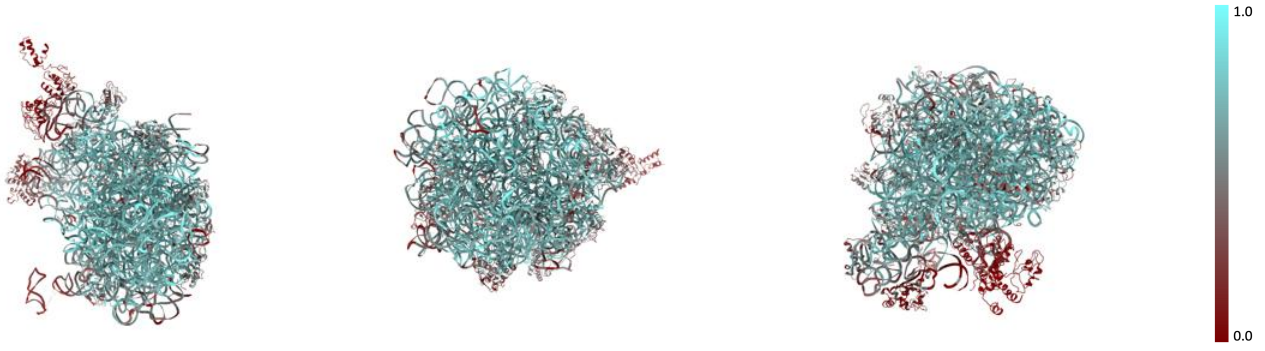
9.2 Q-score mapped to coordinate model



X Y Z

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

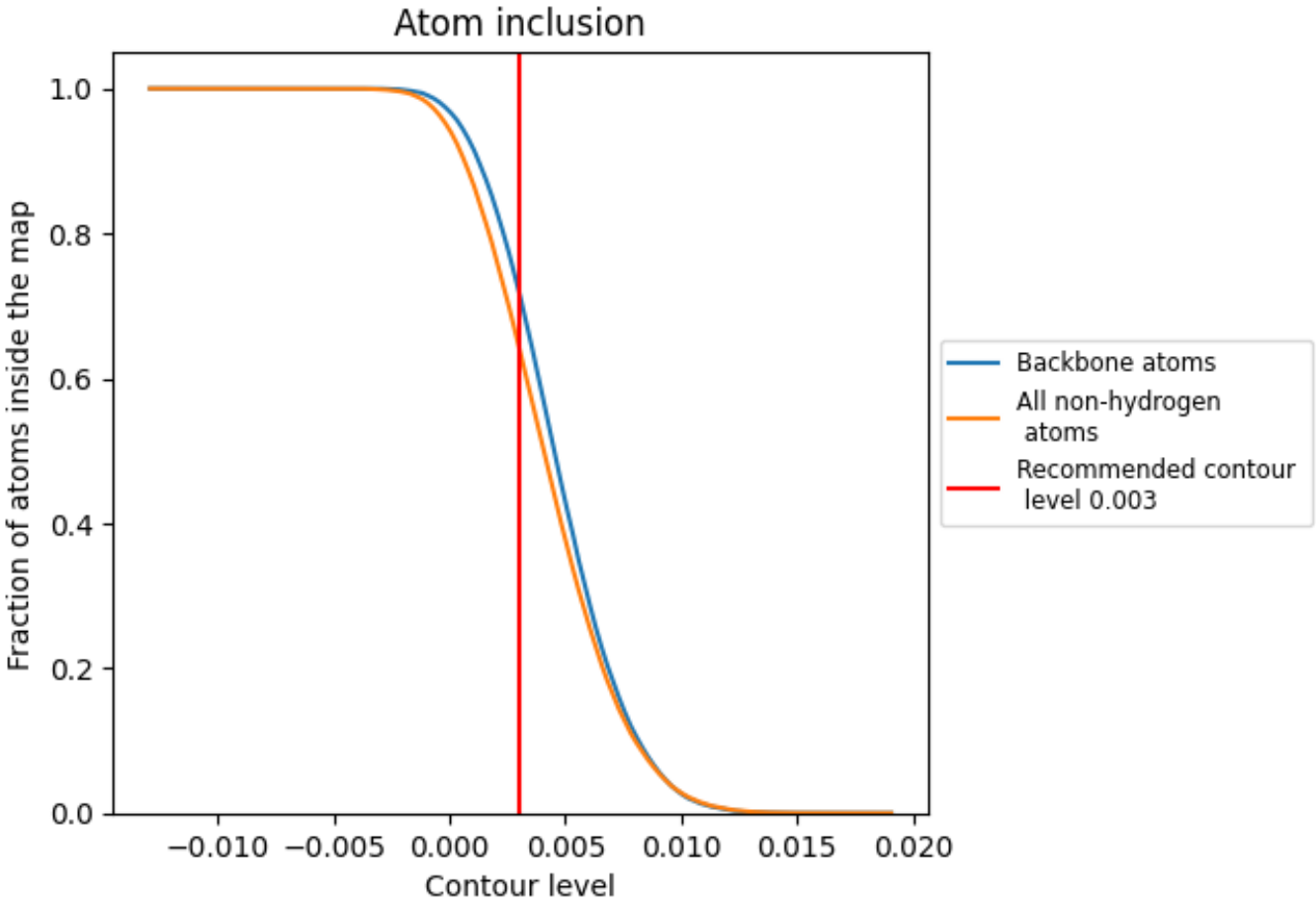
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.003).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6425	0.3120
0	0.5958	0.3310
1	0.1097	0.1330
2	0.6535	0.3740
3	0.6660	0.4030
4	0.6473	0.3940
5	0.0740	0.0490
6	0.0088	0.0340
7	0.8621	0.4460
A	0.7115	0.3290
B	0.5931	0.2290
C	0.6126	0.3460
D	0.5865	0.3600
E	0.5033	0.2980
F	0.1770	-0.0030
G	0.4433	0.2540
H	0.2770	0.2090
I	0.0548	-0.0030
J	0.5936	0.3350
K	0.5838	0.3730
L	0.5354	0.3210
M	0.6046	0.3730
N	0.6399	0.3690
O	0.4762	0.2560
P	0.5732	0.3430
Q	0.6388	0.3450
R	0.5383	0.3170
S	0.5885	0.3470
T	0.5222	0.2860
U	0.4302	0.2430
V	0.5081	0.3020
W	0.5793	0.3410
X	0.5973	0.3600
Y	0.4406	0.2310
Z	0.5721	0.3550
a	0.6667	0.4460