Full wwPDB EM Validation Report ⓘ

Apr 22, 2024 – 06:55 pm BST

PDB ID	:	7BL6
EMDB ID	:	EMD-12219
Title	:	50S-ObgE-GMPPNP particle
Authors	:	Hilal, T.; Nikolay, R.; Schmidt, S.; Spahn, C.M.T.
Deposited on	:	2021-01-18
Resolution	:	4.00 Å(reported)

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:

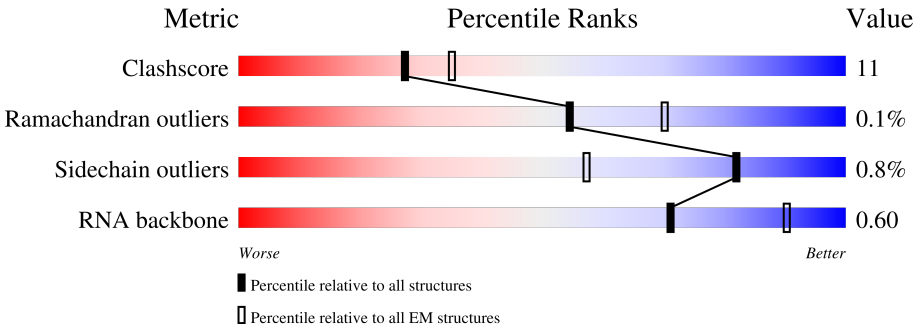
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 4.00 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	g	38	100%
2	C	273	73% 26%
3	D	209	74% 26%
4	E	201	76% 20%
5	F	179	68% 31%
6	G	177	5% 74% 24%
7	J	142	82% 18%

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Mol	Chain	Length	Quality of chain
8	L	144	80% 20%
9	N	120	78% 22%
10	O	117	72% 27%
11	Q	118	81% 18%
12	R	103	76% 24%
13	S	110	71% 29%
14	T	100	64% 29% 7%
15	U	104	82% 16%
16	V	94	74% 24%
17	W	85	72% 18% 11%
18	X	78	71% 28%
19	Y	63	5% 62% 38%
20	Z	59	76% 22%
21	0	57	70% 28%
22	1	55	65% 24% 9%
23	2	46	70% 28%
24	K	123	70% 29%
25	P	115	81% 17%
26	M	136	76% 23%
27	H	149	40% 72% 26%
28	d	70	17% 66% 33%
29	A	2904	48% 47% 6%
30	B	119	48% 49%
31	9	390	7% 71% 16% 13%
32	3	65	71% 26%

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 92769 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 L36.

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

- Molecule 2 is a protein called 50S ribosomal protein L2.

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

- Molecule 3 is a protein called 50S ribosomal protein L3.

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

- Molecule 4 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	193	Total	C	N	O	S	0	0
			1483	932	266	280	5		

- Molecule 5 is a protein called 50S ribosomal protein L5.

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

- Molecule 6 is a protein called 50S ribosomal protein L6.

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

- Molecule 7 is a protein called 50S ribosomal protein L13.

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

- Molecule 8 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 9 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 10 is a protein called 50S ribosomal protein L18.

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

- Molecule 11 is a protein called 50S ribosomal protein L20.

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

- Molecule 12 is a protein called 50S ribosomal protein L21.

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

- Molecule 13 is a protein called 50S ribosomal protein L22.

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

- Molecule 14 is a protein called 50S ribosomal protein L23.

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

- Molecule 15 is a protein called 50S ribosomal protein L24.

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

- Molecule 16 is a protein called 50S ribosomal protein L25.

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

- Molecule 17 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	76	Total	C	N	O	S	0	0
			577	357	117	102	1		

- Molecule 18 is a protein called 50S ribosomal protein L28.

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

- Molecule 19 is a protein called 50S ribosomal protein L29.

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

- Molecule 20 is a protein called 50S ribosomal protein L30.

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

- Molecule 21 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 22 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 23 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 24 is a protein called 50S ribosomal protein L14.

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

- Molecule 25 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	P	113	Total	C	N	O	S	0	0
			911	571	178	161	1		

- Molecule 26 is a protein called 50S ribosomal protein L16.

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

- Molecule 27 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	H	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	47	Total	C	N	O	S	0	0
			364	227	64	67	6		

- Molecule 29 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	A	2897	Total	C	N	O	P	0	0
			62195	27745	11446	20107	2897		

- Molecule 30 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B	119	Total	C	N	O	P	0	0
			2548	1135	466	829	118		

- Molecule 31 is a protein called GTPase ObgE/CgtA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	9	338	Total	C	N	O	S	0	0
			2582	1626	453	490	13		

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

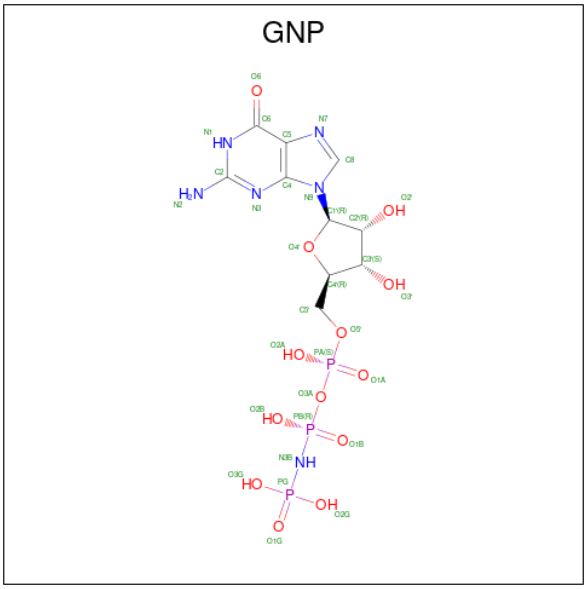
- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
33	g	1	Total	Zn	0
			1	1	
33	d	1	Total	Zn	0
			1	1	

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
34	A	1	Total	Mg	0
			1	1	
34	9	1	Total	Mg	0
			1	1	

- Molecule 35 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
35	9	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 36 is water.

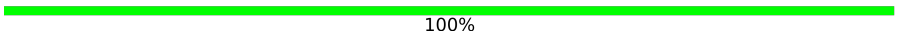
Mol	Chain	Residues	Atoms		AltConf
36	C	1	Total	O	0
			1	1	
36	F	1	Total	O	0
			1	1	
36	N	3	Total	O	0
			3	3	
36	S	1	Total	O	0
			1	1	
36	A	20	Total	O	0
			20	20	
36	B	1	Total	O	0
			1	1	

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 L36

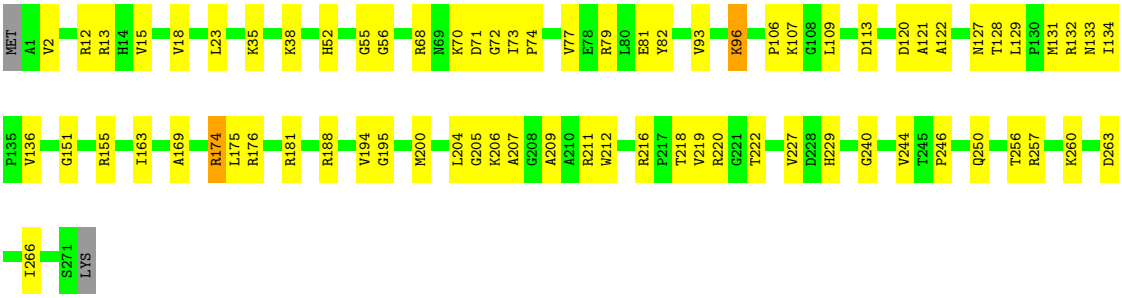
Chain g:



There are no outlier residues recorded for this chain.

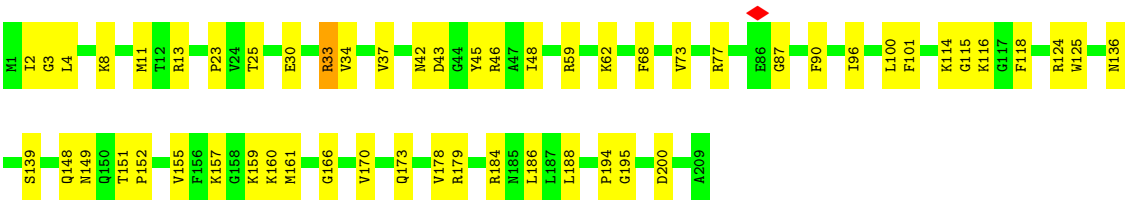
- Molecule 2: 50S ribosomal protein L2

Chain C:



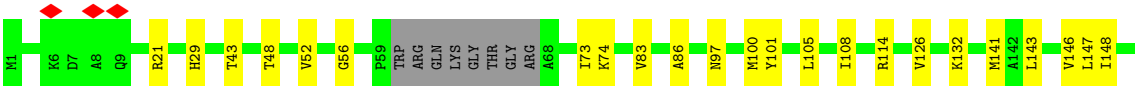
- Molecule 3: 50S ribosomal protein L3

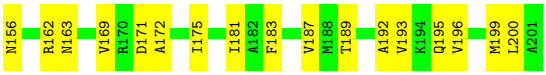
Chain D:



- Molecule 4: 50S ribosomal protein L4

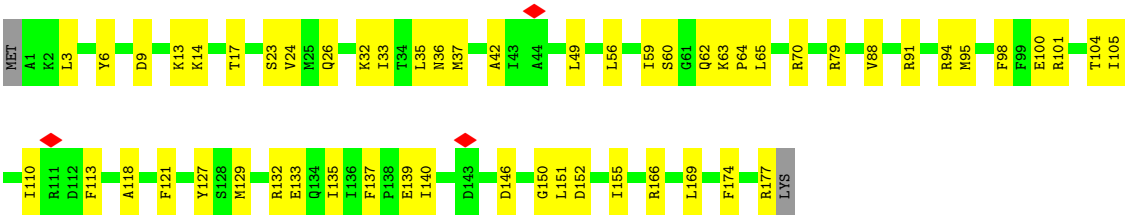
Chain E:





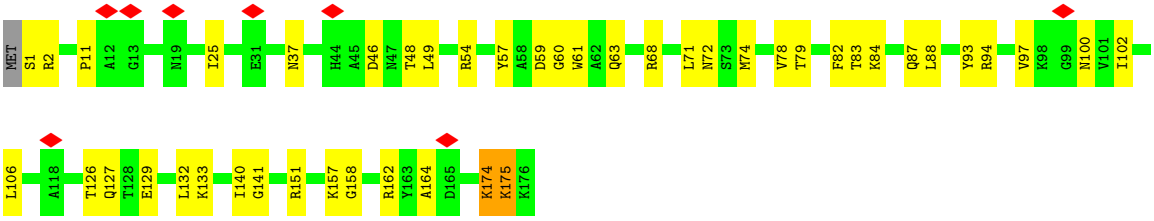
• Molecule 5: 50S ribosomal protein L5

Chain F:



• Molecule 6: 50S ribosomal protein L6

Chain G:

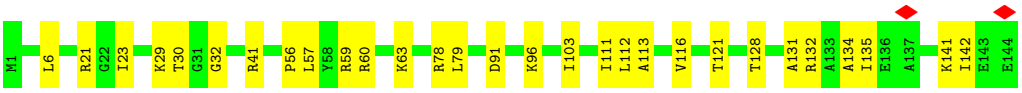


• Molecule 7: 50S ribosomal protein L13

Chain J:

• Molecule 8: 50S ribosomal protein L15

Chain L:

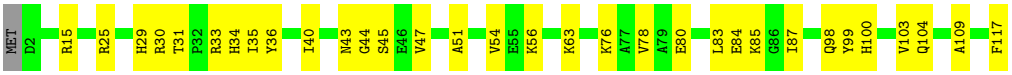


• Molecule 9: 50S ribosomal protein L17

Chain N:

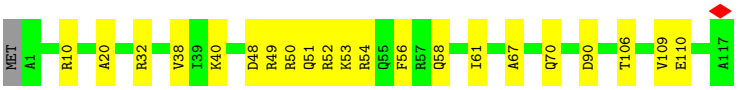
• Molecule 10: 50S ribosomal protein L18

Chain O:



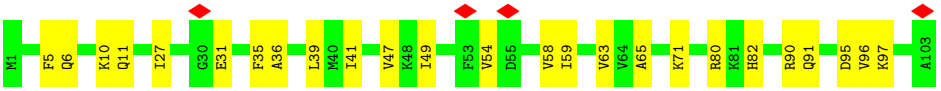
• Molecule 11: 50S ribosomal protein L20

Chain Q:



• Molecule 12: 50S ribosomal protein L21

Chain R:



• Molecule 13: 50S ribosomal protein L22

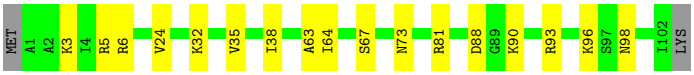
Chain S:

• Molecule 14: 50S ribosomal protein L23

Chain T:

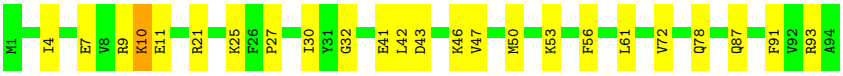
• Molecule 15: 50S ribosomal protein L24

Chain U:



• Molecule 16: 50S ribosomal protein L25

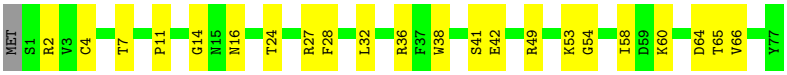
Chain V:



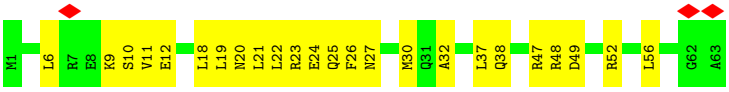
• Molecule 17: 50S ribosomal protein L27

Chain W:

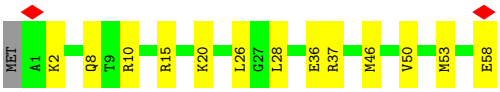
• Molecule 18: 50S ribosomal protein L28



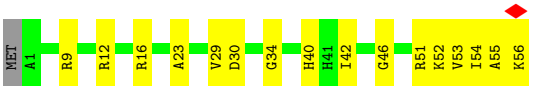
• Molecule 19: 50S ribosomal protein L29



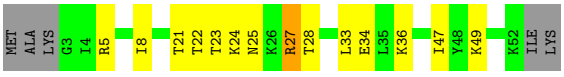
• Molecule 20: 50S ribosomal protein L30



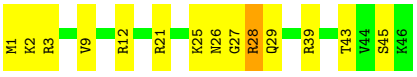
• Molecule 21: 50S ribosomal protein L32



• Molecule 22: 50S ribosomal protein L33

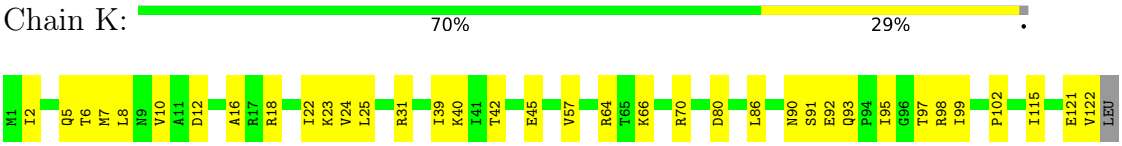


• Molecule 23: 50S ribosomal protein L34



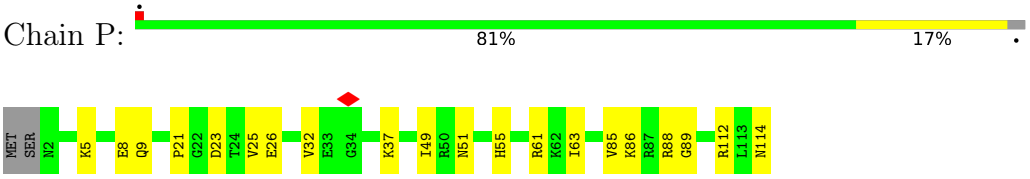
• Molecule 24: 50S ribosomal protein L14

Chain K:



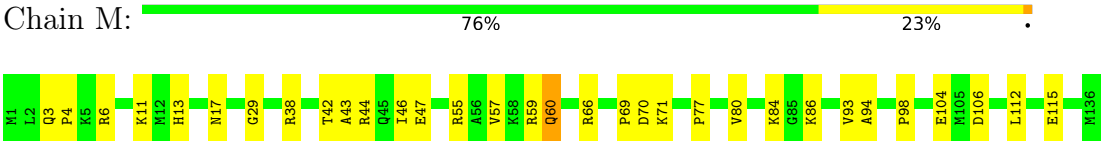
• Molecule 25: 50S ribosomal protein L19

Chain P:



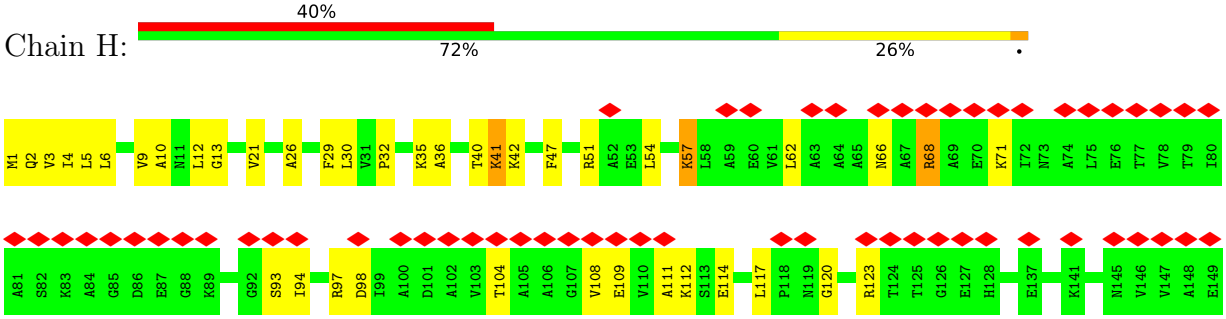
• Molecule 26: 50S ribosomal protein L16

Chain M:



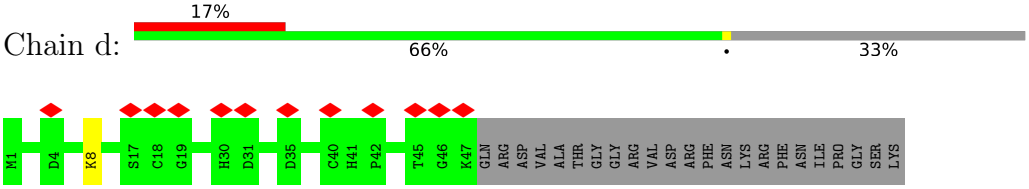
• Molecule 27: 50S ribosomal protein L9

Chain H:



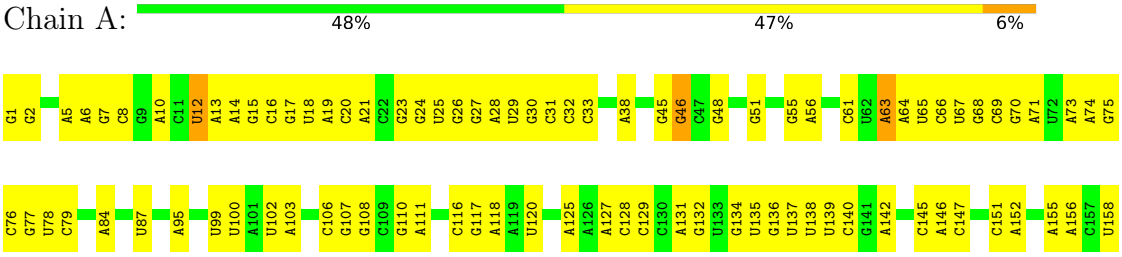
• Molecule 28: 50S ribosomal protein L31

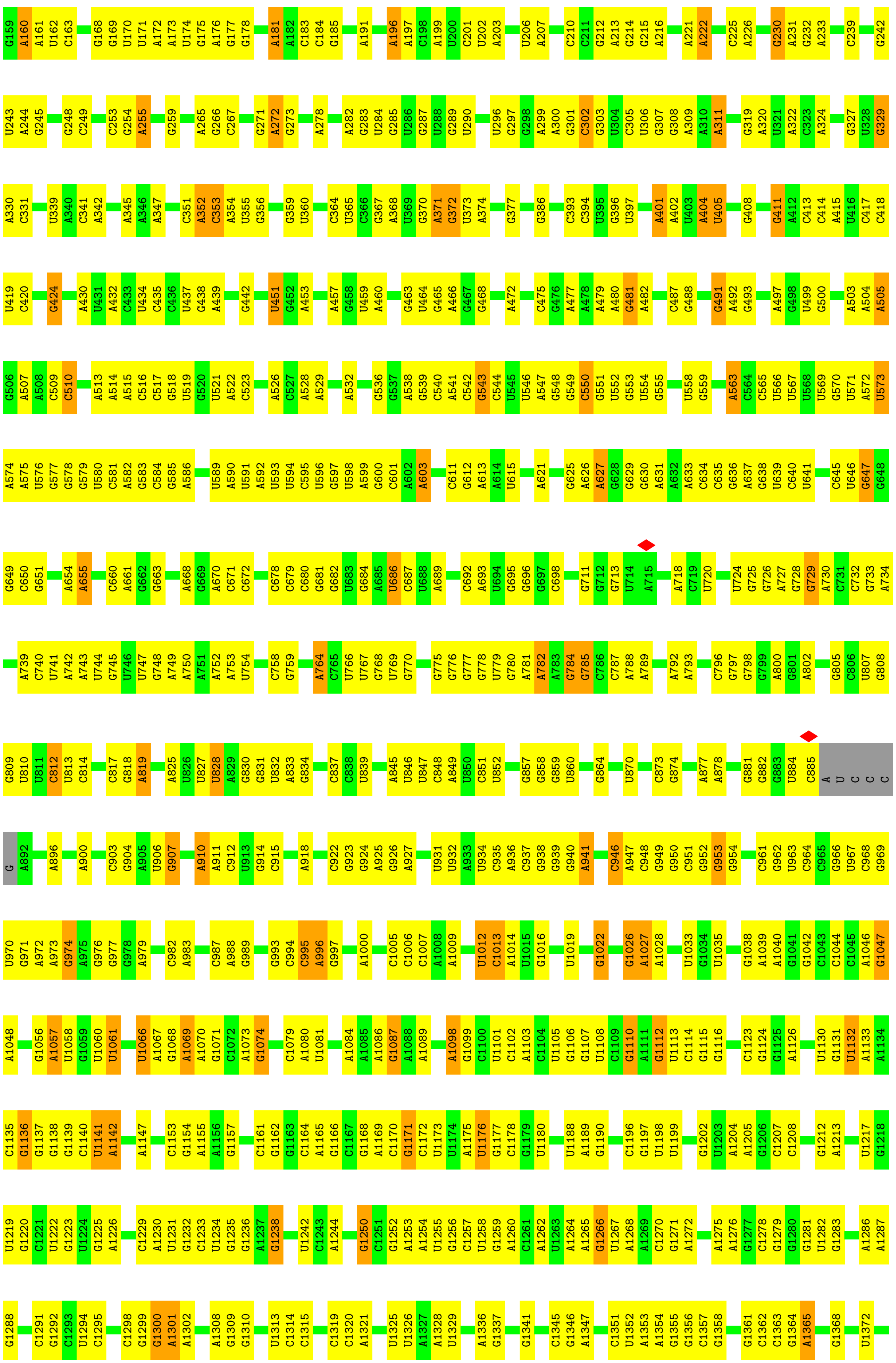
Chain d:

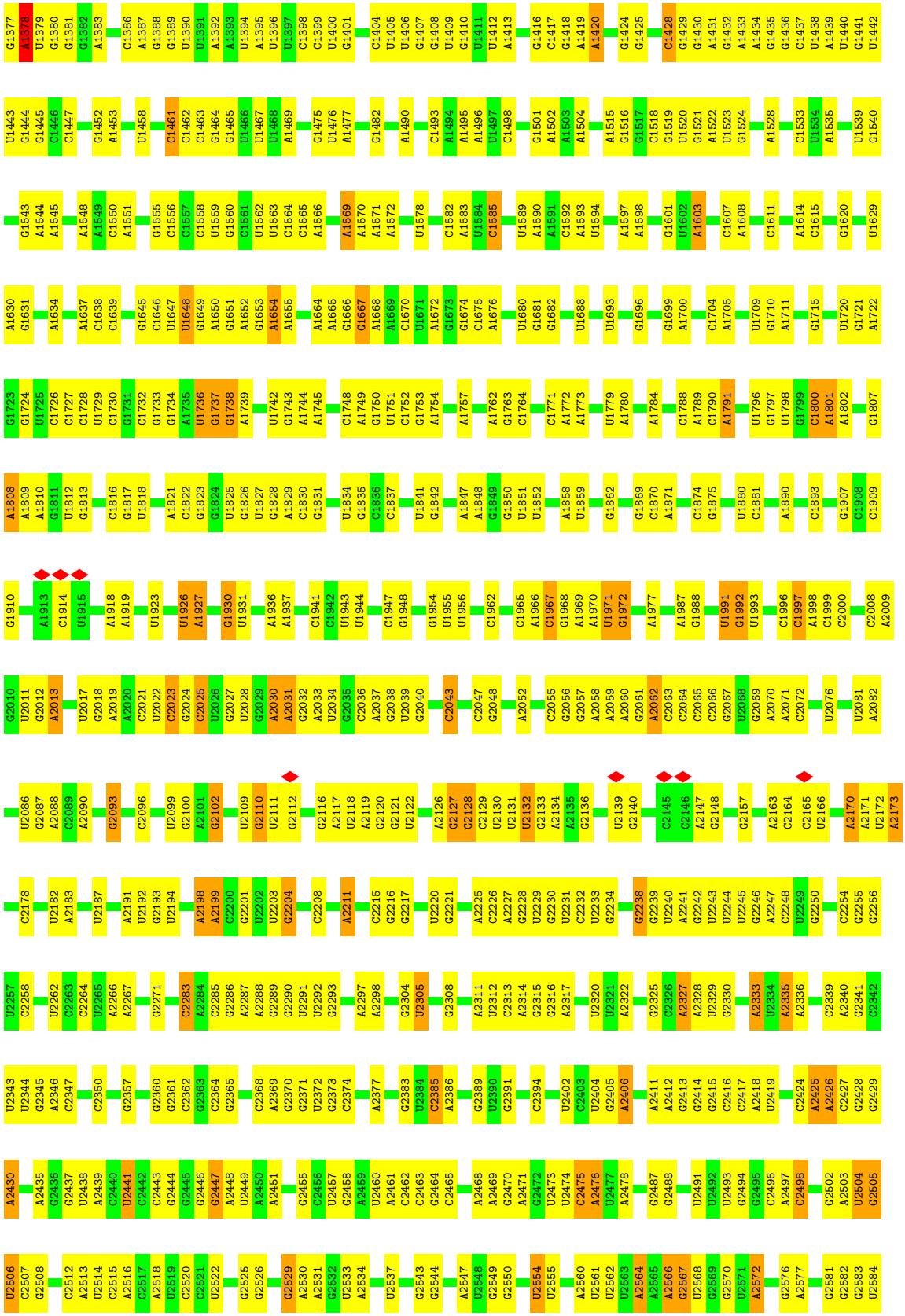


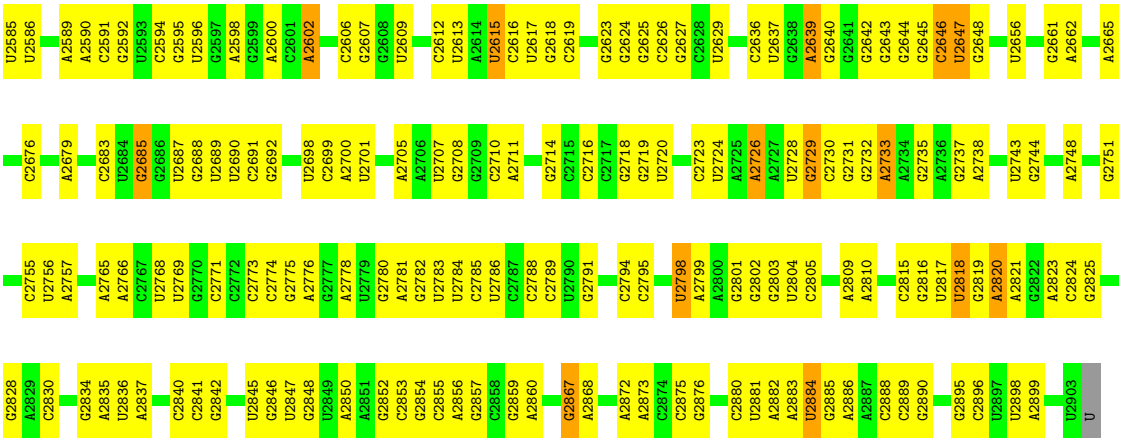
• Molecule 29: 23S ribosomal RNA

Chain A:



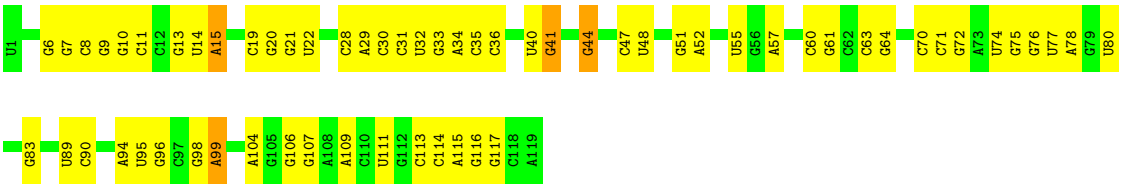

G159 A160 A161 U162 C163 G168 G169 U170 U171 A172 A173 U174 G175 A176 G177 G178 A181 A182 C183 C184 G185 A191 A196 A197 C198 A199 U200 C201 U202 A203 U206 A207 C210 C211 G212 A213 G214 G215 A216 A221 A222 C225 A226 G230 A231 G232 A233 C239 G242
U243 A244 G245 G248 C249 C253 G254 A255 G259 A265 C266 C267 G271 A272 G273 A278 A282 G283 U284 G285 U286 G287 U288 G289 U290 U296 G297 G298 A299 A300 G301 C302 G303 U304 C305 U306 G307 G308 A309 A310 A311 G319 A320 U321 A322 C323 A324 G327 U328 G329
A330 C331 U339 A340 C341 A342 A345 A346 A347 C351 A352 C353 A354 U355 G356 G359 U360 C364 U365 C366 G367 A368 U369 G370 A371 G372 U373 A374 G377 G386 C393 C394 U395 G396 U397 A401 A402 U403 A404 U405 G408 G411 A412 C413 C414 A415 U416 C417 C418
U419 C420 G424 A430 U431 A432 C433 U434 C435 C436 U437 G438 A439 G442 U451 G452 A453 A457 G458 U459 A460 G463 U464 G465 A466 G467 G468 A472 C475 G476 A477 A478 A479 A480 G481 A482 C487 G488 G491 A492 G493 A497 G498 U499 G500 A503 A504 A505
G506 A507 A508 C509 C510 A513 A514 A515 C516 C517 G518 U519 G520 U521 A522 C523 A526 C527 A528 A529 A532 G536 G537 A538 G539 C540 A541 C542 G543 C544 U545 U546 A547 G548 G549 C550 G551 U552 G553 U554 G555 U558 G559 A563 C564 C565 U566 U567 U568 U569 G570 U571 A572 U573
A574 A575 U576 G577 G578 G579 U580 C581 A582 G583 C584 G585 A586 U589 A590 U591 A592 U593 U594 C595 U596 G597 U598 A599 G600 C601 A602 A603 C611 G612 A613 A614 U615 A621 G625 A626 A627 G628 G629 G630 A631 A632 A633 C634 C635 C636 A637 G638 U639 C640 U641 C645 U646 G647 G648
G649 C650 G651 A654 A655 C660 A661 G662 G663 A668 G669 A670 C671 C672 C678 C679 C680 G681 G682 U683 G684 A685 U686 C687 U688 A689 C692 A693 U694 G695 G696 G697 C698 G711 G712 G713 U714 A715 A718 C719 U720 U724 G725 C726 A727 G728 G729 A730 C731 C732 G733 A734
A739 C740 U741 A742 A743 U744 G745 U746 U747 G748 A749 A750 A751 A752 A753 U754 C758 G759 A764 C765 U766 U767 G768 U769 G770 G775 C776 G777 U778 U779 G780 A781 A782 A783 G784 G785 C786 C787 A788 A789 A792 A793 C796 G797 G798 G799 A800 G801 A802 G805 G806 U807 G808
G809 U810 U811 C812 U813 C814 C817 G818 A819 A825 U826 U827 U828 A829 G830 G831 U832 A833 G834 C837 C838 U839 A845 U846 U847 C848 A849 U850 C851 U852 G857 G858 G859 U860 G864 U870 C873 G874 A877 A878 G881 G882 G883 U884 C885 A U C C C
G A892 A896 A900 C903 G904 A905 U906 G907 A910 A911 C912 U913 G914 C915 A918 C922 G923 G924 A925 G926 A927 U931 U932 A933 U934 C935 A936 C937 G938 G939 G940 A941 C946 A947 C948 G949 G950 C951 G952 G953 G954 C961 G962 U963 C964 C965 G966 U967 C968 G969
U970 G971 A972 A973 G974 A975 G976 G977 G978 A979 C982 A983 C987 A988 G989 G993 C994 C995 A996 G997 A1000 C1005 C1006 C1007 A1008 A1009 U1012 C1013 A1014 U1015 G1016 U1019 G1022 G1026 A1027 A1028 U1033 G1034 U1035 G1038 A1039 A1040 G1041 G1042 C1043 C1044 C1045 A1046 G1047
A1048 G1056 A1057 U1058 G1059 U1060 U1061 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1079 A1080 U1081 A1084 A1085 A1086 G1087 A1088 A1089 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 U1108 C1109 G1110 A1111 G1112 U1113 C1114 G1115 G1116 C1123 G1124 G1125 A1126 U1130 G1131 U1132 A1133 A1134
C1135 G1136 G1137 G1138 G1139 C1140 U1141 A1142 A1147 C1153 G1154 A1155 A1156 G1157 C1161 G1162 G1163 C1164 A1165 G1166 C1167 G1168 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1188 A1189 G1190 C1196 G1197 U1198 U1199 G1202 U1203 A1204 A1205 G1206 C1207 C1208 G1212 A1213 U1217 G1218
U1219 G1220 C1221 U1222 G1223 U1224 G1225 A1226 C1229 A1230 U1231 G1232 C1233 U1234 G1235 G1236 A1237 G1238 U1242 C1243 A1244 G1250 C1251 G1252 A1253 A1254 U1255 G1256 C1257 U1258 G1259 A1260 C1261 A1262 U1263 A1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 A1275 A1276 G1277 C1278 G1279 G1280 G1281 U1282 G1283 A1286 A1287
G1288 C1291 G1292 C1293 U1294 C1295 C1298 G1299 G1300 A1301 A1302 A1308 G1309 G1310 U1313 C1314 C1315 C1319 C1320 A1321 U1325 U1326 A1327 A1328 U1329 A1336 G1337 G1341 C1345 G1346 A1347 C1351 U1352 A1353 A1354 G1355 G1356 C1357 G1358 G1361 C1362 C1363 G1364 A1365 G1368 U1372





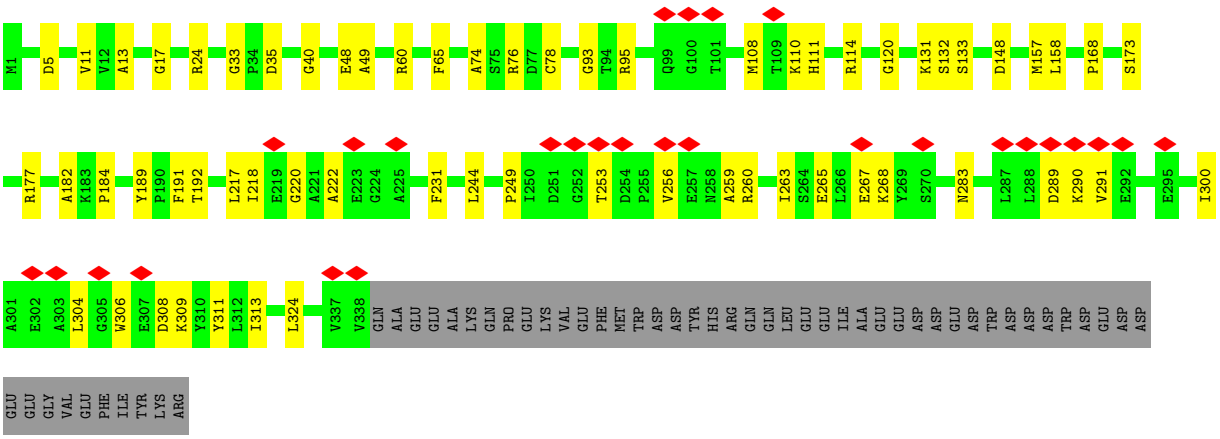
• Molecule 30: 5S ribosomal RNA

Chain B:



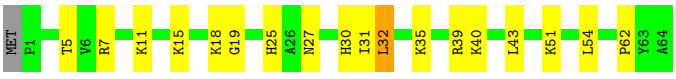
• Molecule 31: GTPase ObgE/CgtA

Chain 9:



• Molecule 32: 50S ribosomal protein L35

Chain 3:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45746	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.195	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.034	Depositor
Map value standard deviation	0.170	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	417.6, 417.6, 417.6	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.74, 1.74, 1.74	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, ZN, MG

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	g	0.23	0/303	0.44	0/397
2	C	0.23	0/2121	0.43	0/2852
3	D	0.24	0/1586	0.45	0/2134
4	E	0.23	0/1499	0.41	0/2016
5	F	0.24	0/1434	0.44	0/1926
6	G	0.24	0/1343	0.45	0/1816
7	J	0.23	0/1152	0.40	0/1551
8	L	0.25	0/1062	0.48	0/1413
9	N	0.24	0/974	0.42	0/1301
10	O	0.25	0/902	0.47	0/1209
11	Q	0.28	0/960	0.40	0/1278
12	R	0.25	0/829	0.46	0/1107
13	S	0.23	0/864	0.41	0/1156
14	T	0.23	0/744	0.44	0/994
15	U	0.24	0/787	0.46	0/1051
16	V	0.25	0/766	0.48	0/1025
17	W	0.25	0/584	0.42	0/772
18	X	0.22	0/635	0.41	0/848
19	Y	0.26	0/510	0.63	0/677
20	Z	0.23	0/453	0.44	0/605
21	0	0.21	0/450	0.48	0/599
22	1	0.24	0/416	0.44	0/554
23	2	0.22	0/380	0.39	0/498
24	K	0.24	0/947	0.47	0/1268
25	P	0.24	0/923	0.42	0/1234
26	M	0.24	0/1093	0.44	0/1460
27	H	0.24	0/1121	0.47	0/1515
28	d	0.24	0/371	0.48	0/496
29	A	0.16	0/69659	0.73	7/108672 (0.0%)
30	B	0.14	0/2847	0.70	0/4440
31	9	0.24	0/2626	0.45	0/3542
32	3	0.23	0/513	0.47	0/676

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.18	0/100854	0.67	7/151082 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	1313	U	C2-N1-C1'	6.94	126.03	117.70
29	A	1893	C	N3-C2-O2	-6.47	117.37	121.90
29	A	1313	U	N1-C2-O2	5.97	126.98	122.80
29	A	1313	U	N3-C2-O2	-5.66	118.24	122.20
29	A	1893	C	N1-C2-O2	5.39	122.13	118.90
29	A	837	C	N3-C2-O2	-5.09	118.34	121.90
29	A	1378	A	OP1-P-O3'	5.03	116.27	105.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	g	302	0	340	0	0
2	C	2082	0	2157	58	0
3	D	1565	0	1616	40	0
4	E	1483	0	1548	25	0
5	F	1410	0	1447	39	0
6	G	1323	0	1374	28	0
7	J	1129	0	1162	19	0
8	L	1053	0	1129	24	0
9	N	961	0	1000	20	0
10	O	892	0	923	22	0
11	Q	947	0	1022	17	0
12	R	816	0	839	18	0
13	S	857	0	922	22	0
14	T	738	0	807	23	0
15	U	779	0	834	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	V	753	0	780	19	0
17	W	577	0	594	12	0
18	X	625	0	655	15	0
19	Y	509	0	543	20	0
20	Z	449	0	491	9	0
21	0	444	0	461	12	0
22	1	409	0	440	12	0
23	2	377	0	418	11	0
24	K	938	0	1012	24	0
25	P	911	0	957	13	0
26	M	1074	0	1157	20	0
27	H	1110	0	1148	30	0
28	d	364	0	364	0	0
29	A	62195	0	31280	1102	0
30	B	2548	0	1292	55	0
31	9	2582	0	2606	40	0
32	3	504	0	574	14	0
33	d	1	0	0	0	0
33	g	1	0	0	0	0
34	9	1	0	0	0	0
34	A	1	0	0	0	0
35	9	32	0	13	2	0
36	A	20	0	0	0	0
36	B	1	0	0	0	0
36	C	1	0	0	0	0
36	F	1	0	0	0	0
36	N	3	0	0	0	0
36	S	1	0	0	0	0
All	All	92769	0	61905	1601	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 (1601) 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)
29:A:1433:A:N6	29:A:1560:G:H1	1.63	0.96
29:A:408:G:H1	29:A:419:U:H3	1.08	0.95
29:A:2102:G:H1	29:A:2187:U:H3	1.17	0.92
29:A:2475:C:H42	29:A:2529:G:H22	1.13	0.91
29:A:377:G:H1	29:A:397:U:H3	0.93	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:1433:A:H61	29:A:1560:G:H1	0.90	0.89
29:A:2204:G:H1	29:A:2220:U:H3	1.20	0.89
29:A:2475:C:H42	29:A:2529:G:N2	1.71	0.88
29:A:78:U:H3	29:A:108:G:H1	1.24	0.84
29:A:285:G:H1	29:A:355:U:H3	1.23	0.84
29:A:1390:U:H3	29:A:1395:A:H62	1.25	0.83
29:A:1171:G:N1	29:A:1178:C:N3	2.26	0.83
29:A:639:U:H3	29:A:649:G:H1	1.27	0.83
29:A:2475:C:N4	29:A:2529:G:H22	1.79	0.80
29:A:284:U:H3	29:A:356:G:H1	1.28	0.79
29:A:950:G:H1	29:A:967:U:H3	1.31	0.79
10:O:100:HIS:HA	10:O:104:GLN:HE22	1.48	0.78
14:T:25:GLU:HG3	14:T:26:LYS:HG2	1.68	0.75
29:A:1664:A:H61	29:A:1996:C:H42	1.33	0.75
23:2:12:ARG:HH22	29:A:464:U:H4'	1.52	0.74
29:A:2857:G:N2	29:A:2860:A:OP2	2.20	0.73
29:A:2898:U:H2'	29:A:2899:A:H8	1.52	0.73
3:D:46:ARG:HH22	3:D:87:GLY:H	1.36	0.73
31:9:244:LEU:HD22	31:9:283:ASN:HB2	1.70	0.73
29:A:171:U:H2'	29:A:172:A:H8	1.54	0.72
29:A:2093:G:N3	29:A:2198:A:N6	2.36	0.72
30:B:114:C:H2'	30:B:115:A:H8	1.54	0.72
31:9:5:ASP:O	31:9:60:ARG:NH1	2.22	0.72
18:X:32:LEU:HD12	18:X:49:ARG:HG2	1.72	0.71
5:F:129:MET:HA	29:A:2304:G:H4'	1.72	0.71
29:A:1105:U:H2'	29:A:1106:G:H8	1.55	0.71
29:A:1270:C:H5"	29:A:1271:G:H5'	1.71	0.71
29:A:488:G:H22	29:A:491:G:H5"	1.56	0.71
29:A:475:C:O2	29:A:479:A:N6	2.23	0.71
29:A:668:A:H2'	29:A:670:A:H62	1.55	0.71
29:A:1597:A:H5"	29:A:1598:A:H5'	1.72	0.70
29:A:160:A:N3	29:A:2208:C:O2'	2.23	0.70
5:F:3:LEU:HA	5:F:6:TYR:HB3	1.72	0.70
29:A:212:G:H2'	29:A:213:A:C8	2.26	0.70
31:9:217:LEU:HB3	31:9:231:PHE:HZ	1.56	0.70
26:M:77:PRO:HG2	26:M:80:VAL:HG21	1.73	0.70
29:A:463:G:N2	29:A:466:A:OP2	2.25	0.70
5:F:36:ASN:HB3	5:F:152:ASP:HB2	1.74	0.69
29:A:1664:A:H61	29:A:1996:C:N4	1.91	0.69
29:A:1040:A:H61	29:A:1115:G:H1	1.38	0.69
29:A:1992:G:N2	29:A:1996:C:O2'	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:2120:G:H2'	29:A:2121:G:H8	1.57	0.69
29:A:1528:A:OP2	29:A:1543:G:N2	2.26	0.69
29:A:371:A:H61	29:A:401:A:H3'	1.58	0.69
29:A:937:C:H2'	29:A:938:G:H8	1.58	0.68
29:A:629:G:N3	29:A:639:U:O2'	2.27	0.68
29:A:1834:U:H5"	29:A:1835:G:H5'	1.74	0.68
31:9:93:GLY:H	31:9:108:MET:HB2	1.58	0.68
29:A:2595:G:N2	29:A:2598:A:OP2	2.22	0.68
4:E:56:GLY:HA2	4:E:73:ILE:HG12	1.75	0.68
4:E:163:ASN:ND2	29:A:320:A:N3	2.42	0.67
29:A:2233:U:H2'	29:A:2234:G:H8	1.59	0.67
29:A:2645:G:OP2	29:A:2645:G:N2	2.20	0.67
2:C:257:ARG:HB2	29:A:1798:U:H5"	1.76	0.67
22:1:24:LYS:NZ	22:1:25:ASN:O	2.27	0.67
24:K:121:GLU:HG2	24:K:122:VAL:H	1.59	0.67
19:Y:23:ARG:O	19:Y:27:ASN:ND2	2.24	0.67
29:A:177:G:OP2	29:A:177:G:N2	2.18	0.67
29:A:1664:A:N6	29:A:1996:C:H42	1.92	0.67
29:A:2258:C:O2'	29:A:2427:C:OP2	2.13	0.67
29:A:629:G:H1'	29:A:639:U:H1'	1.74	0.67
29:A:1057:A:N6	29:A:1087:G:OP2	2.28	0.67
29:A:1086:A:O2'	29:A:1087:G:N7	2.28	0.67
29:A:2229:U:H2'	29:A:2230:G:H8	1.58	0.67
29:A:2656:U:O2	29:A:2665:A:N7	2.27	0.66
2:C:35:LYS:HE3	29:A:1353:A:H4'	1.77	0.66
11:Q:106:THR:O	11:Q:109:VAL:HG12	1.95	0.66
29:A:2468:A:OP2	29:A:2476:A:N6	2.28	0.66
29:A:2497:A:N3	29:A:2498:C:N4	2.44	0.66
8:L:41:ARG:NH1	29:A:807:U:OP2	2.29	0.66
29:A:2581:G:N2	29:A:2581:G:OP2	2.29	0.66
29:A:373:U:H2'	29:A:374:A:H8	1.61	0.66
29:A:1171:G:N2	29:A:1178:C:O2	2.16	0.66
29:A:1779:U:OP2	29:A:1784:A:N6	2.29	0.66
18:X:58:ILE:HG22	18:X:66:VAL:HG11	1.77	0.65
5:F:9:ASP:O	5:F:13:LYS:NZ	2.28	0.65
29:A:2246:G:H2'	29:A:2247:A:H8	1.62	0.65
31:9:260:ARG:HE	31:9:304:LEU:HA	1.61	0.65
25:P:32:VAL:HG12	25:P:37:LYS:HG2	1.79	0.65
8:L:79:LEU:HD23	8:L:112:LEU:HA	1.79	0.65
29:A:1060:U:H4'	29:A:1061:U:H5'	1.77	0.65
29:A:1800:C:H42	29:A:1817:G:H22	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:2514:U:H3	29:A:2570:G:H1	1.41	0.65
29:A:2515:C:H2'	29:A:2516:A:H8	1.62	0.65
12:R:63:VAL:HG22	12:R:96:VAL:HG12	1.79	0.65
29:A:26:G:H1'	29:A:515:A:H61	1.62	0.65
11:Q:48:ASP:HA	11:Q:51:GLN:HB2	1.79	0.65
29:A:2728:U:HO2'	29:A:2729:G:H8	1.45	0.65
29:A:177:G:H3'	29:A:178:G:H8	1.62	0.64
2:C:220:ARG:NH2	29:A:1788:C:OP1	2.31	0.64
29:A:213:A:H2'	29:A:214:G:C8	2.32	0.64
29:A:2816:G:N3	29:A:2883:A:O2'	2.29	0.64
5:F:3:LEU:HD13	5:F:100:GLU:HG2	1.78	0.64
20:Z:2:LYS:NZ	20:Z:58:GLU:OE2	2.30	0.64
29:A:488:G:N1	29:A:491:G:OP2	2.31	0.64
22:1:5:ARG:NH2	29:A:2285:C:OP2	2.28	0.64
29:A:1696:G:N2	29:A:1977:A:O2'	2.28	0.64
4:E:29:HIS:HA	8:L:6:LEU:HD12	1.79	0.64
3:D:124:ARG:NH1	3:D:161:MET:O	2.31	0.64
29:A:222:A:H61	29:A:232:G:H1'	1.63	0.64
29:A:1351:C:O2'	29:A:1571:A:O2'	2.13	0.64
29:A:832:U:H2'	29:A:833:A:H8	1.62	0.64
29:A:848:C:H2'	29:A:849:A:H8	1.63	0.64
14:T:54:GLU:HG3	14:T:88:LYS:HD2	1.80	0.64
29:A:1668:A:N3	29:A:1670:C:N4	2.44	0.64
29:A:2059:A:H61	29:A:2503:A:H3'	1.63	0.64
29:A:1282:U:H3	29:A:1286:A:H62	1.46	0.64
29:A:99:U:H5"	29:A:100:U:H5'	1.78	0.63
29:A:324:A:OP2	29:A:1205:A:N6	2.32	0.63
3:D:62:LYS:HD3	29:A:2810:A:H4'	1.80	0.63
10:O:30:ARG:NH2	30:B:48:U:OP1	2.31	0.63
29:A:594:U:H3	29:A:663:G:H1	1.46	0.63
29:A:1040:A:N6	29:A:1115:G:H1	1.96	0.63
22:1:25:ASN:OD1	22:1:27:ARG:NH1	2.32	0.63
26:M:55:ARG:HE	29:A:2469:A:H4'	1.64	0.63
29:A:514:A:N3	29:A:581:C:O2'	2.30	0.63
29:A:272:A:H2'	29:A:273:G:H8	1.63	0.63
29:A:1629:U:O4	29:A:1630:A:N6	2.31	0.63
29:A:1351:C:HO2'	29:A:1571:A:HO2'	1.47	0.63
29:A:1724:G:O6	29:A:1737:G:N2	2.30	0.63
29:A:2730:C:H2'	29:A:2731:G:C8	2.34	0.62
6:G:106:LEU:HB3	6:G:151:ARG:HE	1.62	0.62
23:2:29:GLN:NE2	29:A:210:C:OP1	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:839:U:H3	29:A:939:G:H1	1.46	0.62
29:A:2163:A:OP1	29:A:2170:A:O2'	2.17	0.62
3:D:13:ARG:HA	3:D:23:PRO:HA	1.80	0.62
22:1:21:THR:HG21	29:A:2419:U:H4'	1.82	0.62
16:V:4:ILE:HD12	16:V:42:LEU:HD11	1.81	0.62
29:A:571:U:O2'	29:A:573:U:OP2	2.17	0.62
29:A:1826:G:O2'	29:A:1971:U:OP2	2.16	0.62
12:R:10:LYS:NZ	29:A:994:C:O2	2.32	0.62
21:0:9:ARG:NH1	29:A:516:C:OP1	2.32	0.62
24:K:23:LYS:HB3	24:K:40:LYS:HB3	1.81	0.62
4:E:97:ASN:HB2	4:E:100:MET:HG2	1.81	0.62
31:9:309:LYS:NZ	31:9:311:TYR:OH	2.33	0.62
10:O:31:THR:OG1	10:O:34:HIS:O	2.15	0.62
17:W:68:LYS:NZ	30:B:11:C:OP1	2.24	0.62
2:C:120:ASP:OD1	2:C:121:ALA:N	2.28	0.62
6:G:106:LEU:O	6:G:151:ARG:NH2	2.32	0.62
10:O:45:SER:HG	30:B:9:G:HO2'	1.46	0.62
29:A:974:G:O2'	29:A:989:G:N2	2.33	0.62
29:A:1204:A:N6	29:A:1242:U:O4	2.32	0.62
29:A:1830:C:H2'	29:A:1831:G:H8	1.65	0.62
29:A:1999:C:O2	29:A:2687:U:O2'	2.17	0.62
5:F:132:ARG:HA	5:F:150:GLY:HA2	1.80	0.62
15:U:81:ARG:NH1	29:A:300:A:O5'	2.33	0.62
27:H:1:MET:N	27:H:21:VAL:O	2.32	0.62
29:A:371:A:N6	29:A:402:A:OP2	2.33	0.62
29:A:1123:C:H2'	29:A:1124:G:H8	1.64	0.62
29:A:2848:G:O2'	29:A:2867:G:N2	2.33	0.62
29:A:962:G:O2'	29:A:2250:G:N2	2.32	0.61
29:A:1353:A:OP2	29:A:1377:G:N1	2.32	0.61
29:A:1681:G:H21	29:A:1762:A:H3'	1.65	0.61
5:F:24:VAL:HG12	30:B:55:U:H4'	1.82	0.61
10:O:76:LYS:HB3	10:O:109:ALA:HB1	1.81	0.61
29:A:1288:G:OP2	29:A:1288:G:N2	2.33	0.61
20:Z:36:GLU:O	20:Z:37:ARG:NH1	2.33	0.61
29:A:787:C:H5"	29:A:788:A:H5'	1.82	0.61
3:D:42:ASN:ND2	3:D:43:ASP:OD2	2.33	0.61
29:A:1278:C:H2'	29:A:1279:G:C8	2.35	0.61
29:A:2081:U:H2'	29:A:2082:A:H8	1.66	0.61
29:A:818:G:N1	29:A:1188:U:OP2	2.28	0.61
31:9:11:VAL:HG12	31:9:65:PHE:HB2	1.81	0.61
19:Y:22:LEU:HD23	19:Y:23:ARG:HH11	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:1278:C:H2'	29:A:1279:G:H8	1.65	0.61
29:A:1721:G:O2'	29:A:1739:A:N6	2.34	0.61
2:C:174:ARG:NH1	2:C:175:LEU:O	2.34	0.61
4:E:132:LYS:NZ	29:A:320:A:OP2	2.29	0.61
29:A:345:A:N3	29:A:347:A:N6	2.49	0.61
29:A:1165:A:H2'	29:A:1166:G:H8	1.66	0.61
29:A:1363:C:O2'	29:A:1809:A:N3	2.28	0.61
30:B:28:C:H2'	30:B:29:A:H8	1.66	0.61
29:A:370:G:O2'	29:A:424:G:OP1	2.19	0.61
29:A:698:C:O2'	29:A:734:A:N6	2.23	0.61
29:A:1408:G:H1	29:A:1594:U:H3	1.48	0.61
29:A:1936:A:OP2	29:A:1962:C:N4	2.30	0.61
12:R:91:GLN:NE2	29:A:993:G:N3	2.47	0.60
17:W:37:ARG:NH2	29:A:2262:U:OP1	2.34	0.60
23:2:2:LYS:HE2	29:A:687:C:H5"	1.82	0.60
27:H:40:THR:O	27:H:41:LYS:HG3	2.01	0.60
29:A:482:A:O2'	29:A:497:A:N1	2.34	0.60
29:A:1443:U:H2'	29:A:1444:G:H8	1.67	0.60
29:A:1791:A:N6	29:A:1828:G:O2'	2.34	0.60
29:A:2735:G:H1	29:A:2769:U:H3	1.49	0.60
3:D:115:GLY:HA2	3:D:166:GLY:HA3	1.83	0.60
29:A:1463:C:H2'	29:A:1464:G:H8	1.67	0.60
2:C:70:LYS:HD2	2:C:73:ILE:HD12	1.83	0.60
2:C:260:LYS:HE2	29:A:2227:A:H5"	1.83	0.60
6:G:88:LEU:HD23	6:G:93:TYR:HB3	1.82	0.60
26:M:43:ALA:HA	26:M:46:ILE:HD12	1.82	0.60
29:A:2692:G:N3	29:A:2847:U:O2'	2.34	0.60
8:L:29:LYS:HE3	29:A:566:U:H5"	1.83	0.60
29:A:174:U:H2'	29:A:175:G:H8	1.67	0.60
29:A:184:C:H2'	29:A:185:G:H8	1.66	0.60
29:A:576:U:H2'	29:A:577:G:C8	2.37	0.60
2:C:23:LEU:HD21	2:C:82:TYR:HB2	1.83	0.60
31:9:13:ALA:HB3	31:9:148:ASP:H	1.67	0.60
2:C:122:ALA:O	2:C:127:ASN:ND2	2.32	0.59
2:C:244:VAL:HG12	2:C:250:GLN:HA	1.85	0.59
20:Z:8:GLN:HB2	20:Z:28:LEU:HD13	1.84	0.59
29:A:1992:G:O2'	29:A:1997:C:N4	2.34	0.59
19:Y:9:LYS:N	19:Y:12:GLU:OE1	2.34	0.59
26:M:70:ASP:OD2	29:A:907:G:N2	2.35	0.59
27:H:111:ALA:HB3	27:H:114:GLU:HB2	1.85	0.59
29:A:23:G:H2'	29:A:24:G:H8	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:97:VAL:HG22	6:G:102:ILE:HG22	1.83	0.59
10:O:51:ALA:HB3	10:O:78:VAL:HG12	1.84	0.59
13:S:22:ASP:OD1	13:S:25:ARG:NH1	2.33	0.59
29:A:158:U:H3	29:A:168:G:H1	1.50	0.59
29:A:1926:U:O2'	29:A:1927:A:N7	2.30	0.59
4:E:101:TYR:OH	4:E:175:ILE:O	2.21	0.59
29:A:1056:G:H5"	29:A:1057:A:H5'	1.84	0.59
29:A:2591:C:N4	29:A:2592:G:O6	2.35	0.59
2:C:52:HIS:HA	2:C:216:ARG:HB2	1.83	0.59
22:1:25:ASN:ND2	29:A:2285:C:OP1	2.36	0.59
24:K:90:ASN:OD1	24:K:91:SER:N	2.36	0.59
29:A:1420:A:O2'	29:A:2211:A:N7	2.36	0.59
29:A:1432:G:H2'	29:A:1433:A:C8	2.37	0.59
29:A:2564:A:C2	29:A:2647:U:H4'	2.38	0.59
2:C:2:VAL:HG12	2:C:18:VAL:HG22	1.84	0.59
29:A:1016:G:O6	29:A:1147:A:N6	2.36	0.59
29:A:272:A:H2'	29:A:273:G:C8	2.37	0.59
29:A:591:U:O4	29:A:592:A:N6	2.35	0.59
29:A:2776:A:O2'	29:A:2782:G:N7	2.32	0.59
5:F:70:ARG:NH2	29:A:2298:A:OP1	2.32	0.59
6:G:126:THR:HB	6:G:129:GLU:HB3	1.83	0.59
24:K:86:LEU:HB3	24:K:95:ILE:HD12	1.85	0.59
26:M:17:ASN:O	26:M:38:ARG:NH2	2.36	0.59
6:G:71:LEU:HA	6:G:74:MET:HG2	1.84	0.58
5:F:35:LEU:HD22	5:F:151:LEU:HD11	1.85	0.58
5:F:133:GLU:HG3	5:F:135:ILE:HG12	1.86	0.58
24:K:7:MET:HE3	24:K:8:LEU:H	1.68	0.58
29:A:1754:A:N1	29:A:2716:C:O2'	2.35	0.58
29:A:2215:C:H2'	29:A:2216:G:H8	1.67	0.58
24:K:23:LYS:NZ	29:A:2561:U:O2	2.36	0.58
29:A:1812:U:H2'	29:A:1813:G:H8	1.68	0.58
2:C:220:ARG:NH1	29:A:1789:A:OP2	2.37	0.58
10:O:40:ILE:HG12	10:O:47:VAL:HG12	1.84	0.58
29:A:1969:A:H2'	29:A:1972:G:H21	1.68	0.58
29:A:2291:U:H1'	29:A:2374:C:H1'	1.86	0.58
29:A:1386:C:H2'	29:A:1387:A:H8	1.68	0.58
29:A:1390:U:H3	29:A:1395:A:N6	1.99	0.58
29:A:1966:A:N6	31:9:133:SER:OG	2.37	0.58
2:C:68:ARG:NH1	2:C:128:THR:OG1	2.36	0.58
25:P:88:ARG:NH1	25:P:114:ASN:OD1	2.36	0.58
29:A:926:G:H2'	29:A:927:A:C8	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:1681:G:OP2	29:A:1757:A:N6	2.34	0.58
29:A:1852:U:O2	29:A:1890:A:N6	2.32	0.58
24:K:64:ARG:HD3	24:K:102:PRO:HG2	1.86	0.58
27:H:104:THR:HG22	27:H:109:GLU:HA	1.86	0.58
29:A:6:A:H2'	29:A:7:G:H8	1.69	0.58
29:A:1469:A:OP2	29:A:1522:A:N6	2.36	0.58
14:T:37:ASP:OD1	14:T:38:ALA:N	2.31	0.58
25:P:5:LYS:HB3	25:P:9:GLN:HE22	1.68	0.58
2:C:181:ARG:NH1	29:A:1800:C:OP2	2.36	0.58
26:M:6:ARG:NH2	29:A:870:U:OP1	2.37	0.58
29:A:1123:C:H2'	29:A:1124:G:C8	2.39	0.58
31:9:48:GLU:OE2	31:9:114:ARG:NH2	2.37	0.58
5:F:33:ILE:HG12	5:F:95:MET:HG2	1.86	0.57
29:A:2245:U:H5"	29:A:2246:G:H5'	1.86	0.57
29:A:2788:C:O2'	29:A:2809:A:N3	2.32	0.57
2:C:206:LYS:NZ	29:A:729:G:OP2	2.35	0.57
14:T:18:GLU:OE2	29:A:1392:A:N6	2.37	0.57
29:A:1528:A:N6	29:A:1543:G:O2'	2.36	0.57
5:F:63:LYS:HD2	5:F:64:PRO:HD2	1.86	0.57
29:A:1682:G:OP2	29:A:1699:G:N2	2.37	0.57
29:A:2417:C:H2'	29:A:2418:A:C8	2.38	0.57
21:0:12:ARG:NH2	29:A:517:C:OP1	2.35	0.57
29:A:453:A:N3	29:A:457:A:O2'	2.38	0.57
29:A:741:U:H2'	29:A:742:A:H8	1.69	0.57
2:C:128:THR:HG22	2:C:188:ARG:HG2	1.87	0.57
15:U:81:ARG:HH12	29:A:300:A:H3'	1.70	0.57
8:L:96:LYS:HD3	8:L:103:ILE:HA	1.85	0.57
29:A:2246:G:H2'	29:A:2247:A:C8	2.39	0.57
29:A:968:C:H2'	29:A:969:G:C8	2.40	0.57
12:R:35:PHE:HB2	12:R:59:ILE:HB	1.87	0.57
24:K:70:ARG:NH1	29:A:2683:C:O2	2.31	0.57
29:A:633:A:O2'	29:A:2404:U:OP1	2.23	0.57
29:A:2730:C:H2'	29:A:2731:G:H8	1.69	0.57
29:A:2898:U:H2'	29:A:2899:A:C8	2.37	0.57
30:B:14:U:OP2	30:B:70:C:O2'	2.22	0.57
29:A:713:G:H21	29:A:718:A:H62	1.51	0.57
29:A:1386:C:H2'	29:A:1387:A:C8	2.39	0.57
29:A:1430:G:H1	29:A:1563:U:H3	1.53	0.57
29:A:2855:C:H2'	29:A:2856:A:H8	1.68	0.57
8:L:116:VAL:HG11	8:L:134:ALA:HB1	1.87	0.56
29:A:6:A:H2'	29:A:7:G:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:1266:G:N2	29:A:2013:A:OP2	2.31	0.56
31:9:313:ILE:HD13	31:9:324:LEU:HD13	1.86	0.56
3:D:136:ASN:ND2	3:D:139:SER:O	2.38	0.56
29:A:1807:G:N2	29:A:1810:A:OP2	2.30	0.56
13:S:99:ARG:NH1	29:A:1262:A:OP1	2.38	0.56
20:Z:10:ARG:HB2	20:Z:53:MET:HB2	1.87	0.56
23:2:25:LYS:HA	23:2:28:ARG:HE	1.70	0.56
24:K:6:THR:HG23	29:A:1666:G:H4'	1.86	0.56
29:A:110:G:H2'	29:A:111:A:H8	1.71	0.56
29:A:377:G:N2	29:A:397:U:O2	2.31	0.56
29:A:948:C:H2'	29:A:949:G:H8	1.70	0.56
29:A:1358:G:N1	29:A:1372:U:OP2	2.31	0.56
29:A:2102:G:O6	29:A:2187:U:O4	2.23	0.56
29:A:2606:C:H2'	29:A:2607:G:C8	2.41	0.56
10:O:80:GLU:HA	10:O:83:LEU:HD12	1.87	0.56
17:W:36:GLN:HE22	17:W:41:PHE:HB2	1.70	0.56
29:A:541:A:N6	29:A:553:G:O6	2.38	0.56
29:A:2327:A:H2'	29:A:2328:A:C8	2.41	0.56
29:A:2443:C:H2'	29:A:2444:G:C8	2.41	0.56
29:A:2818:U:H3	29:A:2828:G:H1	1.54	0.56
2:C:77:VAL:HG12	2:C:93:VAL:HG12	1.88	0.56
29:A:1202:G:O6	29:A:1244:A:N6	2.38	0.56
29:A:2526:G:H1	29:A:2537:U:H3	1.52	0.56
29:A:577:G:O2'	29:A:1254:A:OP1	2.24	0.56
29:A:584:C:N4	29:A:585:G:O6	2.38	0.56
29:A:1196:C:H2'	29:A:1197:G:H8	1.71	0.56
29:A:1812:U:H2'	29:A:1813:G:C8	2.39	0.56
4:E:83:VAL:HB	4:E:86:ALA:HB2	1.87	0.56
14:T:8:LEU:HD12	14:T:50:LEU:HD21	1.87	0.56
29:A:184:C:H2'	29:A:185:G:C8	2.40	0.56
29:A:651:G:H5'	32:3:18:LYS:HG3	1.88	0.56
29:A:1807:G:H2'	29:A:1808:A:H5'	1.88	0.56
11:Q:50:ARG:NH2	29:A:993:G:OP2	2.38	0.56
29:A:935:C:H2'	29:A:936:A:H8	1.71	0.56
29:A:2743:U:OP2	29:A:2755:C:N4	2.39	0.56
4:E:126:VAL:O	4:E:156:ASN:ND2	2.39	0.56
29:A:5:A:H2'	29:A:6:A:H8	1.69	0.56
29:A:727:A:OP2	29:A:1431:A:O2'	2.23	0.56
29:A:780:G:N2	29:A:785:G:N7	2.53	0.56
29:A:2507:C:O3'	31:9:76:ARG:NH2	2.39	0.56
7:J:7:LYS:HG3	29:A:538:A:H4'	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:X:36:ARG:NH2	29:A:2199:A:OP1	2.35	0.56
29:A:2090:A:N6	29:A:2230:G:O6	2.39	0.56
7:J:13:ARG:NH2	7:J:49:ASP:OD2	2.38	0.55
19:Y:20:ASN:HA	19:Y:24:GLU:OE2	2.05	0.55
29:A:213:A:H2'	29:A:214:G:H8	1.72	0.55
29:A:1282:U:O4	29:A:1286:A:N7	2.39	0.55
16:V:7:GLU:HG2	16:V:41:GLU:HB3	1.88	0.55
17:W:63:VAL:HG12	17:W:78:ILE:HG12	1.89	0.55
29:A:631:A:N3	29:A:2415:G:O2'	2.34	0.55
29:A:1429:G:H2'	29:A:1430:G:H8	1.71	0.55
29:A:2345:G:H4'	29:A:2346:A:H3'	1.88	0.55
2:C:155:ARG:HD3	29:A:1818:U:H2'	1.89	0.55
3:D:179:ARG:HB2	3:D:188:LEU:HD12	1.88	0.55
26:M:11:LYS:HD3	26:M:86:LYS:HD3	1.88	0.55
29:A:1438:U:H2'	29:A:1439:A:H8	1.71	0.55
29:A:1709:U:O2'	29:A:2859:G:N3	2.34	0.55
22:1:25:ASN:ND2	22:1:28:THR:OG1	2.40	0.55
29:A:739:A:H1'	29:A:740:C:H5	1.70	0.55
29:A:1539:U:H2'	29:A:1540:G:H8	1.71	0.55
29:A:918:A:N3	30:B:80:U:O2'	2.39	0.55
29:A:1822:C:H2'	29:A:1823:G:H8	1.70	0.55
14:T:92:ASN:OD1	14:T:93:LEU:N	2.39	0.55
22:1:8:ILE:HD13	22:1:24:LYS:HD2	1.88	0.55
29:A:1518:C:H2'	29:A:1519:G:C8	2.41	0.55
31:9:49:ALA:O	31:9:111:HIS:ND1	2.39	0.55
3:D:2:ILE:HD13	3:D:48:ILE:HD11	1.89	0.55
4:E:189:THR:O	4:E:193:VAL:N	2.39	0.55
10:O:63:LYS:NZ	30:B:51:G:OP1	2.36	0.55
16:V:47:VAL:HA	16:V:50:MET:SD	2.46	0.55
29:A:434:U:O2	29:A:435:C:N4	2.33	0.55
29:A:1463:C:H2'	29:A:1464:G:C8	2.42	0.55
10:O:98:GLN:NE2	30:B:47:C:O2'	2.37	0.55
29:A:987:C:O2'	29:A:1000:A:N3	2.37	0.55
29:A:1164:C:H2'	29:A:1165:A:H8	1.72	0.55
29:A:1501:G:H2'	29:A:1502:A:H8	1.71	0.55
29:A:1800:C:H42	29:A:1817:G:N2	2.05	0.55
29:A:2405:G:O2'	29:A:2411:A:N6	2.39	0.55
29:A:968:C:H2'	29:A:969:G:H8	1.71	0.55
29:A:1223:G:N2	29:A:1226:A:OP2	2.24	0.55
29:A:1461:C:H2'	29:A:1462:C:H6	1.72	0.55
29:A:1825:U:H2'	29:A:1826:G:H8	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:2192:U:H2'	29:A:2193:G:H8	1.71	0.55
29:A:2707:U:H2'	29:A:2708:G:H8	1.71	0.55
29:A:31:C:O2'	29:A:1238:G:OP1	2.24	0.54
29:A:739:A:N3	29:A:740:C:N4	2.55	0.54
29:A:2417:C:H2'	29:A:2418:A:H8	1.72	0.54
29:A:174:U:H2'	29:A:175:G:C8	2.41	0.54
29:A:2656:U:C2	29:A:2665:A:N7	2.74	0.54
15:U:81:ARG:NH1	29:A:301:G:OP2	2.38	0.54
29:A:244:A:OP2	32:3:7:ARG:NH2	2.40	0.54
29:A:552:U:H2'	29:A:553:G:H8	1.72	0.54
29:A:1400:U:H2'	29:A:1401:G:C8	2.42	0.54
29:A:1589:U:H2'	29:A:1590:A:C8	2.42	0.54
29:A:1688:U:O2'	29:A:1700:A:N7	2.31	0.54
29:A:1907:G:O6	29:A:1923:U:O2	2.24	0.54
5:F:104:THR:HG23	5:F:105:ILE:HG12	1.90	0.54
29:A:2623:G:H2'	29:A:2624:G:H8	1.73	0.54
29:A:2815:C:H2'	29:A:2816:G:H8	1.72	0.54
32:3:5:THR:HG22	32:3:62:PRO:HD2	1.89	0.54
2:C:15:VAL:HG22	2:C:205:GLY:HA3	1.88	0.54
4:E:43:THR:O	29:A:442:G:N2	2.40	0.54
5:F:127:TYR:HB3	5:F:155:ILE:HB	1.90	0.54
6:G:106:LEU:HD12	6:G:151:ARG:HG2	1.89	0.54
17:W:67:VAL:HG22	17:W:74:LYS:HG2	1.90	0.54
7:J:40:HIS:O	11:Q:70:GLN:NE2	2.38	0.54
9:N:103:ARG:NH1	29:A:1287:A:O4'	2.41	0.54
10:O:54:VAL:O	10:O:56:LYS:NZ	2.39	0.54
29:A:45:G:H5'	29:A:46:G:H5'	1.89	0.54
29:A:1433:A:H2'	29:A:1434:A:H8	1.73	0.54
29:A:2070:A:H2'	29:A:2071:A:H8	1.73	0.54
2:C:132:ARG:HH22	27:H:93:SER:HB3	1.72	0.54
9:N:2:ARG:HD2	29:A:1653:G:H5"	1.90	0.54
29:A:1791:A:OP2	29:A:1828:G:N2	2.40	0.54
15:U:3:LYS:O	15:U:93:ARG:NH2	2.40	0.54
15:U:81:ARG:HG3	15:U:96:LYS:HD3	1.89	0.54
29:A:2320:U:O2'	29:A:2322:A:N6	2.41	0.54
3:D:116:LYS:NZ	29:A:2724:U:OP1	2.37	0.54
9:N:12:ARG:O	9:N:17:ARG:NH2	2.41	0.54
21:0:29:VAL:O	29:A:2885:G:N1	2.35	0.54
26:M:69:PRO:HA	26:M:94:ALA:HB2	1.90	0.54
29:A:937:C:H2'	29:A:938:G:C8	2.42	0.54
23:2:39:ARG:NH2	29:A:468:G:O6	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:2047:C:H2'	29:A:2048:G:H8	1.72	0.54
30:B:114:C:H2'	30:B:115:A:C8	2.39	0.54
5:F:37:MET:HG2	5:F:56:LEU:HD11	1.89	0.53
29:A:2549:G:H2'	29:A:2550:G:H8	1.73	0.53
29:A:2818:U:H2'	29:A:2819:G:C8	2.43	0.53
3:D:148:GLN:O	29:A:2052:A:H4'	2.08	0.53
11:Q:40:LYS:HE3	29:A:563:A:H4'	1.88	0.53
13:S:17:VAL:HG11	13:S:103:ILE:HG12	1.89	0.53
22:1:36:LYS:HG2	22:1:47:ILE:HD13	1.91	0.53
7:J:102:GLU:HB2	7:J:119:PHE:HE2	1.73	0.53
8:L:30:THR:OG1	29:A:1190:G:OP1	2.26	0.53
15:U:67:SER:OG	29:A:327:G:N2	2.41	0.53
29:A:2070:A:H2'	29:A:2071:A:C8	2.43	0.53
4:E:171:ASP:OD2	4:E:172:ALA:N	2.39	0.53
6:G:46:ASP:O	6:G:48:THR:N	2.38	0.53
15:U:96:LYS:NZ	29:A:299:A:OP1	2.40	0.53
21:0:54:ILE:HG23	21:0:56:LYS:H	1.73	0.53
29:A:742:A:H2'	29:A:743:A:H8	1.74	0.53
30:B:72:G:H21	30:B:104:A:H62	1.56	0.53
3:D:159:LYS:NZ	29:A:2512:C:O2'	2.33	0.53
5:F:42:ALA:HB1	5:F:49:LEU:HD21	1.90	0.53
27:H:71:LYS:HZ3	27:H:108:VAL:HG21	1.73	0.53
29:A:873:C:N4	29:A:874:G:O6	2.42	0.53
29:A:2328:A:H2'	29:A:2329:U:C6	2.44	0.53
3:D:37:VAL:HG22	3:D:48:ILE:HG22	1.91	0.53
7:J:17:VAL:HG22	7:J:55:ILE:HB	1.89	0.53
14:T:2:ILE:HA	14:T:3:ARG:C	2.28	0.53
16:V:32:GLY:O	16:V:93:ARG:NH2	2.36	0.53
29:A:574:A:N6	29:A:2034:U:OP1	2.41	0.53
29:A:742:A:H2'	29:A:743:A:C8	2.44	0.53
29:A:1649:G:O6	29:A:2009:A:N6	2.42	0.53
29:A:2059:A:N6	29:A:2504:U:OP2	2.42	0.53
3:D:151:THR:OG1	29:A:2032:G:N2	2.40	0.53
17:W:38:GLY:HA2	29:A:2330:G:H21	1.74	0.53
27:H:6:LEU:HD13	27:H:36:ALA:HA	1.91	0.53
29:A:222:A:N6	29:A:232:G:H1'	2.24	0.53
29:A:711:G:H1	29:A:720:U:H3	1.57	0.53
29:A:741:U:H2'	29:A:742:A:C8	2.44	0.53
29:A:1161:C:H2'	29:A:1162:G:H8	1.74	0.53
29:A:1170:C:N4	29:A:1171:G:O6	2.42	0.53
29:A:2447:G:H1	29:A:2451:A:H62	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:2687:U:H2'	29:A:2688:G:O4'	2.09	0.53
16:V:30:ILE:HD13	16:V:72:VAL:HG11	1.89	0.53
27:H:1:MET:SD	27:H:2:GLN:N	2.82	0.53
29:A:1281:G:H2'	29:A:1282:U:C6	2.44	0.53
29:A:2313:C:H2'	29:A:2314:A:H8	1.73	0.53
30:B:28:C:H2'	30:B:29:A:C8	2.44	0.53
6:G:1:SER:HA	6:G:61:TRP:HB3	1.91	0.53
9:N:114:GLU:HB2	9:N:118:ARG:HD2	1.91	0.53
29:A:796:C:H2'	29:A:797:G:C8	2.44	0.53
29:A:1171:G:O6	29:A:1178:C:N4	2.35	0.53
29:A:2192:U:H2'	29:A:2193:G:C8	2.45	0.53
6:G:158:GLY:O	6:G:162:ARG:NH1	2.41	0.52
13:S:83:LYS:HD2	13:S:95:ARG:HD2	1.91	0.52
13:S:55:ILE:HG23	13:S:66:ILE:HD11	1.92	0.52
25:P:25:VAL:HG22	25:P:85:VAL:HG22	1.91	0.52
29:A:2339:C:H2'	29:A:2340:A:C8	2.44	0.52
29:A:696:G:H1	29:A:766:U:H3	1.57	0.52
29:A:2250:G:O2'	29:A:2496:C:OP1	2.27	0.52
3:D:34:VAL:HG23	3:D:96:ILE:HD11	1.91	0.52
4:E:162:ARG:NE	29:A:322:A:OP1	2.42	0.52
29:A:1048:A:H1'	29:A:1112:G:N2	2.25	0.52
29:A:1310:G:O2'	29:A:1611:C:OP1	2.27	0.52
29:A:2039:U:H2'	29:A:2040:G:C8	2.44	0.52
29:A:2443:C:H2'	29:A:2444:G:H8	1.74	0.52
32:3:51:LYS:HA	32:3:54:LEU:HD23	1.91	0.52
6:G:82:PHE:HB3	6:G:140:ILE:HD13	1.92	0.52
23:2:9:VAL:HG23	29:A:1309:G:H5"	1.90	0.52
29:A:935:C:H2'	29:A:936:A:C8	2.44	0.52
10:O:15:ARG:HH21	30:B:8:C:H5"	1.74	0.52
29:A:373:U:H2'	29:A:374:A:C8	2.42	0.52
29:A:645:C:H2'	29:A:647:G:C8	2.45	0.52
29:A:1013:C:H2'	29:A:1014:A:H8	1.74	0.52
29:A:2028:U:H3	29:A:2033:A:H62	1.57	0.52
29:A:2474:U:H5"	29:A:2475:C:H5	1.74	0.52
5:F:23:SER:OG	30:B:55:U:O2'	2.22	0.52
29:A:20:C:H2'	29:A:21:A:C8	2.44	0.52
29:A:305:C:H2'	29:A:306:U:C6	2.44	0.52
29:A:1161:C:H2'	29:A:1162:G:C8	2.43	0.52
29:A:1176:U:H2'	29:A:1177:G:C8	2.45	0.52
29:A:1380:G:H1'	29:A:1569:A:H61	1.74	0.52
29:A:1681:G:N2	29:A:1763:G:OP2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:1800:C:N4	29:A:1817:G:H22	2.07	0.52
29:A:2728:U:O2'	29:A:2729:G:H8	1.91	0.52
31:9:177:ARG:HH11	31:9:182:ALA:H	1.56	0.52
29:A:145:C:H2'	29:A:146:A:H8	1.75	0.52
29:A:2637:U:H3	29:A:2776:A:H62	1.57	0.52
10:O:33:ARG:HG3	10:O:34:HIS:ND1	2.25	0.52
29:A:1428:C:N4	29:A:1570:A:OP2	2.33	0.52
29:A:1435:G:H2'	29:A:1436:G:H8	1.75	0.52
29:A:2027:G:H2'	29:A:2028:U:C6	2.44	0.52
7:J:21:THR:HG23	7:J:61:LYS:HB3	1.92	0.52
12:R:49:ILE:HG22	12:R:54:VAL:HG23	1.92	0.52
27:H:71:LYS:HE2	27:H:108:VAL:HG11	1.92	0.52
29:A:745:G:O2'	29:A:748:G:H1'	2.09	0.52
29:A:1406:U:H2'	29:A:1407:G:C8	2.45	0.52
29:A:1965:C:H5"	29:A:1966:A:H2'	1.92	0.52
29:A:2372:U:H2'	29:A:2373:G:H8	1.73	0.52
29:A:2819:G:H2'	29:A:2821:A:N7	2.24	0.52
6:G:11:PRO:HG2	6:G:79:THR:HG21	1.91	0.51
29:A:171:U:H2'	29:A:172:A:C8	2.42	0.51
29:A:1748:C:H2'	29:A:1749:A:H8	1.74	0.51
22:1:33:LEU:HD11	29:A:2286:G:C8	2.45	0.51
23:2:1:MET:N	29:A:1620:G:O4'	2.42	0.51
29:A:48:G:H22	29:A:177:G:P	2.32	0.51
29:A:2802:G:H2'	29:A:2803:G:H8	1.75	0.51
2:C:121:ALA:HB3	2:C:129:LEU:HD13	1.90	0.51
29:A:1390:U:O4	29:A:1395:A:N7	2.44	0.51
29:A:1736:U:H3'	29:A:1737:G:C8	2.46	0.51
29:A:2182:U:H2'	29:A:2183:A:H8	1.75	0.51
11:Q:49:ARG:O	11:Q:53:LYS:NZ	2.43	0.51
27:H:117:LEU:HG	27:H:120:GLY:HA2	1.92	0.51
29:A:576:U:H2'	29:A:577:G:H8	1.75	0.51
3:D:118:PHE:O	29:A:1654:A:O2'	2.26	0.51
18:X:49:ARG:NH2	29:A:1364:G:OP2	2.40	0.51
18:X:64:ASP:OD1	18:X:65:THR:N	2.43	0.51
20:Z:8:GLN:NE2	20:Z:10:ARG:O	2.37	0.51
20:Z:15:ARG:O	20:Z:20:LYS:NZ	2.43	0.51
29:A:196:A:H61	29:A:831:G:N2	2.09	0.51
29:A:1137:G:H2'	29:A:1138:G:C8	2.45	0.51
29:A:1138:G:H2'	29:A:1139:G:O4'	2.09	0.51
29:A:2031:A:N3	29:A:2455:G:O2'	2.43	0.51
25:P:112:ARG:HH11	25:P:114:ASN:HD21	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:807:U:H2'	29:A:808:G:H8	1.75	0.51
29:A:1281:G:H2'	29:A:1282:U:H6	1.74	0.51
29:A:1417:C:H2'	29:A:1418:G:O4'	2.10	0.51
29:A:1830:C:H2'	29:A:1831:G:C8	2.45	0.51
4:E:147:LEU:HB2	4:E:183:PHE:HD1	1.74	0.51
8:L:63:LYS:HE2	29:A:2394:C:H5"	1.92	0.51
23:2:43:THR:HG23	23:2:45:SER:H	1.76	0.51
25:P:23:ASP:OD1	25:P:89:GLY:N	2.42	0.51
29:A:639:U:H2'	29:A:640:C:C6	2.46	0.51
29:A:1000:A:OP2	29:A:1154:G:N1	2.31	0.51
29:A:2008:C:H2'	29:A:2009:A:H8	1.74	0.51
29:A:2076:U:OP2	29:A:2238:G:N2	2.37	0.51
29:A:2333:A:H5'	29:A:2335:A:H1'	1.93	0.51
29:A:2781:A:H5"	29:A:2782:G:H5'	1.91	0.51
27:H:94:ILE:HG23	27:H:98:ASP:HB2	1.93	0.51
29:A:5:A:H2'	29:A:6:A:C8	2.45	0.51
29:A:459:U:H2'	29:A:460:A:H8	1.76	0.51
29:A:758:C:H2'	29:A:759:G:C8	2.46	0.51
29:A:1406:U:H2'	29:A:1407:G:H8	1.75	0.51
29:A:2385:C:H2'	29:A:2386:A:C8	2.46	0.51
19:Y:19:LEU:HB3	19:Y:23:ARG:NH2	2.26	0.51
29:A:2291:U:O2'	29:A:2374:C:O2	2.27	0.51
29:A:2836:U:H2'	29:A:2837:A:C8	2.46	0.51
29:A:2853:C:H2'	29:A:2854:G:C8	2.45	0.51
30:B:60:C:H2'	30:B:61:G:H8	1.75	0.51
30:B:78:A:H62	30:B:98:G:H21	1.58	0.51
2:C:257:ARG:NH1	2:C:263:ASP:OD2	2.43	0.51
9:N:44:LEU:HD22	9:N:113:ILE:HD13	1.92	0.51
29:A:910:A:H2'	29:A:911:A:C8	2.45	0.51
29:A:1589:U:H2'	29:A:1590:A:H8	1.76	0.51
29:A:2788:C:H2'	29:A:2789:C:C6	2.46	0.51
12:R:27:ILE:HG21	12:R:63:VAL:HG21	1.93	0.50
29:A:758:C:H2'	29:A:759:G:H8	1.75	0.50
29:A:951:C:N4	29:A:952:G:O6	2.44	0.50
29:A:2836:U:H2'	29:A:2837:A:H8	1.77	0.50
31:9:218:ILE:HG23	31:9:220:GLY:H	1.75	0.50
4:E:21:ARG:O	4:E:114:ARG:NH1	2.39	0.50
19:Y:47:ARG:NH1	29:A:61:C:OP2	2.45	0.50
29:A:69:C:O2	29:A:73:A:O2'	2.23	0.50
29:A:414:C:H2'	29:A:415:A:C8	2.46	0.50
29:A:2065:C:H2'	29:A:2066:C:H6	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:2131:U:H5'	29:A:2132:U:H5"	1.91	0.50
29:A:2463:C:H2'	29:A:2464:G:H8	1.76	0.50
29:A:2514:U:H2'	29:A:2515:C:C6	2.47	0.50
6:G:94:ARG:HA	6:G:127:GLN:HE22	1.76	0.50
9:N:24:MET:HG3	9:N:44:LEU:HD12	1.93	0.50
12:R:49:ILE:O	12:R:49:ILE:HG13	2.12	0.50
12:R:97:LYS:HE2	12:R:97:LYS:HA	1.93	0.50
16:V:30:ILE:HG12	16:V:91:PHE:HB2	1.92	0.50
16:V:50:MET:HB2	16:V:53:LYS:HZ2	1.76	0.50
25:P:21:PRO:HG3	25:P:49:ILE:HD13	1.93	0.50
26:M:38:ARG:HG2	26:M:98:PRO:HD3	1.92	0.50
29:A:145:C:H2'	29:A:146:A:C8	2.46	0.50
29:A:1518:C:H2'	29:A:1519:G:H8	1.75	0.50
29:A:2698:U:H2'	29:A:2699:C:C6	2.47	0.50
2:C:129:LEU:HD12	2:C:133:ASN:HB2	1.92	0.50
15:U:5:ARG:HG2	15:U:6:ARG:H	1.76	0.50
29:A:750:A:OP1	29:A:1615:C:N4	2.38	0.50
29:A:828:U:H4'	29:A:831:G:N1	2.26	0.50
29:A:1997:C:H2'	29:A:1998:A:H8	1.75	0.50
29:A:2460:U:H2'	29:A:2461:A:H8	1.74	0.50
19:Y:32:ALA:HB2	19:Y:37:LEU:HD13	1.93	0.50
22:1:5:ARG:NH1	22:1:23:THR:O	2.45	0.50
29:A:1432:G:H2'	29:A:1433:A:H8	1.75	0.50
29:A:2233:U:H2'	29:A:2234:G:C8	2.43	0.50
29:A:2241:A:H2'	29:A:2242:G:C8	2.47	0.50
29:A:2841:C:H2'	29:A:2842:G:H8	1.76	0.50
29:A:2848:G:H1'	29:A:2868:A:H61	1.77	0.50
29:A:465:G:N2	29:A:684:G:H1'	2.27	0.50
29:A:825:A:N1	29:A:833:A:N6	2.59	0.50
29:A:911:A:H5"	29:A:912:C:H5"	1.94	0.50
29:A:1672:A:C6	29:A:2582:G:H5'	2.46	0.50
29:A:2329:U:H2'	29:A:2330:G:C8	2.45	0.50
29:A:2855:C:H2'	29:A:2856:A:C8	2.46	0.50
22:1:34:GLU:OE1	22:1:49:LYS:NZ	2.35	0.50
29:A:581:C:H2'	29:A:582:A:C8	2.46	0.50
29:A:639:U:H2'	29:A:640:C:H6	1.77	0.50
5:F:118:ALA:O	5:F:166:ARG:NH1	2.44	0.50
6:G:87:GLN:HE22	6:G:164:ALA:HA	1.76	0.50
29:A:954:G:H1	29:A:963:U:H3	1.59	0.50
29:A:1042:G:H1	29:A:1113:U:H3	1.59	0.50
29:A:2505:G:N2	29:A:2576:G:N7	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:2594:C:H2'	29:A:2595:G:C8	2.46	0.50
2:C:106:PRO:HG2	2:C:109:LEU:HB2	1.94	0.50
3:D:149:ASN:O	3:D:152:PRO:HD2	2.12	0.50
12:R:65:ALA:HB3	12:R:95:ASP:HB2	1.94	0.50
12:R:71:LYS:HA	12:R:90:ARG:HG2	1.93	0.50
14:T:38:ALA:HB3	14:T:81:LYS:HD2	1.93	0.50
15:U:32:LYS:HB3	15:U:63:ALA:HB1	1.94	0.50
18:X:53:LYS:NZ	29:A:373:U:OP2	2.36	0.50
19:Y:6:LEU:HD23	19:Y:56:LEU:HD11	1.93	0.50
29:A:23:G:H2'	29:A:24:G:C8	2.46	0.50
29:A:881:G:H2'	29:A:882:G:H8	1.76	0.50
29:A:1026:G:H2'	29:A:1027:A:H8	1.77	0.50
29:A:1073:A:H3'	29:A:1074:G:H5"	1.92	0.50
29:A:1710:G:H2'	29:A:1711:A:C8	2.47	0.50
29:A:2656:U:N3	29:A:2665:A:C8	2.77	0.50
20:Z:50:VAL:HB	20:Z:53:MET:SD	2.52	0.49
26:M:57:VAL:O	26:M:60:GLN:HG3	2.12	0.49
29:A:580:U:H2'	29:A:581:C:C6	2.47	0.49
29:A:1539:U:H2'	29:A:1540:G:C8	2.46	0.49
13:S:31:GLN:O	13:S:35:ILE:HG12	2.13	0.49
21:0:51:ARG:NH1	21:0:53:VAL:HG12	2.27	0.49
29:A:1102:C:H2'	29:A:1103:A:H8	1.77	0.49
29:A:1582:C:O2'	29:A:1585:C:N3	2.42	0.49
8:L:121:THR:HG22	8:L:141:LYS:HB3	1.94	0.49
16:V:56:PHE:CE1	16:V:61:LEU:HD11	2.48	0.49
21:0:52:LYS:HD3	21:0:55:ALA:HA	1.94	0.49
29:A:226:A:H1'	29:A:230:G:N2	2.28	0.49
29:A:308:G:N2	29:A:477:A:N7	2.59	0.49
29:A:351:C:H2'	29:A:352:A:C8	2.47	0.49
29:A:417:C:H2'	29:A:418:C:C6	2.47	0.49
29:A:2036:C:H2'	29:A:2037:A:H8	1.77	0.49
29:A:2685:G:H21	29:A:2726:A:N6	2.10	0.49
9:N:106:ASP:OD1	29:A:1649:G:O2'	2.27	0.49
29:A:175:G:H2'	29:A:176:A:C8	2.47	0.49
29:A:1267:U:H2'	29:A:1268:A:H8	1.77	0.49
29:A:1443:U:H2'	29:A:1444:G:C8	2.46	0.49
29:A:1563:U:H2'	29:A:1564:C:C6	2.48	0.49
30:B:40:U:N3	30:B:44:G:OP2	2.44	0.49
30:B:95:U:H2'	30:B:96:G:H8	1.76	0.49
29:A:13:A:O2'	29:A:15:G:N7	2.46	0.49
29:A:581:C:H2'	29:A:582:A:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:767:U:H2'	29:A:768:G:H8	1.77	0.49
29:A:966:G:H4'	29:A:2271:G:H22	1.78	0.49
29:A:1748:C:H2'	29:A:1749:A:C8	2.48	0.49
2:C:151:GLY:O	2:C:155:ARG:NH1	2.32	0.49
29:A:922:C:H2'	29:A:923:G:H8	1.76	0.49
29:A:967:U:H2'	29:A:968:C:C6	2.48	0.49
29:A:1264:A:H4'	29:A:2615:U:H5'	1.95	0.49
29:A:1447:C:O2'	29:A:1544:A:N3	2.42	0.49
29:A:2127:G:H2'	29:A:2128:G:C8	2.48	0.49
30:B:13:G:O2'	30:B:15:A:OP2	2.23	0.49
2:C:71:ASP:OD1	2:C:72:GLY:N	2.46	0.49
17:W:22:PHE:N	17:W:25:GLU:OE2	2.46	0.49
29:A:55:G:H2'	29:A:56:A:H8	1.78	0.49
29:A:230:G:H2'	29:A:231:A:H8	1.78	0.49
29:A:438:G:H2'	29:A:439:A:C8	2.48	0.49
29:A:538:A:H62	29:A:555:G:N2	2.11	0.49
29:A:1315:C:O2'	29:A:1392:A:N3	2.38	0.49
29:A:1431:A:H2'	29:A:1432:G:H8	1.78	0.49
29:A:1441:G:H2'	29:A:1442:U:C6	2.48	0.49
29:A:1726:C:H2'	29:A:1727:C:C6	2.48	0.49
29:A:2109:U:N3	29:A:2110:G:O6	2.45	0.49
31:9:168:PRO:HB3	31:9:191:PHE:H	1.77	0.49
32:3:32:LEU:HD23	32:3:40:LYS:HG2	1.94	0.49
5:F:135:ILE:HA	5:F:140:ILE:HD11	1.95	0.49
6:G:25:ILE:HG23	6:G:78:VAL:HG11	1.94	0.49
25:P:61:ARG:HE	25:P:63:ILE:HD11	1.77	0.49
29:A:953:G:O2'	29:A:2266:A:OP2	2.28	0.49
29:A:1433:A:H2'	29:A:1434:A:C8	2.47	0.49
29:A:1798:U:O2'	29:A:1802:A:N3	2.38	0.49
29:A:1808:A:H3'	29:A:1809:A:C8	2.48	0.49
29:A:2441:U:OP2	29:A:2586:U:O2'	2.31	0.49
29:A:2841:C:H2'	29:A:2842:G:C8	2.48	0.49
3:D:157:LYS:HG2	29:A:2619:C:H5"	1.95	0.49
5:F:110:ILE:HG23	5:F:113:PHE:HB2	1.94	0.49
8:L:112:LEU:O	29:A:627:A:N6	2.39	0.49
29:A:1259:G:H2'	29:A:1260:A:C8	2.47	0.49
29:A:2473:U:OP1	29:A:2529:G:N2	2.45	0.49
29:A:2847:U:H2'	29:A:2848:G:O4'	2.13	0.49
8:L:132:ARG:O	8:L:135:ILE:HG22	2.13	0.49
29:A:1435:G:H2'	29:A:1436:G:C8	2.47	0.49
29:A:2304:G:H22	29:A:2312:U:H3	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:3:THR:OG1	29:A:995:C:O2	2.26	0.48
29:A:924:G:H2'	29:A:925:A:H8	1.78	0.48
29:A:1131:G:N2	29:A:1132:U:O4	2.34	0.48
29:A:2737:G:H2'	29:A:2738:A:C8	2.48	0.48
30:B:77:U:O2	30:B:99:A:N7	2.46	0.48
2:C:107:LYS:HA	2:C:195:GLY:HA2	1.95	0.48
3:D:155:VAL:HG21	29:A:2618:G:H21	1.78	0.48
29:A:20:C:H2'	29:A:21:A:H8	1.78	0.48
29:A:249:C:O2	32:3:11:LYS:NZ	2.45	0.48
29:A:299:A:N1	29:A:322:A:O2'	2.41	0.48
29:A:457:A:N7	29:A:472:A:N6	2.60	0.48
29:A:579:G:H2'	29:A:580:U:C6	2.48	0.48
29:A:833:A:H2'	29:A:834:G:C8	2.48	0.48
29:A:1400:U:H2'	29:A:1401:G:H8	1.77	0.48
3:D:4:LEU:HD21	3:D:100:LEU:HD21	1.95	0.48
26:M:3:GLN:HG2	26:M:4:PRO:HD2	1.95	0.48
29:A:306:U:H2'	29:A:307:G:O4'	2.12	0.48
29:A:1704:C:H2'	29:A:1705:A:C8	2.48	0.48
29:A:1801:A:H5'	29:A:2203:U:H2'	1.95	0.48
29:A:2229:U:H2'	29:A:2230:G:C8	2.46	0.48
31:9:13:ALA:HB1	31:9:120:GLY:HA2	1.94	0.48
3:D:45:TYR:OH	29:A:2636:C:O2'	2.30	0.48
3:D:125:TRP:CD1	3:D:160:LYS:HB3	2.48	0.48
12:R:41:ILE:HB	12:R:47:VAL:HB	1.96	0.48
13:S:25:ARG:NH2	13:S:74:ILE:O	2.45	0.48
29:A:499:U:H2'	29:A:500:G:O4'	2.13	0.48
29:A:749:A:H5'	29:A:1271:G:H1'	1.93	0.48
29:A:1434:A:H2'	29:A:1435:G:H8	1.78	0.48
29:A:2120:G:H2'	29:A:2121:G:C8	2.45	0.48
29:A:2637:U:O4	29:A:2776:A:N7	2.46	0.48
30:B:70:C:H2'	30:B:71:C:H6	1.77	0.48
3:D:151:THR:HB	3:D:152:PRO:HD3	1.96	0.48
5:F:118:ALA:HB2	5:F:177:ARG:HA	1.95	0.48
13:S:73:LYS:HB2	13:S:106:VAL:HB	1.94	0.48
29:A:864:G:O2'	29:A:914:G:O6	2.30	0.48
29:A:1038:G:H2'	29:A:1039:A:C8	2.48	0.48
29:A:1207:C:H2'	29:A:1208:C:C6	2.49	0.48
29:A:1637:A:H2'	29:A:1638:C:C6	2.48	0.48
32:3:30:HIS:O	32:3:32:LEU:N	2.45	0.48
13:S:67:ASP:OD2	13:S:68:ASP:N	2.46	0.48
14:T:22:THR:HA	14:T:25:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:851:C:H2'	29:A:852:U:C6	2.49	0.48
29:A:1013:C:H2'	29:A:1014:A:C8	2.49	0.48
30:B:29:A:H2'	30:B:30:C:C6	2.49	0.48
31:9:290:LYS:HG3	31:9:291:VAL:H	1.79	0.48
2:C:194:VAL:HG22	2:C:195:GLY:H	1.77	0.48
3:D:173:GLN:NE2	29:A:2771:C:O2'	2.42	0.48
7:J:120:ARG:NE	29:A:2780:G:OP2	2.47	0.48
29:A:87:U:H3	29:A:95:A:H61	1.60	0.48
29:A:2439:A:O2'	29:A:2600:A:OP1	2.30	0.48
2:C:74:PRO:HD2	2:C:96:LYS:HG2	1.96	0.48
3:D:8:LYS:NZ	3:D:195:GLY:O	2.42	0.48
6:G:175:LYS:HE2	29:A:2530:A:H5'	1.96	0.48
27:H:62:LEU:O	27:H:66:ASN:ND2	2.47	0.48
29:A:155:A:H2'	29:A:156:A:C8	2.49	0.48
29:A:946:C:H2'	29:A:947:A:C8	2.49	0.48
29:A:1495:A:H2	29:A:1578:U:H1'	1.79	0.48
29:A:1564:C:H2'	29:A:1565:C:C6	2.48	0.48
29:A:2231:U:H2'	29:A:2232:C:C6	2.49	0.48
29:A:2385:C:H2'	29:A:2386:A:H8	1.78	0.48
29:A:2824:C:H3'	29:A:2825:G:H21	1.79	0.48
29:A:877:A:O2'	29:A:900:A:N6	2.47	0.48
29:A:934:U:H2'	29:A:935:C:H6	1.79	0.48
29:A:1441:G:H2'	29:A:1442:U:H6	1.79	0.48
29:A:1444:G:H2'	29:A:1445:G:H8	1.79	0.48
29:A:1936:A:H2	29:A:1943:U:H3	1.62	0.48
29:A:2345:G:H5'	29:A:2347:C:H5'	1.96	0.48
3:D:178:VAL:HG12	3:D:179:ARG:HG3	1.95	0.48
18:X:2:ARG:NH2	29:A:1365:A:OP1	2.41	0.48
24:K:40:LYS:HD2	24:K:57:VAL:HG12	1.96	0.48
29:A:319:G:H2'	29:A:320:A:C8	2.49	0.48
29:A:539:G:H1	29:A:554:U:H3	1.61	0.48
29:A:2840:C:H2'	29:A:2841:C:H6	1.79	0.48
30:B:116:G:H2'	30:B:117:G:H8	1.79	0.48
2:C:222:THR:N	29:A:1826:G:OP1	2.47	0.47
3:D:3:GLY:HA2	3:D:101:PHE:HZ	1.79	0.47
29:A:924:G:H2'	29:A:925:A:C8	2.49	0.47
29:A:2204:G:O6	29:A:2220:U:O4	2.32	0.47
3:D:77:ARG:NH2	3:D:200:ASP:OD1	2.47	0.47
29:A:625:G:H2'	29:A:626:A:C8	2.49	0.47
29:A:1275:A:N1	29:A:1295:C:O2'	2.39	0.47
29:A:1378:A:O2'	29:A:1380:G:OP2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:1709:U:H2'	29:A:1710:G:C8	2.49	0.47
29:A:2719:G:H4'	29:A:2846:G:H4'	1.95	0.47
14:T:8:LEU:HD11	19:Y:26:PHE:HB2	1.97	0.47
16:V:21:ARG:NH1	30:B:77:U:OP1	2.35	0.47
29:A:64:A:H2'	29:A:65:U:H6	1.79	0.47
29:A:2057:G:H2'	29:A:2058:A:C8	2.50	0.47
29:A:2127:G:H21	29:A:2173:A:H1'	1.79	0.47
29:A:2688:G:N1	29:A:2720:U:OP2	2.37	0.47
29:A:2834:G:H1'	29:A:2883:A:H61	1.80	0.47
9:N:3:HIS:ND1	29:A:2820:A:H4'	2.29	0.47
14:T:61:LEU:HD11	14:T:82:LYS:HD3	1.96	0.47
24:K:80:ASP:OD2	25:P:61:ARG:NH1	2.47	0.47
29:A:155:A:H2'	29:A:156:A:H8	1.78	0.47
29:A:172:A:H2'	29:A:173:A:H8	1.79	0.47
29:A:671:C:H2'	29:A:672:C:H6	1.78	0.47
29:A:1357:C:H2'	29:A:1358:G:O4'	2.14	0.47
29:A:2470:G:H2'	29:A:2471:A:H8	1.79	0.47
30:B:6:G:H2'	30:B:7:G:C8	2.49	0.47
4:E:108:ILE:HD12	4:E:181:ILE:HD11	1.97	0.47
12:R:6:GLN:HB3	12:R:11:GLN:HG2	1.95	0.47
24:K:5:GLN:H	24:K:22:ILE:HA	1.78	0.47
25:P:55:HIS:HB3	29:A:2683:C:H5"	1.97	0.47
29:A:419:U:H2'	29:A:420:C:C6	2.48	0.47
29:A:437:U:H2'	29:A:438:G:H8	1.80	0.47
29:A:1346:G:N2	29:A:1347:A:H1'	2.29	0.47
29:A:1438:U:H2'	29:A:1439:A:C8	2.48	0.47
29:A:1520:U:H2'	29:A:1521:G:O4'	2.13	0.47
29:A:2215:C:H2'	29:A:2216:G:C8	2.49	0.47
29:A:2606:C:H2'	29:A:2607:G:H8	1.79	0.47
29:A:2818:U:H2'	29:A:2819:G:H8	1.80	0.47
13:S:3:THR:OG1	13:S:62:ASP:OD2	2.31	0.47
17:W:73:ARG:NH2	29:A:2333:A:OP2	2.47	0.47
29:A:414:C:H2'	29:A:415:A:H8	1.80	0.47
29:A:589:U:H2'	29:A:590:A:H8	1.80	0.47
29:A:948:C:H2'	29:A:949:G:C8	2.49	0.47
29:A:1141:U:H4'	29:A:1142:A:O4'	2.15	0.47
29:A:1353:A:H2'	29:A:1354:A:H8	1.79	0.47
29:A:2577:A:O4'	29:A:2612:C:N4	2.48	0.47
4:E:196:VAL:HA	4:E:199:MET:HG3	1.96	0.47
15:U:38:ILE:HG21	15:U:64:ILE:HG13	1.97	0.47
27:H:47:PHE:O	27:H:51:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:302:C:H2'	29:A:303:G:C8	2.50	0.47
29:A:996:A:H2'	29:A:997:G:C8	2.50	0.47
29:A:1720:U:H2'	29:A:1721:G:O4'	2.14	0.47
29:A:1801:A:N6	29:A:2201:G:O2'	2.39	0.47
29:A:1930:G:N2	29:A:1969:A:O5'	2.42	0.47
29:A:2039:U:H2'	29:A:2040:G:H8	1.79	0.47
29:A:2064:C:H2'	29:A:2065:C:H6	1.80	0.47
29:A:2372:U:H2'	29:A:2373:G:C8	2.50	0.47
29:A:2636:C:H2'	29:A:2637:U:H6	1.79	0.47
32:3:32:LEU:HA	32:3:35:LYS:HE3	1.97	0.47
9:N:22:ARG:HG3	9:N:70:THR:HA	1.97	0.47
13:S:78:GLU:OE2	29:A:24:G:N2	2.47	0.47
29:A:16:C:H2'	29:A:17:G:H8	1.77	0.47
29:A:1752:C:H2'	29:A:1753:G:C8	2.50	0.47
29:A:2011:U:H2'	29:A:2012:G:O4'	2.14	0.47
29:A:2182:U:H2'	29:A:2183:A:C8	2.50	0.47
29:A:2228:G:H2'	29:A:2229:U:C6	2.50	0.47
3:D:30:GLU:OE1	3:D:33:ARG:NH2	2.47	0.47
8:L:96:LYS:HB3	8:L:103:ILE:HD13	1.96	0.47
10:O:25:ARG:NH1	30:B:8:C:O3'	2.48	0.47
11:Q:54:ARG:HD3	29:A:1155:A:H5"	1.96	0.47
13:S:77:ASP:HB3	29:A:24:G:H1'	1.95	0.47
24:K:18:ARG:NH2	24:K:45:GLU:HG2	2.30	0.47
27:H:97:ARG:HH21	27:H:112:LYS:HZ3	1.62	0.47
29:A:987:C:H2'	29:A:988:A:O4'	2.15	0.47
29:A:1733:G:H2'	29:A:1734:G:C8	2.50	0.47
29:A:2066:C:H2'	29:A:2067:G:C8	2.49	0.47
29:A:2707:U:H2'	29:A:2708:G:C8	2.49	0.47
30:B:51:G:O6	30:B:52:A:N6	2.47	0.47
30:B:83:G:O6	30:B:94:A:N6	2.47	0.47
5:F:98:PHE:HA	5:F:101:ARG:HG2	1.96	0.47
6:G:2:ARG:NH1	29:A:2751:G:OP2	2.46	0.47
29:A:307:G:N2	29:A:309:A:H3'	2.30	0.47
29:A:582:A:H2'	29:A:583:G:H8	1.78	0.47
29:A:996:A:H2'	29:A:997:G:H8	1.79	0.47
29:A:1431:A:H2'	29:A:1432:G:C8	2.49	0.47
29:A:2425:A:H4'	29:A:2426:A:O5'	2.14	0.47
31:9:24:ARG:HB2	31:9:35:ASP:HB2	1.97	0.47
2:C:38:LYS:NZ	2:C:55:GLY:O	2.42	0.46
4:E:52:VAL:HB	4:E:74:LYS:HD2	1.96	0.46
29:A:630:G:N2	29:A:633:A:OP2	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:1079:C:H2'	29:A:1080:A:O4'	2.15	0.46
29:A:1821:A:H2'	29:A:1822:C:C6	2.50	0.46
29:A:2329:U:H2'	29:A:2330:G:H8	1.80	0.46
5:F:121:PHE:HE2	5:F:166:ARG:HH12	1.63	0.46
6:G:84:LYS:HB3	6:G:132:LEU:HB2	1.98	0.46
16:V:50:MET:O	16:V:53:LYS:NZ	2.43	0.46
19:Y:26:PHE:O	19:Y:30:MET:HG2	2.15	0.46
29:A:491:G:H3'	29:A:492:A:H8	1.79	0.46
29:A:777:G:H2'	29:A:778:G:H8	1.79	0.46
29:A:1355:G:H2'	29:A:1356:G:H8	1.80	0.46
29:A:2036:C:H2'	29:A:2037:A:C8	2.50	0.46
11:Q:67:ALA:HA	11:Q:70:GLN:OE1	2.15	0.46
13:S:24:ILE:HD13	13:S:36:LEU:HD11	1.96	0.46
16:V:9:ARG:HE	16:V:27:PRO:HB3	1.80	0.46
17:W:66:GLU:OE1	17:W:68:LYS:HG2	2.15	0.46
27:H:97:ARG:NH2	29:A:2220:U:O3'	2.49	0.46
29:A:282:A:H2'	29:A:283:G:C8	2.51	0.46
29:A:979:A:H2'	29:A:982:C:H42	1.80	0.46
29:A:1394:U:H4'	29:A:1603:A:H4'	1.97	0.46
29:A:1809:A:H2'	29:A:1810:A:C8	2.50	0.46
29:A:1847:A:O2'	29:A:1848:A:H8	1.99	0.46
31:9:263:ILE:HG22	31:9:267:GLU:HG3	1.98	0.46
9:N:5:LYS:NZ	29:A:2000:C:OP1	2.47	0.46
10:O:29:HIS:HB3	10:O:36:TYR:HB2	1.96	0.46
29:A:577:G:H2'	29:A:578:G:C8	2.50	0.46
29:A:1114:C:N4	29:A:1115:G:O6	2.48	0.46
29:A:2266:A:H4'	29:A:2267:A:N3	2.30	0.46
29:A:2328:A:H2'	29:A:2329:U:H6	1.80	0.46
29:A:2626:C:H2'	29:A:2627:G:C8	2.50	0.46
30:B:116:G:H2'	30:B:117:G:C8	2.50	0.46
4:E:141:MET:HG2	4:E:143:LEU:HG	1.97	0.46
25:P:5:LYS:HA	25:P:8:GLU:HB2	1.98	0.46
29:A:566:U:H2'	29:A:567:U:C6	2.50	0.46
29:A:903:C:H2'	29:A:904:G:C8	2.50	0.46
29:A:1098:A:H3'	29:A:1099:G:H8	1.81	0.46
29:A:1550:C:H2'	29:A:1551:A:H8	1.81	0.46
29:A:2446:G:N2	29:A:2449:U:O2	2.44	0.46
29:A:2845:U:H2'	29:A:2846:G:C8	2.49	0.46
6:G:59:ASP:OD1	6:G:60:GLY:N	2.40	0.46
19:Y:9:LYS:HD3	19:Y:10:SER:N	2.31	0.46
30:B:9:G:H1	30:B:111:U:H3	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:157:MET:HE3	31:9:158:LEU:H	1.79	0.46
31:9:289:ASP:OD1	31:9:289:ASP:N	2.47	0.46
2:C:209:ALA:HA	2:C:212:TRP:CZ2	2.51	0.46
2:C:219:VAL:HG21	29:A:782:A:C8	2.50	0.46
14:T:10:VAL:HG21	14:T:42:GLU:HB3	1.97	0.46
16:V:61:LEU:N	16:V:72:VAL:O	2.46	0.46
27:H:9:VAL:HG22	27:H:10:ALA:H	1.81	0.46
29:A:67:U:C2	29:A:68:G:C8	3.03	0.46
29:A:582:A:H2'	29:A:583:G:C8	2.51	0.46
29:A:970:U:H2'	29:A:971:G:C8	2.51	0.46
29:A:1164:C:H2'	29:A:1165:A:C8	2.50	0.46
29:A:1571:A:H2'	29:A:1572:A:H8	1.81	0.46
29:A:1638:C:O2	29:A:2698:U:O2'	2.34	0.46
31:9:177:ARG:NH2	31:9:184:PRO:HD2	2.30	0.46
18:X:16:ASN:HB2	18:X:24:THR:HB	1.96	0.46
21:0:30:ASP:HB3	21:0:34:GLY:H	1.81	0.46
27:H:4:ILE:HG21	27:H:51:ARG:HH22	1.80	0.46
29:A:732:C:H2'	29:A:733:G:O4'	2.16	0.46
29:A:793:A:OP2	29:A:2071:A:O2'	2.34	0.46
29:A:1665:A:H2'	29:A:1666:G:H8	1.80	0.46
29:A:1826:G:H2'	29:A:1827:U:C6	2.51	0.46
29:A:2030:A:H4'	29:A:2031:A:H8	1.80	0.46
29:A:2047:C:O2'	29:A:2823:A:N1	2.42	0.46
29:A:2241:A:H2'	29:A:2242:G:H8	1.80	0.46
29:A:2414:G:C2	29:A:2415:G:C8	3.04	0.46
29:A:2642:G:H2'	29:A:2643:G:H8	1.81	0.46
2:C:240:GLY:O	29:A:2596:U:O2'	2.34	0.46
4:E:43:THR:HB	29:A:38:A:N3	2.31	0.46
9:N:34:ILE:HD12	29:A:1278:C:H4'	1.97	0.46
10:O:117:PHE:O	29:A:2377:A:O2'	2.34	0.46
11:Q:106:THR:O	11:Q:110:GLU:OE1	2.34	0.46
29:A:1084:A:N3	29:A:1105:U:O2'	2.48	0.46
29:A:1751:U:H2'	29:A:1752:C:C6	2.50	0.46
29:A:1862:G:H1	29:A:1880:U:H3	1.64	0.46
29:A:2364:C:H2'	29:A:2365:G:O4'	2.16	0.46
29:A:2416:C:C2	29:A:2417:C:C5	3.03	0.46
29:A:2625:G:H2'	29:A:2626:C:C6	2.51	0.46
31:9:177:ARG:NH1	31:9:182:ALA:H	2.14	0.46
31:9:306:TRP:CE3	31:9:308:ASP:HB2	2.51	0.46
29:A:24:G:H2'	29:A:25:U:C6	2.50	0.46
29:A:355:U:H2'	29:A:356:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:680:C:H2'	29:A:681:G:C8	2.50	0.46
29:A:926:G:H2'	29:A:927:A:H8	1.81	0.46
29:A:2391:G:O2'	29:A:2424:C:N4	2.42	0.46
29:A:2457:U:H2'	29:A:2458:G:C8	2.50	0.46
31:9:222:ALA:HB1	31:9:268:LYS:HD2	1.98	0.46
9:N:39:PRO:HG2	29:A:1651:G:H5'	1.98	0.45
19:Y:48:ARG:NH1	29:A:76:C:OP1	2.49	0.45
29:A:419:U:H2'	29:A:420:C:H6	1.82	0.45
29:A:551:G:H2'	29:A:552:U:C6	2.51	0.45
29:A:599:A:H2'	29:A:600:G:C8	2.51	0.45
29:A:695:G:H1	29:A:767:U:H3	1.62	0.45
29:A:832:U:H2'	29:A:833:A:C8	2.48	0.45
29:A:934:U:H2'	29:A:935:C:C6	2.51	0.45
30:B:6:G:H2'	30:B:7:G:H8	1.80	0.45
30:B:70:C:H2'	30:B:71:C:C6	2.51	0.45
4:E:192:ALA:HA	4:E:195:GLN:HE21	1.81	0.45
6:G:157:LYS:HE3	6:G:157:LYS:HB3	1.72	0.45
11:Q:56:PHE:HZ	29:A:536:G:H4'	1.80	0.45
19:Y:49:ASP:HA	19:Y:52:ARG:HG2	1.98	0.45
29:A:106:C:H2'	29:A:107:G:H8	1.81	0.45
29:A:301:G:O2'	29:A:302:C:O5'	2.32	0.45
29:A:523:C:H5"	29:A:540:C:O2'	2.16	0.45
29:A:558:U:H2'	29:A:559:G:H8	1.81	0.45
29:A:589:U:H2'	29:A:590:A:C8	2.51	0.45
29:A:638:G:H2'	29:A:639:U:H6	1.82	0.45
29:A:1298:C:H2'	29:A:1299:G:O4'	2.16	0.45
29:A:1496:A:H2'	29:A:1498:C:C5	2.51	0.45
29:A:2460:U:O2	29:A:2493:U:N3	2.50	0.45
29:A:2731:G:H2'	29:A:2732:G:C8	2.51	0.45
7:J:95:ARG:HG2	7:J:96:ARG:HD3	1.98	0.45
12:R:27:ILE:HG23	12:R:31:GLU:OE2	2.16	0.45
29:A:2254:C:C2	29:A:2255:G:C8	3.05	0.45
29:A:2784:U:H2'	29:A:2785:C:H6	1.81	0.45
30:B:20:G:H2'	30:B:21:G:H8	1.82	0.45
3:D:194:PRO:HB3	29:A:2679:A:H4'	1.97	0.45
29:A:69:C:H2'	29:A:70:G:C8	2.50	0.45
29:A:411:G:OP2	29:A:2406:A:O2'	2.30	0.45
29:A:558:U:H2'	29:A:559:G:C8	2.52	0.45
29:A:1326:U:N3	29:A:1648:U:O2'	2.45	0.45
29:A:2357:G:N2	29:A:2360:G:OP2	2.35	0.45
29:A:2370:G:H2'	29:A:2371:G:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:2584:U:H2'	29:A:2585:U:O4'	2.16	0.45
29:A:2623:G:H2'	29:A:2624:G:C8	2.51	0.45
32:3:15:LYS:HD2	32:3:19:GLY:HA2	1.99	0.45
26:M:112:LEU:O	26:M:115:GLU:HG3	2.17	0.45
29:A:341:C:H2'	29:A:342:A:C8	2.52	0.45
29:A:364:C:H2'	29:A:365:U:C6	2.51	0.45
29:A:541:A:H2'	29:A:542:C:C6	2.51	0.45
29:A:946:C:H2'	29:A:947:A:H8	1.82	0.45
29:A:1019:U:OP1	29:A:1035:U:O2'	2.26	0.45
29:A:1841:U:H2'	29:A:1842:G:H8	1.81	0.45
29:A:2023:C:H2'	29:A:2024:G:H8	1.80	0.45
29:A:2315:G:H2'	29:A:2316:G:H8	1.81	0.45
30:B:9:G:C2	30:B:10:G:C8	3.04	0.45
27:H:1:MET:SD	27:H:3:VAL:N	2.89	0.45
29:A:55:G:H2'	29:A:56:A:C8	2.52	0.45
29:A:599:A:H2'	29:A:600:G:H8	1.82	0.45
29:A:807:U:H2'	29:A:808:G:C8	2.51	0.45
29:A:1442:U:H2'	29:A:1443:U:C6	2.52	0.45
29:A:1825:U:H2'	29:A:1826:G:C8	2.50	0.45
29:A:2028:U:O4	29:A:2033:A:N7	2.49	0.45
8:L:23:ILE:HG12	12:R:82:HIS:NE2	2.32	0.45
29:A:2065:C:H2'	29:A:2066:C:C6	2.51	0.45
29:A:2340:A:H2'	29:A:2341:G:H8	1.81	0.45
32:3:27:ASN:O	32:3:32:LEU:HD21	2.17	0.45
2:C:256:THR:OG1	29:A:1797:G:O2'	2.34	0.45
11:Q:20:ALA:HB2	11:Q:38:VAL:HG23	1.99	0.45
27:H:30:LEU:HB3	27:H:36:ALA:HB3	1.99	0.45
29:A:451:U:O2	29:A:453:A:N6	2.50	0.45
29:A:1231:U:H2'	29:A:1232:G:H8	1.81	0.45
29:A:1389:G:H2'	29:A:1390:U:C6	2.52	0.45
29:A:1464:G:H2'	29:A:1465:G:C8	2.52	0.45
29:A:2081:U:H2'	29:A:2082:A:C8	2.49	0.45
6:G:54:ARG:HH11	6:G:57:TYR:HE2	1.65	0.45
25:P:26:GLU:HB2	25:P:86:LYS:NZ	2.32	0.45
29:A:243:U:OP2	32:3:7:ARG:NH1	2.50	0.45
29:A:1005:C:H2'	29:A:1006:C:C6	2.52	0.45
29:A:1222:U:H2'	29:A:1223:G:C8	2.52	0.45
29:A:1361:G:H2'	29:A:1362:C:H6	1.81	0.45
29:A:1409:U:H2'	29:A:1410:G:H8	1.82	0.45
29:A:2339:C:H2'	29:A:2340:A:H8	1.82	0.45
32:3:30:HIS:C	32:3:32:LEU:H	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:80:HIS:ND1	7:J:81:ILE:HG22	2.32	0.45
7:J:101:ILE:HD13	7:J:124:VAL:HG21	1.99	0.45
27:H:29:PHE:O	27:H:35:LYS:NZ	2.40	0.45
29:A:639:U:C2	29:A:640:C:C5	3.05	0.45
29:A:727:A:H2'	29:A:728:G:C8	2.52	0.45
29:A:1028:A:OP2	29:A:1126:A:N6	2.50	0.45
29:A:1744:A:H3'	29:A:1745:A:H8	1.82	0.45
29:A:2291:U:H2'	29:A:2292:U:C6	2.52	0.45
29:A:2487:G:H2'	29:A:2488:G:C8	2.52	0.45
29:A:2602:A:H8	31:9:33:GLY:HA2	1.81	0.45
29:A:2804:U:H2'	29:A:2805:C:H6	1.82	0.45
30:B:22:U:H3	30:B:61:G:H1	1.63	0.45
30:B:32:U:H2'	30:B:33:G:C8	2.52	0.45
5:F:14:LYS:O	5:F:17:THR:N	2.49	0.44
26:M:13:HIS:O	26:M:71:LYS:NZ	2.49	0.44
29:A:1434:A:H2'	29:A:1435:G:C8	2.52	0.44
29:A:1874:C:H2'	29:A:1875:G:O4'	2.17	0.44
2:C:204:LEU:HB3	2:C:209:ALA:HB3	1.99	0.44
7:J:102:GLU:HA	7:J:105:VAL:HB	1.98	0.44
9:N:28:LEU:HD22	9:N:44:LEU:HD21	1.99	0.44
18:X:54:GLY:O	18:X:58:ILE:HG23	2.17	0.44
26:M:84:LYS:NZ	29:A:2250:G:OP1	2.41	0.44
29:A:63:A:H2'	29:A:64:A:H8	1.82	0.44
29:A:296:U:H2'	29:A:297:G:C8	2.53	0.44
29:A:743:A:H2'	29:A:744:U:C6	2.51	0.44
29:A:1404:C:H2'	29:A:1405:U:H6	1.83	0.44
29:A:1630:A:N1	29:A:1637:A:N6	2.66	0.44
29:A:2636:C:H2'	29:A:2637:U:C6	2.52	0.44
30:B:30:C:H2'	30:B:31:C:O4'	2.18	0.44
3:D:184:ARG:HB3	3:D:186:LEU:HD13	1.99	0.44
13:S:16:LYS:NZ	29:A:2011:U:OP2	2.44	0.44
18:X:4:CYS:SG	18:X:7:THR:OG1	2.70	0.44
24:K:25:LEU:HD22	29:A:2562:U:H4'	1.99	0.44
27:H:26:ALA:O	27:H:30:LEU:HB2	2.17	0.44
29:A:404:A:H4'	29:A:405:U:O5'	2.16	0.44
29:A:689:A:N3	29:A:779:U:O2'	2.42	0.44
29:A:724:U:H2'	29:A:725:G:O4'	2.18	0.44
29:A:796:C:H2'	29:A:797:G:H8	1.80	0.44
29:A:940:G:H2'	29:A:941:A:O4'	2.16	0.44
29:A:1219:U:H2'	29:A:1220:G:C8	2.53	0.44
29:A:1850:G:H2'	29:A:1851:U:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:2087:G:H2'	29:A:2088:A:H8	1.83	0.44
13:S:92:ARG:O	29:A:1614:A:N6	2.46	0.44
24:K:2:ILE:HD12	24:K:8:LEU:HD21	2.00	0.44
29:A:526:A:O2'	29:A:2043:C:O2	2.32	0.44
29:A:595:C:H2'	29:A:596:U:C6	2.53	0.44
29:A:819:A:N6	29:A:1189:A:H1'	2.33	0.44
29:A:2710:C:H2'	29:A:2711:A:C8	2.53	0.44
29:A:2774:C:H2'	29:A:2775:G:O4'	2.17	0.44
29:A:2888:C:H2'	29:A:2889:C:C6	2.53	0.44
31:9:173:SER:N	35:9:402:GNP:O2B	2.39	0.44
31:9:192:THR:N	35:9:402:GNP:O3G	2.39	0.44
10:O:99:TYR:O	10:O:103:VAL:HB	2.18	0.44
14:T:6:ARG:NH2	14:T:37:ASP:OD2	2.51	0.44
29:A:500:G:N1	29:A:503:A:OP2	2.39	0.44
29:A:513:A:H4'	29:A:1217:U:H5'	1.99	0.44
29:A:579:G:H2'	29:A:580:U:H6	1.83	0.44
29:A:967:U:H2'	29:A:968:C:H6	1.81	0.44
29:A:1352:U:H1'	29:A:1570:A:H2	1.82	0.44
29:A:1558:C:H4'	29:A:1559:U:H3'	1.99	0.44
29:A:1749:A:H2'	29:A:1750:G:H8	1.82	0.44
29:A:2582:G:C2	29:A:2583:G:C8	3.05	0.44
5:F:32:LYS:HD3	5:F:91:ARG:HH22	1.82	0.44
5:F:150:GLY:HA3	29:A:2305:U:N3	2.33	0.44
8:L:111:ILE:HG21	29:A:636:G:C6	2.53	0.44
13:S:58:ALA:O	13:S:62:ASP:HB2	2.18	0.44
27:H:5:LEU:HD22	27:H:13:GLY:HA3	1.98	0.44
29:A:201:C:H2'	29:A:202:U:C6	2.53	0.44
29:A:594:U:H2'	29:A:595:C:C6	2.53	0.44
29:A:596:U:H2'	29:A:597:G:C8	2.52	0.44
29:A:680:C:H2'	29:A:681:G:H8	1.83	0.44
3:D:48:ILE:HG21	3:D:90:PHE:HB2	1.99	0.44
3:D:149:ASN:HB3	29:A:2572:A:OP2	2.18	0.44
13:S:46:LEU:O	13:S:50:VAL:HG23	2.17	0.44
26:M:42:THR:HG22	26:M:93:VAL:HG12	2.00	0.44
29:A:16:C:H2'	29:A:17:G:C8	2.52	0.44
29:A:25:U:H2'	29:A:26:G:O4'	2.18	0.44
29:A:686:U:H2'	29:A:788:A:N1	2.33	0.44
29:A:781:A:H5"	29:A:782:A:N7	2.32	0.44
29:A:1066:U:N3	29:A:1069:A:OP2	2.51	0.44
29:A:2130:U:O2'	29:A:2134:A:O4'	2.34	0.44
29:A:2368:C:H2'	29:A:2369:A:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:2639:A:H2'	29:A:2640:G:O4'	2.18	0.44
29:A:2705:A:O2'	29:A:2852:G:OP1	2.28	0.44
3:D:170:VAL:HG11	29:A:2679:A:H5'	2.00	0.44
8:L:56:PRO:HG2	8:L:59:ARG:HD3	2.00	0.44
12:R:5:PHE:HA	12:R:39:LEU:HD23	2.00	0.44
29:A:1047:G:N2	29:A:1110:G:O2'	2.47	0.44
29:A:1136:G:H2'	29:A:1137:G:C8	2.52	0.44
29:A:1954:G:O2'	29:A:1956:U:O4	2.28	0.44
29:A:438:G:H2'	29:A:439:A:H8	1.83	0.44
29:A:475:C:H4'	29:A:510:C:H5'	1.99	0.44
29:A:1987:A:H2'	29:A:1988:G:H8	1.82	0.44
29:A:2099:U:H2'	29:A:2100:G:H8	1.83	0.44
29:A:2554:U:H2'	29:A:2555:U:C6	2.53	0.44
29:A:2798:U:O2	29:A:2799:A:N6	2.51	0.44
30:B:74:U:H2'	30:B:75:G:O4'	2.18	0.44
11:Q:90:ASP:N	11:Q:90:ASP:OD1	2.51	0.43
16:V:21:ARG:HA	16:V:25:LYS:O	2.18	0.43
24:K:31:ARG:NH2	29:A:2676:C:OP1	2.48	0.43
29:A:78:U:O4	29:A:108:G:O6	2.35	0.43
29:A:287:G:H1	29:A:353:C:H42	1.66	0.43
29:A:1026:G:H2'	29:A:1027:A:C8	2.52	0.43
29:A:1654:A:H2'	29:A:1655:A:H8	1.84	0.43
29:A:2018:G:H2'	29:A:2019:A:H8	1.83	0.43
29:A:2412:A:H2'	29:A:2413:G:O4'	2.18	0.43
29:A:2470:G:H2'	29:A:2471:A:C8	2.53	0.43
30:B:20:G:H2'	30:B:21:G:C8	2.53	0.43
30:B:40:U:H3'	30:B:41:G:H4'	1.99	0.43
30:B:60:C:H2'	30:B:61:G:C8	2.52	0.43
12:R:36:ALA:HA	12:R:58:VAL:HG23	2.00	0.43
27:H:112:LYS:HZ3	29:A:2220:U:H5'	1.84	0.43
29:A:172:A:H2'	29:A:173:A:C8	2.54	0.43
29:A:285:G:N2	29:A:355:U:O2	2.39	0.43
29:A:289:G:H2'	29:A:290:U:C6	2.53	0.43
29:A:693:A:O2'	29:A:1353:A:N3	2.52	0.43
29:A:1407:G:H2'	29:A:1408:G:H8	1.82	0.43
29:A:1722:A:N6	29:A:1738:G:H1'	2.33	0.43
29:A:2647:U:H2'	29:A:2648:G:H8	1.83	0.43
31:9:249:PRO:HG2	31:9:253:THR:H	1.82	0.43
5:F:33:ILE:HD12	5:F:155:ILE:HD12	2.00	0.43
6:G:83:THR:HG22	6:G:133:LYS:HE3	2.00	0.43
7:J:37:ARG:NH2	29:A:1007:C:H5"	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:95:ARG:NH2	29:A:2768:U:O2'	2.51	0.43
9:N:29:VAL:HG13	9:N:75:ILE:HD12	1.98	0.43
29:A:800:A:O4'	29:A:802:A:H5'	2.19	0.43
29:A:813:U:H2'	29:A:814:C:H6	1.83	0.43
29:A:1040:A:N1	29:A:1115:G:N2	2.66	0.43
29:A:1107:G:H2'	29:A:1108:U:C6	2.54	0.43
29:A:1229:C:H2'	29:A:1230:A:C8	2.53	0.43
29:A:1234:U:H2'	29:A:1235:G:O4'	2.18	0.43
29:A:1550:C:H2'	29:A:1551:A:C8	2.53	0.43
29:A:1967:C:H2'	29:A:1968:G:O4'	2.18	0.43
29:A:1987:A:H2'	29:A:1988:G:C8	2.53	0.43
29:A:2315:G:H2'	29:A:2316:G:C8	2.53	0.43
29:A:2785:C:H2'	29:A:2786:U:H6	1.84	0.43
29:A:2848:G:H1'	29:A:2868:A:N6	2.32	0.43
29:A:2875:C:H2'	29:A:2876:G:C8	2.53	0.43
2:C:151:GLY:O	2:C:155:ARG:HD2	2.18	0.43
17:W:73:ARG:HH22	29:A:2333:A:P	2.40	0.43
19:Y:18:LEU:CD2	19:Y:23:ARG:HH12	2.32	0.43
23:2:3:ARG:HD3	23:2:3:ARG:HA	1.87	0.43
26:M:66:ARG:NH2	29:A:906:U:O2'	2.52	0.43
29:A:191:A:O2'	29:A:678:C:O2	2.31	0.43
29:A:311:A:N6	29:A:329:G:OP1	2.51	0.43
29:A:1112:G:H2'	29:A:1113:U:C6	2.54	0.43
29:A:1258:U:H2'	29:A:1259:G:C8	2.54	0.43
29:A:1779:U:H5"	29:A:1780:A:H5"	2.00	0.43
29:A:1880:U:H2'	29:A:1881:C:C6	2.53	0.43
29:A:2027:G:H2'	29:A:2028:U:H6	1.81	0.43
29:A:2087:G:H2'	29:A:2088:A:C8	2.54	0.43
29:A:2589:A:H2'	29:A:2590:A:H8	1.83	0.43
29:A:2804:U:H2'	29:A:2805:C:C6	2.53	0.43
6:G:49:LEU:HD13	6:G:71:LEU:HD23	2.01	0.43
8:L:78:ARG:HH11	29:A:627:A:H5"	1.83	0.43
9:N:4:ARG:NH2	29:A:2875:C:OP1	2.51	0.43
29:A:106:C:H2'	29:A:107:G:C8	2.53	0.43
29:A:128:C:H2'	29:A:129:C:H6	1.82	0.43
29:A:253:C:H2'	29:A:254:G:O4'	2.18	0.43
29:A:923:G:H2'	29:A:924:G:H8	1.83	0.43
29:A:1219:U:H2'	29:A:1220:G:H8	1.84	0.43
29:A:1544:A:H2'	29:A:1545:A:C8	2.54	0.43
29:A:2139:U:H2'	29:A:2140:G:H8	1.82	0.43
6:G:37:ASN:HD22	6:G:63:GLN:CD	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:2:26:ASN:CG	29:A:682:G:H5'	2.39	0.43
29:A:1444:G:H2'	29:A:1445:G:C8	2.54	0.43
29:A:2522:U:O2'	29:A:2647:U:OP1	2.25	0.43
2:C:131:MET:HA	2:C:134:ILE:HD12	2.00	0.43
9:N:71:ARG:HA	9:N:71:ARG:HD2	1.77	0.43
14:T:59:ASN:HB2	14:T:84:TYR:HB2	2.01	0.43
16:V:50:MET:HB2	16:V:53:LYS:NZ	2.33	0.43
29:A:634:C:H2'	29:A:635:C:H6	1.83	0.43
29:A:753:A:H2'	29:A:754:U:C6	2.54	0.43
29:A:817:C:H2'	29:A:818:G:O4'	2.19	0.43
29:A:1168:G:H2'	29:A:1169:A:C8	2.53	0.43
29:A:1412:U:H2'	29:A:1413:A:C8	2.53	0.43
29:A:1721:G:N1	29:A:1738:G:N7	2.67	0.43
29:A:1827:U:H2'	29:A:1828:G:O4'	2.19	0.43
29:A:2289:G:H2'	29:A:2290:G:H8	1.84	0.43
29:A:2505:G:H1'	29:A:2506:U:OP2	2.18	0.43
30:B:115:A:H2'	30:B:116:G:H8	1.82	0.43
31:9:74:ALA:HB3	31:9:78:CYS:HB2	2.00	0.43
4:E:192:ALA:HA	4:E:195:GLN:HG2	2.01	0.43
24:K:42:THR:HG22	24:K:57:VAL:HG22	2.01	0.43
24:K:97:THR:O	24:K:98:ARG:NE	2.49	0.43
29:A:196:A:N6	29:A:831:G:H21	2.17	0.43
29:A:324:A:N6	29:A:339:U:O4'	2.51	0.43
29:A:596:U:H2'	29:A:597:G:H8	1.84	0.43
29:A:629:G:H5"	29:A:650:C:O2'	2.18	0.43
29:A:1395:A:O2'	29:A:1396:U:H3'	2.19	0.43
29:A:1562:U:H2'	29:A:1563:U:C6	2.53	0.43
29:A:1562:U:H2'	29:A:1563:U:H6	1.84	0.43
29:A:1869:G:N2	29:A:1871:A:O2'	2.52	0.43
29:A:2064:C:H2'	29:A:2065:C:C6	2.53	0.43
29:A:2794:C:H2'	29:A:2795:C:C6	2.54	0.43
2:C:207:ALA:HB2	29:A:1790:C:O2'	2.19	0.43
10:O:31:THR:HG21	30:B:28:C:H5"	2.00	0.43
11:Q:32:ARG:O	29:A:1252:G:N2	2.52	0.43
29:A:181:A:H1'	29:A:435:C:H5'	1.99	0.43
29:A:183:C:H1'	29:A:432:A:C2	2.54	0.43
29:A:475:C:N3	29:A:479:A:N7	2.67	0.43
29:A:976:G:H2'	29:A:977:G:H8	1.84	0.43
29:A:1139:G:H2'	29:A:1140:C:C6	2.54	0.43
29:A:2515:C:H2'	29:A:2516:A:C8	2.48	0.43
5:F:13:LYS:O	5:F:17:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:23:LEU:HD22	21:0:23:ALA:HB2	2.01	0.43
13:S:96:ILE:HD11	29:A:2012:G:H4'	2.01	0.43
27:H:54:LEU:O	27:H:57:LYS:HG3	2.19	0.43
29:A:78:U:H2'	29:A:79:C:C6	2.54	0.43
29:A:1207:C:H2'	29:A:1208:C:H6	1.83	0.43
29:A:1291:C:H2'	29:A:1292:G:C8	2.53	0.43
29:A:1424:G:H2'	29:A:1425:G:C8	2.54	0.43
29:A:1440:U:H2'	29:A:1441:G:C8	2.53	0.43
29:A:1476:U:H2'	29:A:1477:A:H8	1.84	0.43
29:A:1796:U:H2'	29:A:1797:G:C8	2.53	0.43
29:A:1858:A:H2'	29:A:1859:U:O4'	2.19	0.43
31:9:17:GLY:N	31:9:40:GLY:O	2.49	0.43
31:9:189:TYR:CE2	31:9:192:THR:HA	2.54	0.43
3:D:68:PHE:HB3	3:D:73:VAL:O	2.19	0.42
3:D:155:VAL:O	29:A:2618:G:O2'	2.34	0.42
5:F:60:SER:HA	5:F:98:PHE:CZ	2.54	0.42
6:G:174:LYS:O	6:G:174:LYS:HD2	2.19	0.42
9:N:35:LYS:HD3	9:N:112:TYR:CZ	2.54	0.42
14:T:50:LEU:HD23	19:Y:26:PHE:CZ	2.54	0.42
26:M:55:ARG:HA	26:M:59:ARG:NH1	2.34	0.42
29:A:76:C:H2'	29:A:77:G:H8	1.84	0.42
29:A:244:A:H2'	29:A:245:G:O4'	2.19	0.42
29:A:1169:A:H2'	29:A:1170:C:C6	2.54	0.42
29:A:1429:G:H2'	29:A:1430:G:C8	2.53	0.42
29:A:1738:G:O2'	29:A:1739:A:H8	2.01	0.42
29:A:2220:U:H2'	29:A:2221:G:H8	1.83	0.42
29:A:2547:A:OP2	29:A:2566:A:O2'	2.29	0.42
29:A:2783:U:H2'	29:A:2784:U:H6	1.84	0.42
29:A:2840:C:H2'	29:A:2841:C:C6	2.53	0.42
30:B:63:C:H2'	30:B:64:G:C8	2.54	0.42
2:C:136:VAL:HG13	2:C:163:ILE:HG22	2.01	0.42
29:A:528:A:H2'	29:A:529:A:H5"	2.00	0.42
29:A:797:G:H2'	29:A:798:G:C8	2.54	0.42
29:A:1276:A:N6	29:A:1645:G:O6	2.52	0.42
29:A:1299:G:O6	29:A:1639:C:H5"	2.19	0.42
29:A:1733:G:H2'	29:A:1734:G:H8	1.83	0.42
29:A:2047:C:H2'	29:A:2048:G:C8	2.53	0.42
29:A:2411:A:H2'	29:A:2412:A:H8	1.84	0.42
2:C:79:ARG:NH2	2:C:81:GLU:OE2	2.52	0.42
2:C:181:ARG:HG3	2:C:266:ILE:HG12	2.01	0.42
5:F:146:ASP:OD1	5:F:146:ASP:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:21:ARG:HE	16:V:87:GLN:HA	1.84	0.42
19:Y:37:LEU:HD23	19:Y:37:LEU:O	2.19	0.42
29:A:134:G:H2'	29:A:135:U:C6	2.55	0.42
29:A:239:C:N3	29:A:259:G:N1	2.67	0.42
29:A:1106:G:H2'	29:A:1107:G:H8	1.84	0.42
29:A:1336:A:H2'	29:A:1337:G:C8	2.54	0.42
29:A:1941:C:H1'	31:9:131:LYS:O	2.19	0.42
29:A:2018:G:H2'	29:A:2019:A:C8	2.55	0.42
29:A:2316:G:H2'	29:A:2317:A:C8	2.54	0.42
29:A:2888:C:H2'	29:A:2889:C:H6	1.84	0.42
30:B:72:G:N2	30:B:104:A:H62	2.15	0.42
3:D:11:MET:HB2	3:D:25:THR:HA	2.00	0.42
8:L:78:ARG:HG2	8:L:113:ALA:HB3	2.01	0.42
10:O:87:ILE:O	10:O:87:ILE:HG22	2.19	0.42
11:Q:52:ARG:NH2	29:A:994:C:OP1	2.52	0.42
27:H:97:ARG:HH21	27:H:112:LYS:NZ	2.17	0.42
29:A:48:G:N2	29:A:177:G:OP2	2.52	0.42
29:A:136:G:H2'	29:A:137:U:C6	2.54	0.42
29:A:173:A:H2'	29:A:174:U:C6	2.55	0.42
29:A:1198:U:H2'	29:A:1199:U:C6	2.54	0.42
29:A:1361:G:H2'	29:A:1362:C:C6	2.54	0.42
7:J:30:THR:HG21	29:A:1012:U:O4	2.20	0.42
26:M:44:ARG:HA	26:M:47:GLU:OE2	2.20	0.42
27:H:97:ARG:HH22	29:A:2221:G:P	2.41	0.42
29:A:634:C:H2'	29:A:635:C:C6	2.54	0.42
29:A:641:U:O4	29:A:647:G:O6	2.37	0.42
29:A:2700:A:H2'	29:A:2701:U:C6	2.54	0.42
29:A:2815:C:H2'	29:A:2816:G:C8	2.54	0.42
29:A:2881:U:H2'	29:A:2882:A:C8	2.54	0.42
30:B:115:A:H2'	30:B:116:G:C8	2.53	0.42
12:R:80:ARG:NH1	29:A:572:A:OP2	2.53	0.42
29:A:12:U:O2	29:A:2626:C:H4'	2.20	0.42
29:A:128:C:H2'	29:A:129:C:C6	2.53	0.42
29:A:593:U:H2'	29:A:594:U:H6	1.83	0.42
29:A:600:G:H2'	29:A:601:C:H6	1.84	0.42
29:A:903:C:H2'	29:A:904:G:H8	1.83	0.42
29:A:1022:G:N7	29:A:1140:C:N4	2.68	0.42
29:A:1346:G:N1	29:A:1601:G:C6	2.87	0.42
29:A:2086:U:H2'	29:A:2087:G:C8	2.54	0.42
2:C:77:VAL:HG22	2:C:113:ASP:H	1.84	0.42
2:C:169:ALA:HA	27:H:123:ARG:HH22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:64:PRO:HA	5:F:88:VAL:HG22	2.02	0.42
7:J:15:TRP:CE2	7:J:135:GLN:HG2	2.54	0.42
8:L:132:ARG:HG3	8:L:142:ILE:HG13	2.02	0.42
18:X:41:SER:OG	18:X:42:GLU:OE1	2.26	0.42
18:X:60:LYS:HE2	29:A:372:G:C8	2.54	0.42
20:Z:46:MET:O	20:Z:50:VAL:HG22	2.19	0.42
29:A:1:G:H2'	29:A:2:G:H8	1.84	0.42
29:A:18:U:H2'	29:A:19:A:C8	2.54	0.42
29:A:65:U:H2'	29:A:66:C:H6	1.85	0.42
29:A:161:A:OP2	29:A:162:U:O2'	2.28	0.42
29:A:202:U:H2'	29:A:203:A:O4'	2.19	0.42
29:A:543:G:C2	29:A:551:G:C2	3.08	0.42
29:A:769:U:H2'	29:A:770:G:C8	2.55	0.42
29:A:812:C:H5"	29:A:1250:G:O2'	2.20	0.42
29:A:947:A:H2'	29:A:948:C:C6	2.54	0.42
29:A:1319:C:H2'	29:A:1320:C:C6	2.54	0.42
29:A:1464:G:H2'	29:A:1465:G:H8	1.85	0.42
29:A:1630:A:H2'	29:A:1631:G:O4'	2.19	0.42
29:A:1675:C:H2'	29:A:1676:A:O4'	2.19	0.42
29:A:1727:C:H2'	29:A:1728:C:O4'	2.20	0.42
29:A:1771:C:H2'	29:A:1772:A:C8	2.54	0.42
29:A:2691:C:H2'	29:A:2692:G:C8	2.54	0.42
29:A:2788:C:H2'	29:A:2789:C:H6	1.84	0.42
5:F:62:GLN:HG3	5:F:94:ARG:NH2	2.34	0.42
6:G:140:ILE:HG13	6:G:141:GLY:N	2.35	0.42
10:O:30:ARG:HA	10:O:35:ILE:HG22	2.01	0.42
14:T:61:LEU:HB3	29:A:1341:G:H5'	2.02	0.42
16:V:78:GLN:OE1	30:B:76:G:O2'	2.31	0.42
21:0:16:ARG:NE	29:A:1266:G:OP2	2.48	0.42
29:A:481:G:N1	29:A:507:A:H1'	2.35	0.42
29:A:1267:U:H2'	29:A:1268:A:C8	2.54	0.42
29:A:1409:U:H2'	29:A:1410:G:C8	2.55	0.42
29:A:2391:G:C6	29:A:2427:C:H1'	2.55	0.42
29:A:2464:G:H2'	29:A:2465:C:C6	2.55	0.42
29:A:2644:G:N2	29:A:2733:A:OP2	2.52	0.42
29:A:131:A:H2'	29:A:132:G:C8	2.54	0.42
29:A:282:A:N6	29:A:359:G:O6	2.52	0.42
29:A:492:A:H2'	29:A:493:G:O4'	2.20	0.42
29:A:505:A:O2'	29:A:509:C:O2'	2.26	0.42
29:A:565:C:H2'	29:A:566:U:C6	2.55	0.42
29:A:1153:C:H2'	29:A:1154:G:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:1300:G:H4'	29:A:1301:A:H5"	2.01	0.42
29:A:1308:A:H2'	29:A:1309:G:O4'	2.20	0.42
29:A:1386:C:O2'	29:A:1469:A:N3	2.45	0.42
29:A:1475:G:H1'	29:A:1476:U:H5	1.85	0.42
29:A:2216:G:H2'	29:A:2217:G:H8	1.85	0.42
29:A:2773:C:H2'	29:A:2774:C:H6	1.84	0.42
2:C:227:VAL:HG11	29:A:784:G:C4	2.55	0.42
4:E:48:THR:O	4:E:52:VAL:HG23	2.20	0.42
11:Q:10:ARG:NH2	29:A:28:A:N3	2.68	0.42
16:V:43:ASP:OD2	16:V:46:LYS:NZ	2.40	0.42
18:X:38:TRP:CG	27:H:32:PRO:HA	2.55	0.42
21:0:42:ILE:HD12	21:0:46:GLY:HA2	2.02	0.42
22:1:22:THR:HG21	29:A:2286:G:H1	1.85	0.42
27:H:68:ARG:HG3	27:H:71:LYS:HZ2	1.85	0.42
29:A:538:A:H62	29:A:555:G:H21	1.67	0.42
29:A:932:U:O2'	29:A:934:U:O4	2.25	0.42
29:A:1106:G:H2'	29:A:1107:G:C8	2.55	0.42
29:A:1268:A:H1'	29:A:2013:A:H61	1.84	0.42
29:A:1790:C:H2'	29:A:1791:A:C5	2.55	0.42
29:A:1947:C:H2'	29:A:1948:G:H8	1.84	0.42
29:A:2616:C:H2'	29:A:2617:U:C6	2.54	0.42
31:9:132:SER:OG	31:9:133:SER:N	2.53	0.42
2:C:13:ARG:NH2	29:A:1693:U:O2'	2.52	0.41
6:G:25:ILE:HG13	6:G:78:VAL:HG21	2.01	0.41
8:L:32:GLY:HA2	29:A:1190:G:H5"	2.02	0.41
13:S:109:ASP:OD2	13:S:109:ASP:N	2.53	0.41
24:K:99:ILE:HG13	24:K:115:ILE:HG23	2.02	0.41
29:A:146:A:H2'	29:A:147:C:C6	2.54	0.41
29:A:299:A:H2'	29:A:300:A:C4	2.55	0.41
29:A:611:C:H2'	29:A:612:G:O4'	2.20	0.41
29:A:678:C:H2'	29:A:679:C:C6	2.55	0.41
29:A:1398:C:H2'	29:A:1399:C:H6	1.85	0.41
29:A:1442:U:H2'	29:A:1443:U:H6	1.85	0.41
29:A:1749:A:H2'	29:A:1750:G:C8	2.55	0.41
29:A:2314:A:H2'	29:A:2315:G:H8	1.85	0.41
29:A:2362:C:OP1	32:3:39:ARG:HD2	2.20	0.41
7:J:15:TRP:HE3	7:J:55:ILE:HD11	1.86	0.41
9:N:2:ARG:HH22	29:A:2819:G:P	2.43	0.41
14:T:1:MET:C	14:T:3:ARG:HB2	2.41	0.41
14:T:11:LEU:HD11	14:T:32:LEU:HD13	2.02	0.41
20:Z:26:LEU:HD23	20:Z:26:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:K:12:ASP:N	24:K:12:ASP:OD1	2.53	0.41
29:A:603:A:N6	29:A:655:A:O4'	2.53	0.41
29:A:640:C:H2'	29:A:641:U:C6	2.55	0.41
29:A:1440:U:H2'	29:A:1441:G:H8	1.86	0.41
29:A:2766:A:N3	29:A:2766:A:H2'	2.35	0.41
30:B:113:C:H2'	30:B:114:C:C6	2.55	0.41
8:L:128:THR:HG23	8:L:131:ALA:H	1.85	0.41
10:O:84:GLU:HG2	10:O:85:LYS:HD3	2.02	0.41
13:S:51:LEU:O	13:S:55:ILE:HG12	2.20	0.41
15:U:88:ASP:O	15:U:90:LYS:N	2.54	0.41
24:K:24:VAL:HG13	24:K:39:ILE:HG22	2.01	0.41
26:M:66:ARG:NH1	26:M:104:GLU:OE2	2.53	0.41
29:A:569:U:H2'	29:A:570:G:O4'	2.20	0.41
29:A:600:G:H2'	29:A:601:C:C6	2.55	0.41
29:A:1067:A:H2'	29:A:1067:A:N3	2.34	0.41
29:A:1130:U:N3	29:A:2025:C:OP1	2.50	0.41
29:A:1259:G:H2'	29:A:1260:A:H8	1.85	0.41
29:A:1380:G:H2'	29:A:1381:G:H8	1.84	0.41
29:A:1398:C:H2'	29:A:1399:C:C6	2.55	0.41
29:A:2037:A:H2'	29:A:2038:G:C8	2.55	0.41
29:A:2062:A:H2'	29:A:2063:C:C6	2.55	0.41
29:A:2193:G:H2'	29:A:2194:U:C6	2.55	0.41
29:A:2193:G:H2'	29:A:2194:U:H6	1.85	0.41
29:A:2290:G:H2'	29:A:2291:U:C6	2.55	0.41
31:9:259:ALA:HB1	31:9:304:LEU:HD21	2.02	0.41
31:9:290:LYS:HA	31:9:290:LYS:HD3	1.81	0.41
2:C:200:MET:N	2:C:200:MET:SD	2.93	0.41
14:T:6:ARG:O	14:T:10:VAL:HG23	2.20	0.41
24:K:92:GLU:O	24:K:93:GLN:NE2	2.54	0.41
29:A:32:C:H2'	29:A:33:C:C6	2.55	0.41
29:A:922:C:H2'	29:A:923:G:C8	2.55	0.41
29:A:1652:A:H2'	29:A:1653:G:O4'	2.21	0.41
29:A:1665:A:H2'	29:A:1666:G:C8	2.54	0.41
29:A:1680:U:H2'	29:A:1681:G:O4'	2.21	0.41
29:A:1909:C:H2'	29:A:1910:G:C8	2.55	0.41
29:A:2645:G:H3'	29:A:2646:C:H5'	2.02	0.41
4:E:148:ILE:HB	4:E:169:VAL:HG22	2.01	0.41
8:L:91:ASP:N	8:L:91:ASP:OD1	2.52	0.41
13:S:28:LYS:H	13:S:31:GLN:HE21	1.69	0.41
16:V:72:VAL:HB	16:V:91:PHE:HB3	2.02	0.41
29:A:151:C:H2'	29:A:152:A:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:418:C:H2'	29:A:419:U:C6	2.56	0.41
29:A:487:C:H2'	29:A:488:G:O4'	2.19	0.41
29:A:679:C:H2'	29:A:680:C:C6	2.55	0.41
29:A:2292:U:H2'	29:A:2293:G:C8	2.55	0.41
29:A:2533:U:H2'	29:A:2534:A:O4'	2.20	0.41
29:A:2543:G:H2'	29:A:2544:G:C8	2.55	0.41
29:A:2889:C:H2'	29:A:2890:G:O4'	2.21	0.41
2:C:12:ARG:HA	2:C:15:VAL:HG23	2.02	0.41
3:D:59:ARG:HG3	29:A:2830:C:OP1	2.21	0.41
5:F:65:LEU:HD11	30:B:41:G:C8	2.55	0.41
5:F:169:LEU:HB3	5:F:174:PHE:HB3	2.02	0.41
21:0:40:HIS:HE2	29:A:2884:U:P	2.43	0.41
24:K:10:VAL:HG21	24:K:16:ALA:O	2.20	0.41
29:A:242:G:N2	29:A:255:A:OP2	2.36	0.41
29:A:393:C:C2	29:A:394:C:C5	3.09	0.41
29:A:540:C:N4	29:A:541:A:H62	2.18	0.41
29:A:598:U:H2'	29:A:599:A:H8	1.84	0.41
29:A:809:G:H2'	29:A:810:U:C6	2.55	0.41
29:A:858:G:H3'	29:A:859:G:C8	2.55	0.41
29:A:1387:A:H5'	29:A:1469:A:H1'	2.03	0.41
29:A:1667:G:O2'	29:A:1991:U:O4	2.38	0.41
29:A:2247:A:H2'	29:A:2248:C:C6	2.55	0.41
29:A:2368:C:H2'	29:A:2369:A:C8	2.56	0.41
29:A:2462:C:H2'	29:A:2463:C:C6	2.56	0.41
29:A:2508:G:H5'	31:9:76:ARG:HH22	1.86	0.41
29:A:2560:A:H2'	29:A:2561:U:C6	2.55	0.41
29:A:2816:G:H2'	29:A:2817:U:H6	1.84	0.41
2:C:176:ARG:HA	2:C:176:ARG:HD2	1.87	0.41
6:G:100:ASN:O	6:G:100:ASN:OD1	2.39	0.41
19:Y:21:LEU:O	19:Y:25:GLN:HB3	2.21	0.41
29:A:671:C:H2'	29:A:672:C:C6	2.55	0.41
29:A:1264:A:O5'	29:A:1265:A:H2'	2.20	0.41
29:A:2128:G:H2'	29:A:2129:C:C6	2.55	0.41
29:A:2413:G:C4	29:A:2414:G:C8	3.09	0.41
29:A:2425:A:H5"	29:A:2427:C:O4'	2.21	0.41
29:A:2549:G:H2'	29:A:2550:G:C8	2.53	0.41
4:E:105:LEU:HD23	4:E:200:LEU:HD13	2.02	0.41
24:K:66:LYS:HZ3	24:K:80:ASP:HA	1.84	0.41
27:H:10:ALA:O	27:H:12:LEU:HD23	2.21	0.41
29:A:19:A:H2'	29:A:20:C:C6	2.56	0.41
29:A:413:C:H2'	29:A:414:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:592:A:H2'	29:A:593:U:C6	2.56	0.41
29:A:593:U:H2'	29:A:594:U:C6	2.56	0.41
29:A:638:G:H2'	29:A:639:U:C6	2.56	0.41
29:A:1437:C:O2'	29:A:1516:G:O2'	2.27	0.41
29:A:1841:U:C2	29:A:1842:G:C8	3.08	0.41
29:A:2191:A:H2'	29:A:2192:U:H6	1.84	0.41
29:A:2283:C:OP2	29:A:2389:G:O2'	2.37	0.41
29:A:2644:G:O6	29:A:2771:C:N4	2.54	0.41
2:C:55:GLY:H	29:A:692:C:P	2.44	0.41
2:C:56:GLY:HA2	2:C:212:TRP:HA	2.02	0.41
2:C:218:THR:O	29:A:1789:A:H5"	2.21	0.41
5:F:127:TYR:CE1	5:F:169:LEU:HD21	2.56	0.41
7:J:57:LEU:HD21	7:J:130:HIS:HB3	2.03	0.41
8:L:29:LYS:HB2	12:R:82:HIS:CD2	2.56	0.41
8:L:57:LEU:HD13	8:L:60:ARG:HH11	1.86	0.41
14:T:2:ILE:HG12	14:T:49:LYS:HE3	2.03	0.41
14:T:38:ALA:HB1	14:T:43:ILE:HD11	2.03	0.41
21:0:30:ASP:HB3	21:0:34:GLY:N	2.35	0.41
29:A:7:G:H2'	29:A:8:C:C6	2.55	0.41
29:A:243:U:H2'	29:A:244:A:C8	2.55	0.41
29:A:367:G:C6	29:A:368:A:C6	3.09	0.41
29:A:963:U:H2'	29:A:964:C:C6	2.56	0.41
29:A:1592:C:H2'	29:A:1593:A:C8	2.56	0.41
29:A:1826:G:H2'	29:A:1827:U:H6	1.86	0.41
29:A:1918:A:O2'	29:A:1919:A:N7	2.39	0.41
29:A:2017:U:O2'	29:A:2019:A:OP2	2.35	0.41
29:A:2166:U:O4	29:A:2170:A:N6	2.46	0.41
29:A:2411:A:H2'	29:A:2412:A:C8	2.56	0.41
4:E:146:VAL:HG21	4:E:187:VAL:HG23	2.03	0.41
5:F:118:ALA:HB1	5:F:166:ARG:CZ	2.50	0.41
9:N:37:THR:HA	9:N:109:PRO:O	2.21	0.41
15:U:24:VAL:HA	15:U:35:VAL:HG22	2.02	0.41
17:W:37:ARG:HH12	29:A:2262:U:H5"	1.86	0.41
18:X:14:GLY:HA3	18:X:28:PHE:HE2	1.86	0.41
19:Y:9:LYS:NZ	19:Y:11:VAL:HG23	2.36	0.41
29:A:64:A:H2'	29:A:65:U:C6	2.55	0.41
29:A:116:C:H2'	29:A:117:G:O4'	2.21	0.41
29:A:249:C:OP2	29:A:2394:C:O2'	2.27	0.41
29:A:640:C:C2	29:A:641:U:C5	3.08	0.41
29:A:1880:U:H2'	29:A:1881:C:H6	1.85	0.41
29:A:2615:U:H2'	29:A:2616:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B:33:G:H2'	30:B:34:A:C8	2.56	0.41
5:F:26:GLN:HG3	30:B:57:A:O2'	2.20	0.40
15:U:81:ARG:HH11	29:A:300:A:P	2.44	0.40
25:P:51:ASN:O	29:A:2845:U:H5"	2.21	0.40
26:M:29:GLY:HA2	26:M:106:ASP:OD2	2.20	0.40
29:A:29:U:H2'	29:A:30:G:H8	1.85	0.40
29:A:116:C:H1'	29:A:127:A:N3	2.36	0.40
29:A:175:G:H2'	29:A:176:A:H8	1.84	0.40
29:A:518:G:H2'	29:A:519:U:C6	2.57	0.40
29:A:594:U:H2'	29:A:595:C:H6	1.86	0.40
29:A:660:C:H2'	29:A:661:A:H8	1.87	0.40
29:A:910:A:H1'	29:A:2264:C:O2'	2.21	0.40
29:A:1213:A:H4'	29:A:1238:G:H21	1.85	0.40
29:A:2292:U:H2'	29:A:2293:G:H8	1.86	0.40
29:A:2514:U:H2'	29:A:2515:C:H6	1.86	0.40
32:3:25:HIS:HD1	32:3:43:LEU:HD23	1.85	0.40
5:F:137:PHE:HE2	5:F:151:LEU:HD22	1.86	0.40
7:J:81:ILE:HD11	29:A:2514:U:H4'	2.03	0.40
10:O:43:ASN:OD1	10:O:44:GLY:N	2.54	0.40
14:T:8:LEU:HD21	19:Y:21:LEU:O	2.21	0.40
29:A:225:C:H2'	29:A:226:A:O4'	2.22	0.40
29:A:554:U:H2'	29:A:555:G:O4'	2.20	0.40
29:A:1233:C:H2'	29:A:1234:U:H6	1.86	0.40
29:A:1837:C:O2'	29:A:1927:A:N3	2.41	0.40
29:A:2255:G:C6	29:A:2256:G:C5	3.09	0.40
29:A:2464:G:H2'	29:A:2465:C:H6	1.86	0.40
29:A:2567:G:H2'	29:A:2568:U:C6	2.57	0.40
29:A:2895:G:H2'	29:A:2896:C:C6	2.55	0.40
31:9:256:VAL:HA	31:9:300:ILE:HD11	2.03	0.40
2:C:77:VAL:HG11	2:C:109:LEU:HD21	2.02	0.40
2:C:229:HIS:CD2	2:C:246:PRO:HB3	2.56	0.40
8:L:21:ARG:HD3	8:L:21:ARG:HA	1.91	0.40
9:N:38:LEU:HD23	9:N:109:PRO:HB2	2.03	0.40
11:Q:58:GLN:HA	11:Q:61:ILE:HG22	2.03	0.40
16:V:10:LYS:HD2	16:V:11:GLU:HB2	2.04	0.40
17:W:52:ASP:OD1	17:W:54:THR:OG1	2.37	0.40
19:Y:22:LEU:HD23	19:Y:23:ARG:HD3	2.03	0.40
29:A:63:A:H2'	29:A:64:A:C8	2.55	0.40
29:A:170:U:H2'	29:A:171:U:C6	2.56	0.40
29:A:197:A:H62	29:A:2430:A:H2'	1.86	0.40
29:A:1257:C:H2'	29:A:1258:U:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:1649:G:H2'	29:A:1650:A:H8	1.87	0.40
29:A:2191:A:H2'	29:A:2192:U:C6	2.56	0.40
29:A:2313:C:H2'	29:A:2314:A:C8	2.54	0.40
2:C:211:ARG:NH2	29:A:764:A:N3	2.69	0.40
3:D:4:LEU:HD23	3:D:101:PHE:CZ	2.56	0.40
5:F:59:ILE:HD13	5:F:139:GLU:HB2	2.03	0.40
11:Q:54:ARG:HH11	29:A:1155:A:H5"	1.87	0.40
23:2:21:ARG:O	23:2:27:GLY:HA3	2.22	0.40
29:A:206:U:C2	29:A:207:A:C8	3.09	0.40
29:A:1282:U:H2'	29:A:1283:G:O4'	2.22	0.40
29:A:1387:A:H2'	29:A:1388:G:C8	2.57	0.40
29:A:2243:U:H2'	29:A:2244:U:C6	2.55	0.40
29:A:2543:G:H2'	29:A:2544:G:H8	1.87	0.40
29:A:2881:U:H2'	29:A:2882:A:H8	1.87	0.40
30:B:95:U:H2'	30:B:96:G:C8	2.55	0.40
30:B:106:G:H2'	30:B:107:G:O4'	2.20	0.40
31:9:217:LEU:HD11	31:9:265:GLU:OE2	2.21	0.40
2:C:155:ARG:HB2	29:A:1818:U:H2'	2.03	0.40
2:C:211:ARG:HD2	2:C:211:ARG:HA	1.89	0.40
3:D:114:LYS:NZ	29:A:2723:C:OP1	2.43	0.40
14:T:58:VAL:HG22	14:T:85:VAL:HG22	2.03	0.40
15:U:73:ASN:HD21	15:U:98:ASN:ND2	2.20	0.40
18:X:11:PRO:HB2	18:X:27:ARG:HH21	1.85	0.40
29:A:169:G:H2'	29:A:170:U:C6	2.56	0.40
29:A:287:G:O6	29:A:354:A:N6	2.55	0.40
29:A:359:G:H2'	29:A:360:U:C6	2.56	0.40
29:A:521:U:H2'	29:A:522:A:H8	1.87	0.40
29:A:549:G:H5"	29:A:550:C:C6	2.57	0.40
29:A:971:G:H2'	29:A:972:A:O4'	2.22	0.40
29:A:1254:A:H5"	29:A:1255:U:H5"	2.04	0.40
29:A:1380:G:H2'	29:A:1381:G:C8	2.56	0.40
29:A:1462:C:C2	29:A:1463:C:C5	3.09	0.40
29:A:1738:G:HO2'	29:A:1739:A:H8	1.69	0.40
29:A:1742:U:H2'	29:A:1743:G:O4'	2.21	0.40
29:A:2240:U:H2'	29:A:2241:A:H8	1.87	0.40
29:A:2437:G:H2'	29:A:2438:U:C6	2.56	0.40
29:A:2845:U:H2'	29:A:2846:G:H8	1.86	0.40
30:B:19:C:H2'	30:B:20:G:C8	2.56	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	g	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
2	C	269/273 (98%)	258 (96%)	11 (4%)	0	100	100
3	D	207/209 (99%)	195 (94%)	12 (6%)	0	100	100
4	E	189/201 (94%)	180 (95%)	9 (5%)	0	100	100
5	F	175/179 (98%)	163 (93%)	12 (7%)	0	100	100
6	G	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
7	J	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
8	L	142/144 (99%)	129 (91%)	13 (9%)	0	100	100
9	N	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
10	O	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
11	Q	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
12	R	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
13	S	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
14	T	91/100 (91%)	85 (93%)	6 (7%)	0	100	100
15	U	100/104 (96%)	91 (91%)	9 (9%)	0	100	100
16	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
17	W	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
18	X	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
19	Y	61/63 (97%)	54 (88%)	7 (12%)	0	100	100
20	Z	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
21	0	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
22	1	48/55 (87%)	48 (100%)	0	0	100	100
23	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
24	K	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
25	P	111/115 (96%)	108 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
26	M	134/136 (98%)	131 (98%)	3 (2%)	0	100 100
27	H	147/149 (99%)	131 (89%)	16 (11%)	0	100 100
28	d	45/70 (64%)	44 (98%)	1 (2%)	0	100 100
31	9	336/390 (86%)	321 (96%)	15 (4%)	0	100 100
32	3	62/65 (95%)	59 (95%)	1 (2%)	2 (3%)	4 31
All	All	3538/3720 (95%)	3370 (95%)	166 (5%)	2 (0%)	54 84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	3	31	ILE
32	3	32	LEU

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	g	34/34 (100%)	34 (100%)	0	100 100
2	C	216/218 (99%)	214 (99%)	2 (1%)	78 88
3	D	164/164 (100%)	163 (99%)	1 (1%)	86 92
4	E	159/165 (96%)	159 (100%)	0	100 100
5	F	148/150 (99%)	147 (99%)	1 (1%)	84 90
6	G	137/138 (99%)	133 (97%)	4 (3%)	42 65
7	J	116/116 (100%)	114 (98%)	2 (2%)	60 78
8	L	103/103 (100%)	103 (100%)	0	100 100
9	N	100/100 (100%)	100 (100%)	0	100 100
10	O	86/87 (99%)	86 (100%)	0	100 100
11	Q	89/90 (99%)	89 (100%)	0	100 100
12	R	84/84 (100%)	84 (100%)	0	100 100
13	S	93/93 (100%)	93 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	T	80/84 (95%)	80 (100%)	0	100 100
15	U	83/85 (98%)	83 (100%)	0	100 100
16	V	78/78 (100%)	77 (99%)	1 (1%)	69 82
17	W	57/63 (90%)	57 (100%)	0	100 100
18	X	67/68 (98%)	67 (100%)	0	100 100
19	Y	55/55 (100%)	54 (98%)	1 (2%)	59 77
20	Z	48/49 (98%)	48 (100%)	0	100 100
21	0	47/48 (98%)	47 (100%)	0	100 100
22	1	45/49 (92%)	44 (98%)	1 (2%)	52 71
23	2	38/38 (100%)	37 (97%)	1 (3%)	46 67
24	K	103/104 (99%)	103 (100%)	0	100 100
25	P	98/100 (98%)	98 (100%)	0	100 100
26	M	109/109 (100%)	108 (99%)	1 (1%)	78 88
27	H	114/114 (100%)	110 (96%)	4 (4%)	36 61
28	d	43/62 (69%)	42 (98%)	1 (2%)	50 70
31	9	273/321 (85%)	271 (99%)	2 (1%)	84 90
32	3	51/52 (98%)	51 (100%)	0	100 100
All	All	2918/3021 (97%)	2896 (99%)	22 (1%)	82 89

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	96	LYS
2	C	174	ARG
3	D	33	ARG
5	F	79	ARG
6	G	68	ARG
6	G	72	ASN
6	G	174	LYS
6	G	175	LYS
7	J	96	ARG
7	J	128	ASN
16	V	10	LYS
19	Y	38	GLN
22	1	27	ARG
23	2	28	ARG

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Mol	Chain	Res	Type
26	M	60	GLN
27	H	41	LYS
27	H	42	LYS
27	H	57	LYS
27	H	68	ARG
28	d	8	LYS
31	9	95	ARG
31	9	110	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	g	37	GLN
5	F	126	ASN
15	U	73	ASN
16	V	87	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	A	2895/2904 (99%)	390 (13%)	9 (0%)
30	B	118/119 (99%)	9 (7%)	0
All	All	3013/3023 (99%)	399 (13%)	9 (0%)

All (399) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	A	10	A
29	A	12	U
29	A	14	A
29	A	27	G
29	A	46	G
29	A	51	G
29	A	63	A
29	A	71	A
29	A	74	A
29	A	75	G
29	A	84	A
29	A	102	U
29	A	103	A

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Mol	Chain	Res	Type
29	A	118	A
29	A	120	U
29	A	125	A
29	A	138	U
29	A	139	U
29	A	140	C
29	A	142	A
29	A	160	A
29	A	163	C
29	A	181	A
29	A	196	A
29	A	199	A
29	A	215	G
29	A	216	A
29	A	221	A
29	A	222	A
29	A	230	G
29	A	233	A
29	A	248	G
29	A	255	A
29	A	265	A
29	A	266	G
29	A	267	C
29	A	271	G
29	A	272	A
29	A	278	A
29	A	302	C
29	A	311	A
29	A	329	G
29	A	330	A
29	A	331	C
29	A	352	A
29	A	353	C
29	A	371	A
29	A	372	G
29	A	386	G
29	A	396	G
29	A	401	A
29	A	404	A
29	A	405	U
29	A	411	G
29	A	424	G

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Mol	Chain	Res	Type
29	A	430	A
29	A	451	U
29	A	480	A
29	A	481	G
29	A	491	G
29	A	504	A
29	A	505	A
29	A	510	C
29	A	532	A
29	A	543	G
29	A	544	C
29	A	546	U
29	A	547	A
29	A	548	G
29	A	550	C
29	A	563	A
29	A	573	U
29	A	575	A
29	A	586	A
29	A	603	A
29	A	613	A
29	A	615	U
29	A	621	A
29	A	627	A
29	A	637	A
29	A	646	U
29	A	647	G
29	A	654	A
29	A	655	A
29	A	686	U
29	A	726	G
29	A	729	G
29	A	730	A
29	A	747	U
29	A	752	A
29	A	764	A
29	A	775	G
29	A	776	G
29	A	782	A
29	A	784	G
29	A	785	G
29	A	789	A

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Mol	Chain	Res	Type
29	A	792	A
29	A	805	G
29	A	812	C
29	A	819	A
29	A	827	U
29	A	828	U
29	A	830	G
29	A	845	A
29	A	846	U
29	A	847	U
29	A	857	G
29	A	860	U
29	A	878	A
29	A	884	U
29	A	885	C
29	A	896	A
29	A	907	G
29	A	910	A
29	A	915	C
29	A	931	U
29	A	941	A
29	A	946	C
29	A	953	G
29	A	961	C
29	A	973	A
29	A	974	G
29	A	983	A
29	A	995	C
29	A	996	A
29	A	1009	A
29	A	1012	U
29	A	1013	C
29	A	1022	G
29	A	1026	G
29	A	1027	A
29	A	1033	U
29	A	1044	C
29	A	1046	A
29	A	1047	G
29	A	1058	U
29	A	1061	U
29	A	1066	U

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Mol	Chain	Res	Type
29	A	1068	G
29	A	1069	A
29	A	1070	A
29	A	1071	G
29	A	1074	G
29	A	1081	U
29	A	1087	G
29	A	1089	A
29	A	1098	A
29	A	1101	U
29	A	1110	G
29	A	1112	G
29	A	1116	G
29	A	1132	U
29	A	1133	A
29	A	1135	C
29	A	1136	G
29	A	1141	U
29	A	1142	A
29	A	1157	G
29	A	1171	G
29	A	1172	C
29	A	1173	U
29	A	1175	A
29	A	1176	U
29	A	1180	U
29	A	1212	G
29	A	1225	G
29	A	1236	G
29	A	1238	G
29	A	1250	G
29	A	1253	A
29	A	1256	G
29	A	1266	G
29	A	1272	A
29	A	1294	U
29	A	1300	G
29	A	1301	A
29	A	1302	A
29	A	1314	C
29	A	1321	A
29	A	1325	U

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Mol	Chain	Res	Type
29	A	1329	U
29	A	1345	C
29	A	1365	A
29	A	1368	G
29	A	1378	A
29	A	1379	U
29	A	1383	A
29	A	1416	G
29	A	1419	A
29	A	1420	A
29	A	1428	C
29	A	1452	G
29	A	1453	A
29	A	1458	U
29	A	1461	C
29	A	1467	U
29	A	1482	G
29	A	1490	A
29	A	1493	C
29	A	1504	A
29	A	1515	A
29	A	1523	U
29	A	1524	G
29	A	1533	C
29	A	1535	A
29	A	1548	A
29	A	1555	G
29	A	1556	C
29	A	1566	A
29	A	1569	A
29	A	1583	A
29	A	1585	C
29	A	1603	A
29	A	1607	C
29	A	1608	A
29	A	1634	A
29	A	1646	C
29	A	1647	U
29	A	1648	U
29	A	1654	A
29	A	1667	G
29	A	1674	G

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Mol	Chain	Res	Type
29	A	1715	G
29	A	1729	U
29	A	1730	C
29	A	1732	C
29	A	1736	U
29	A	1737	G
29	A	1738	G
29	A	1764	C
29	A	1773	A
29	A	1791	A
29	A	1800	C
29	A	1801	A
29	A	1808	A
29	A	1816	C
29	A	1829	A
29	A	1870	C
29	A	1914	C
29	A	1926	U
29	A	1927	A
29	A	1930	G
29	A	1931	U
29	A	1937	A
29	A	1944	U
29	A	1955	U
29	A	1967	C
29	A	1970	A
29	A	1971	U
29	A	1972	G
29	A	1991	U
29	A	1992	G
29	A	1993	U
29	A	1997	C
29	A	2013	A
29	A	2021	C
29	A	2022	U
29	A	2023	C
29	A	2025	C
29	A	2030	A
29	A	2031	A
29	A	2043	C
29	A	2055	C
29	A	2056	G

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Mol	Chain	Res	Type
29	A	2060	A
29	A	2061	G
29	A	2062	A
29	A	2069	G
29	A	2072	C
29	A	2093	G
29	A	2096	C
29	A	2102	G
29	A	2110	G
29	A	2111	U
29	A	2112	G
29	A	2116	G
29	A	2117	A
29	A	2118	U
29	A	2119	A
29	A	2122	U
29	A	2126	A
29	A	2128	G
29	A	2132	U
29	A	2133	G
29	A	2136	G
29	A	2147	A
29	A	2148	G
29	A	2157	G
29	A	2164	C
29	A	2165	C
29	A	2170	A
29	A	2171	A
29	A	2172	U
29	A	2173	A
29	A	2178	C
29	A	2198	A
29	A	2199	A
29	A	2204	G
29	A	2211	A
29	A	2225	A
29	A	2226	C
29	A	2238	G
29	A	2239	G
29	A	2283	C
29	A	2287	A
29	A	2288	A

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Mol	Chain	Res	Type
29	A	2297	A
29	A	2305	U
29	A	2308	G
29	A	2311	A
29	A	2325	G
29	A	2327	A
29	A	2333	A
29	A	2335	A
29	A	2336	A
29	A	2343	U
29	A	2344	U
29	A	2350	C
29	A	2361	G
29	A	2383	G
29	A	2385	C
29	A	2402	U
29	A	2406	A
29	A	2425	A
29	A	2426	A
29	A	2428	G
29	A	2429	G
29	A	2430	A
29	A	2435	A
29	A	2441	U
29	A	2447	G
29	A	2448	A
29	A	2475	C
29	A	2476	A
29	A	2478	A
29	A	2491	U
29	A	2494	G
29	A	2498	C
29	A	2502	G
29	A	2504	U
29	A	2505	G
29	A	2506	U
29	A	2513	A
29	A	2518	A
29	A	2520	C
29	A	2525	G
29	A	2529	G
29	A	2531	A

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Mol	Chain	Res	Type
29	A	2554	U
29	A	2564	A
29	A	2566	A
29	A	2567	G
29	A	2572	A
29	A	2602	A
29	A	2609	U
29	A	2613	U
29	A	2615	U
29	A	2629	U
29	A	2639	A
29	A	2646	C
29	A	2647	U
29	A	2661	G
29	A	2662	A
29	A	2685	G
29	A	2689	U
29	A	2690	U
29	A	2714	G
29	A	2718	G
29	A	2726	A
29	A	2729	G
29	A	2733	A
29	A	2744	G
29	A	2748	A
29	A	2757	A
29	A	2765	A
29	A	2778	A
29	A	2791	G
29	A	2798	U
29	A	2801	G
29	A	2818	U
29	A	2820	A
29	A	2835	A
29	A	2850	A
29	A	2867	G
29	A	2872	A
29	A	2873	A
29	A	2880	C
29	A	2884	U
29	A	2886	A
30	B	15	A

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Mol	Chain	Res	Type
30	B	35	C
30	B	36	C
30	B	41	G
30	B	44	G
30	B	89	U
30	B	90	C
30	B	99	A
30	B	109	A

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	A	271	G
29	A	404	A
29	A	1057	A
29	A	1328	A
29	A	1378	A
29	A	2127	G
29	A	2425	A
29	A	2505	G
29	A	2756	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	GNP	9	402	34	29,34,34	1.63	7 (24%)	33,54,54	2.11	6 (18%)

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
35	GNP	9	402	34	-	4/14/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	9	402	GNP	PB-O3A	4.53	1.64	1.59
35	9	402	GNP	C6-N1	3.14	1.38	1.33
35	9	402	GNP	PB-O1B	3.12	1.51	1.46
35	9	402	GNP	PG-N3B	3.04	1.71	1.63
35	9	402	GNP	PG-O1G	2.73	1.50	1.46
35	9	402	GNP	PB-O2B	-2.22	1.50	1.56
35	9	402	GNP	C5-C6	2.06	1.44	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	9	402	GNP	C5-C6-N1	-8.42	111.91	123.43
35	9	402	GNP	C2-N1-C6	5.82	125.18	115.93
35	9	402	GNP	N3-C2-N1	-2.71	123.60	127.22
35	9	402	GNP	PB-O3A-PA	-2.59	123.49	132.62
35	9	402	GNP	C4-C5-C6	-2.59	118.33	120.80
35	9	402	GNP	C2-N3-C4	-2.22	112.82	115.36

There are no chirality outliers.

All (4) torsion outliers are listed below:

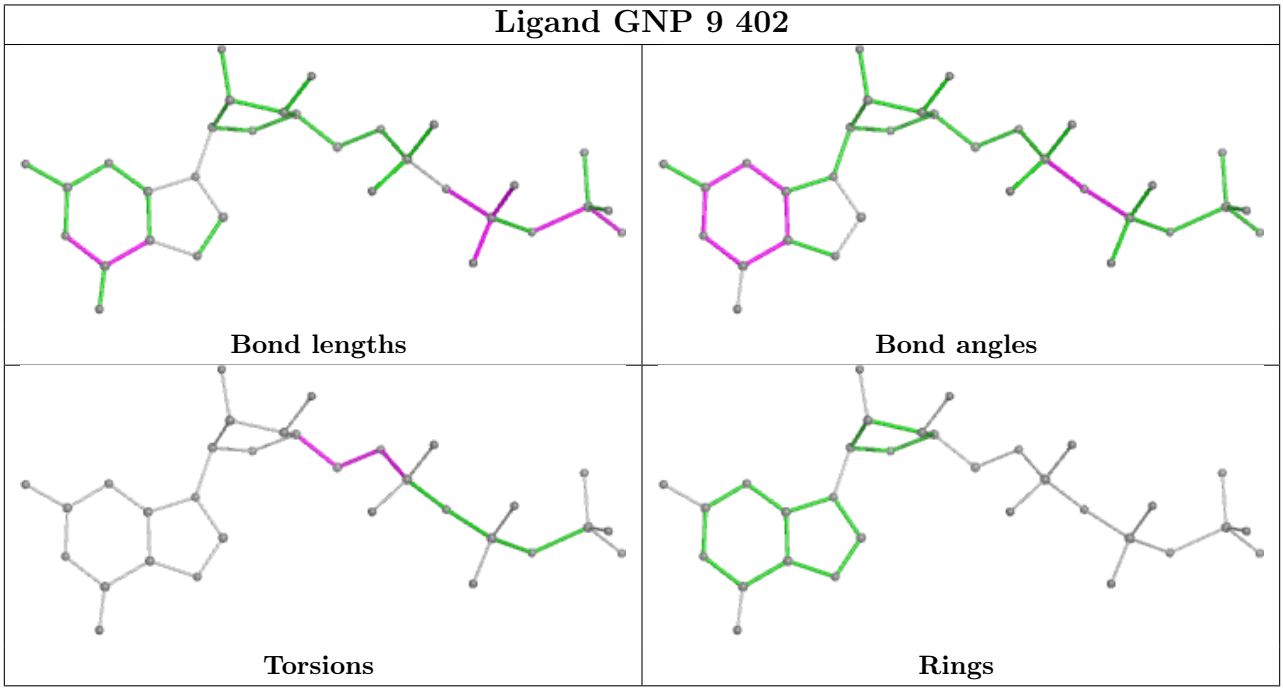
Mol	Chain	Res	Type	Atoms
35	9	402	GNP	C4'-C5'-O5'-PA
35	9	402	GNP	O4'-C4'-C5'-O5'
35	9	402	GNP	C5'-O5'-PA-O3A
35	9	402	GNP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	9	402	GNP	2	0

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



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

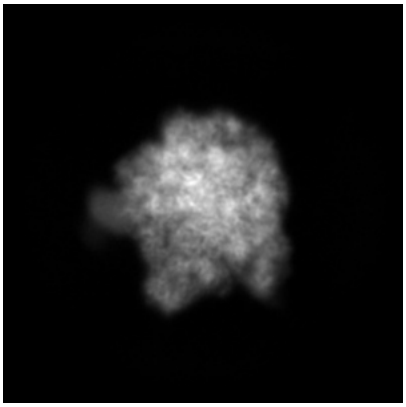
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12219. These allow visual inspection of the internal detail of the map and identification of artifacts.

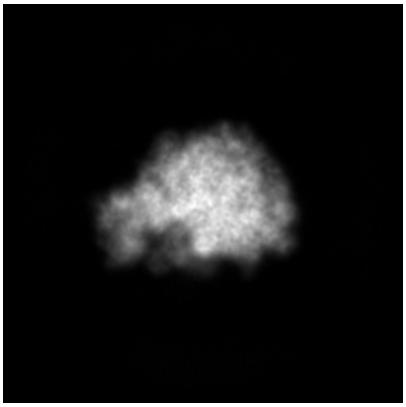
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

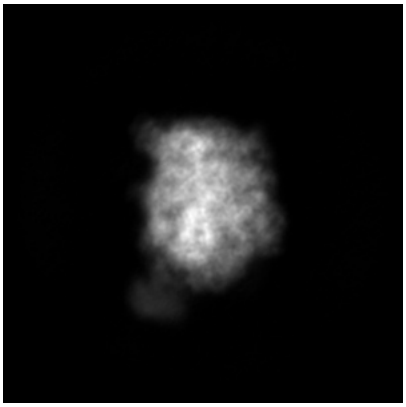
6.1.1 Primary map



X



Y

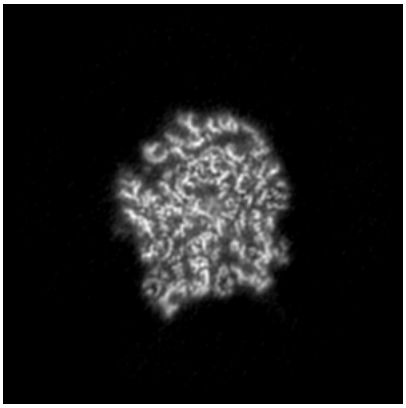


Z

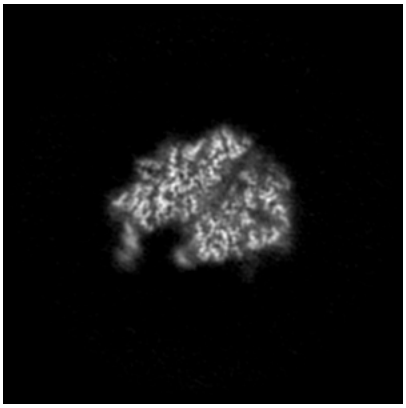
The images above show the map projected in three orthogonal directions.

6.2 Central slices

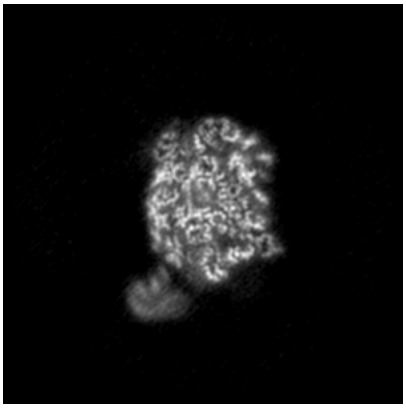
6.2.1 Primary map



X Index: 120



Y Index: 120

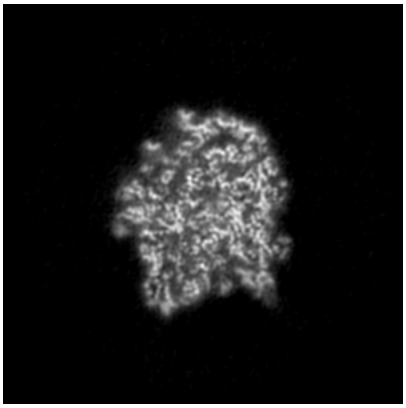


Z Index: 120

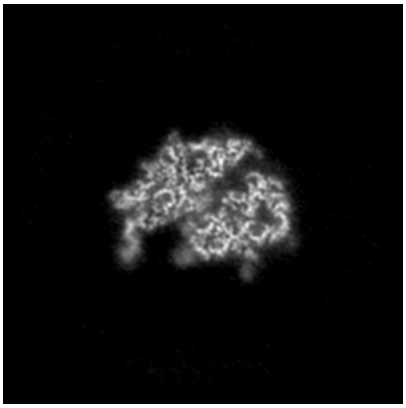
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

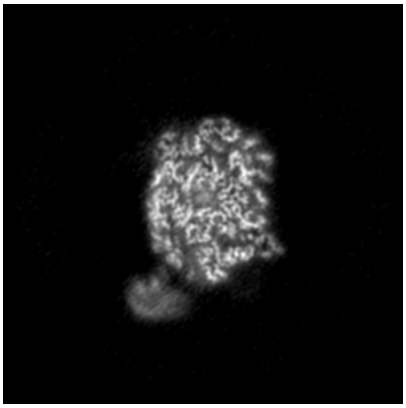
6.3.1 Primary map



X Index: 117



Y Index: 123

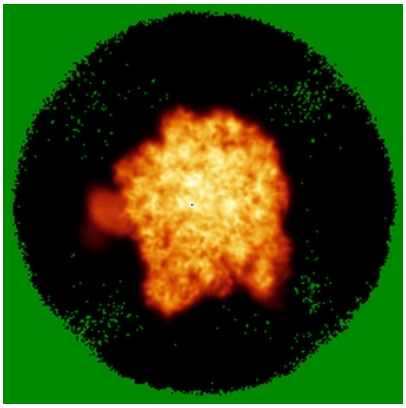


Z Index: 119

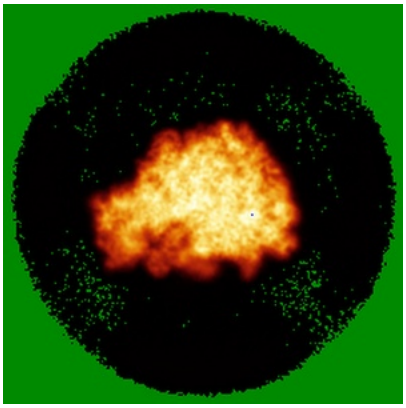
The images above show the largest variance slices of the map in three orthogonal directions.

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

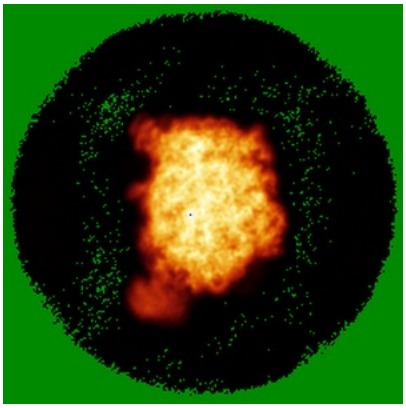
6.4.1 Primary map



X



Y

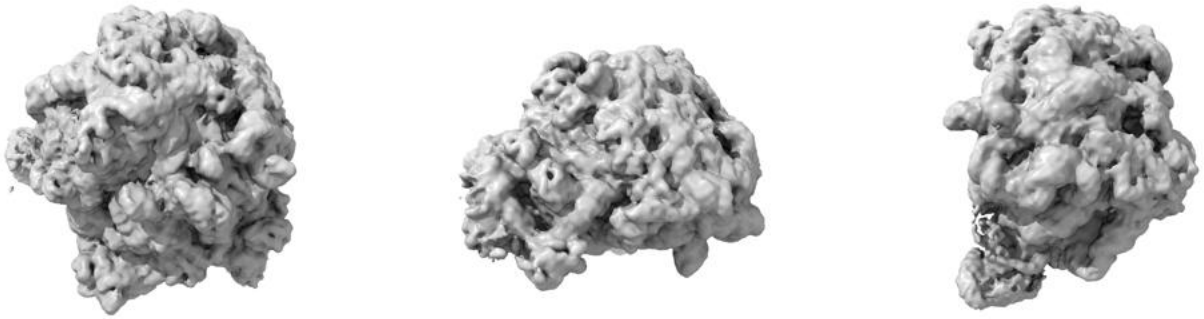


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

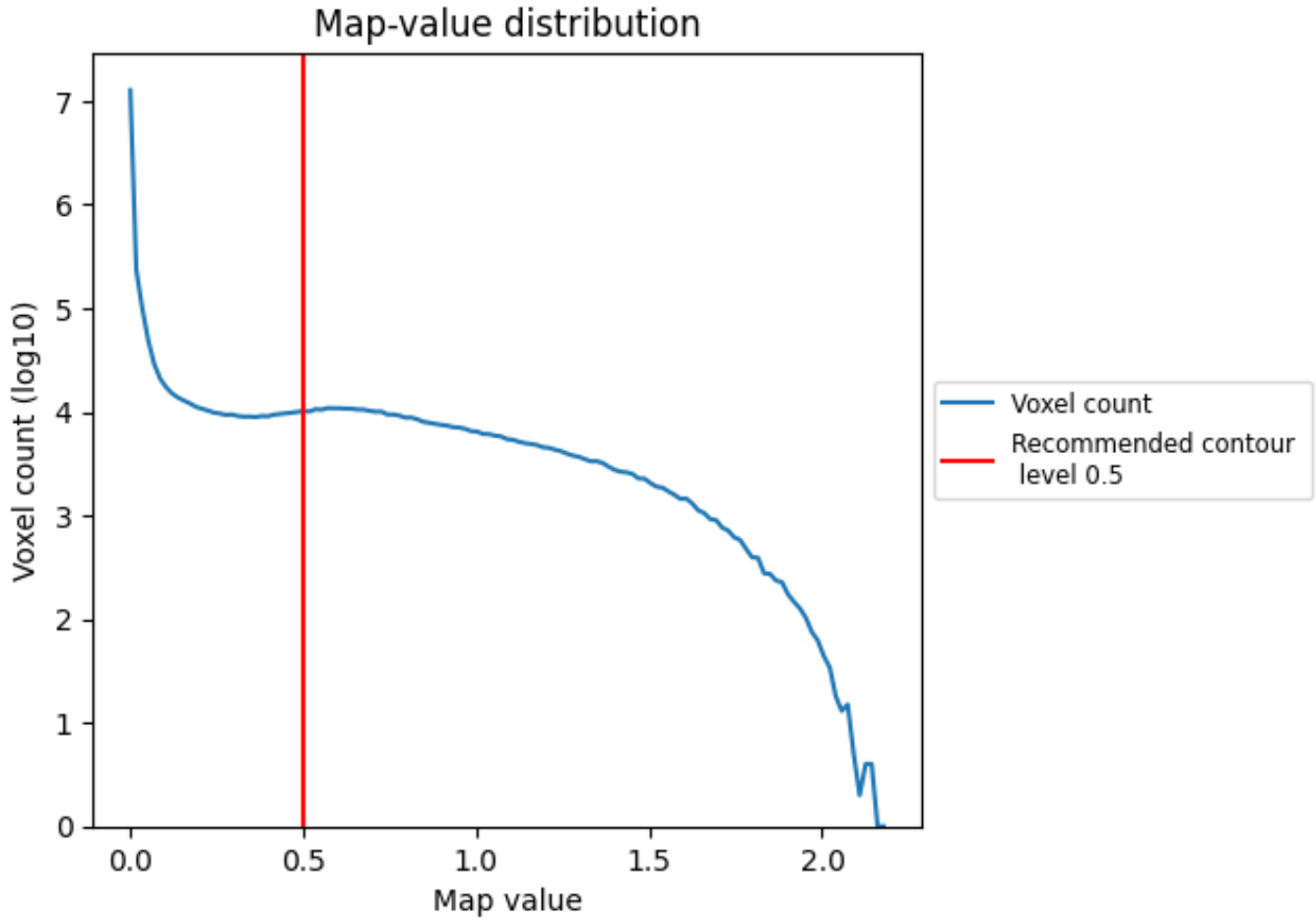
6.6 Mask visualisation (i)

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

7 Map analysis

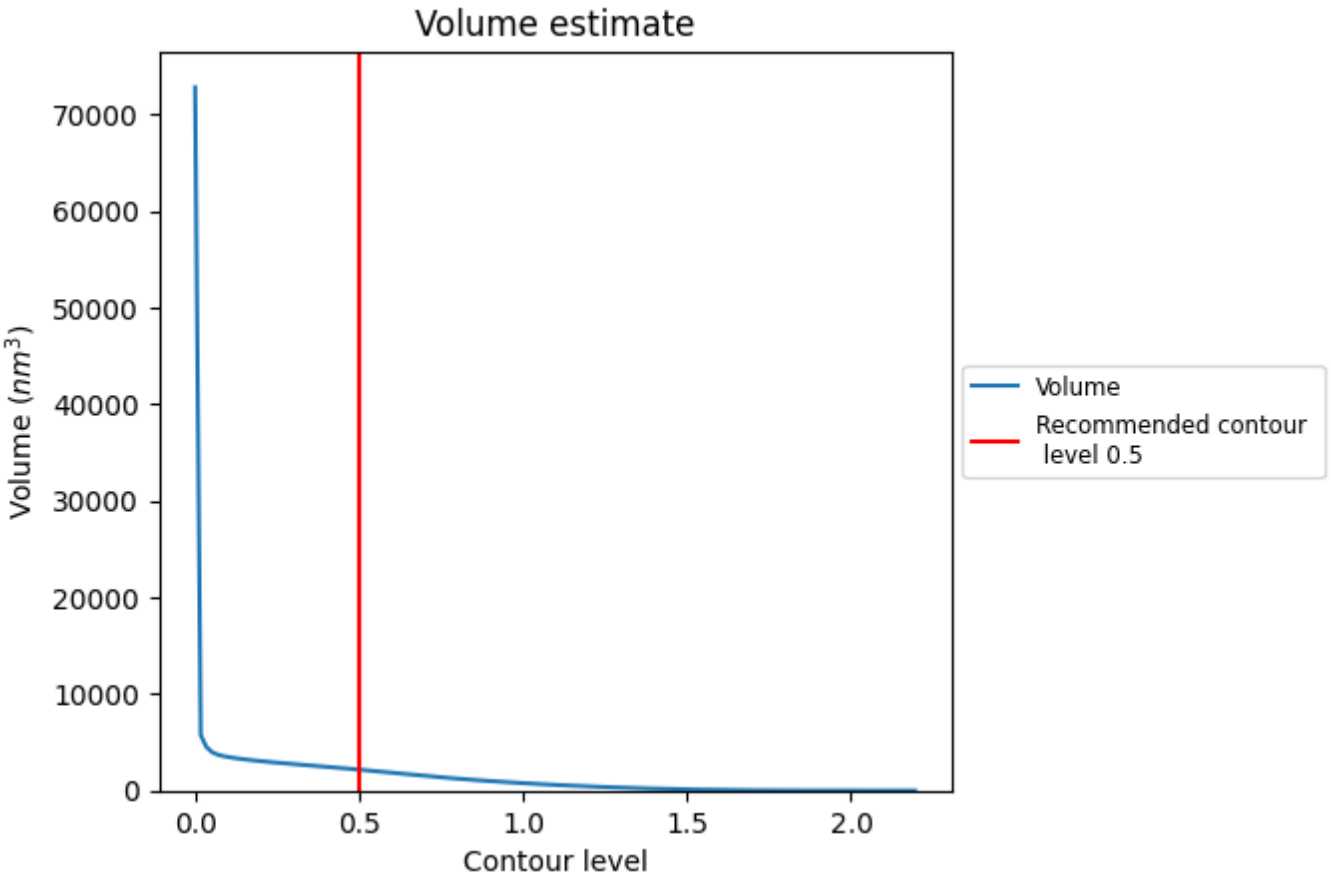
This section contains the results of statistical analysis of the map.

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.

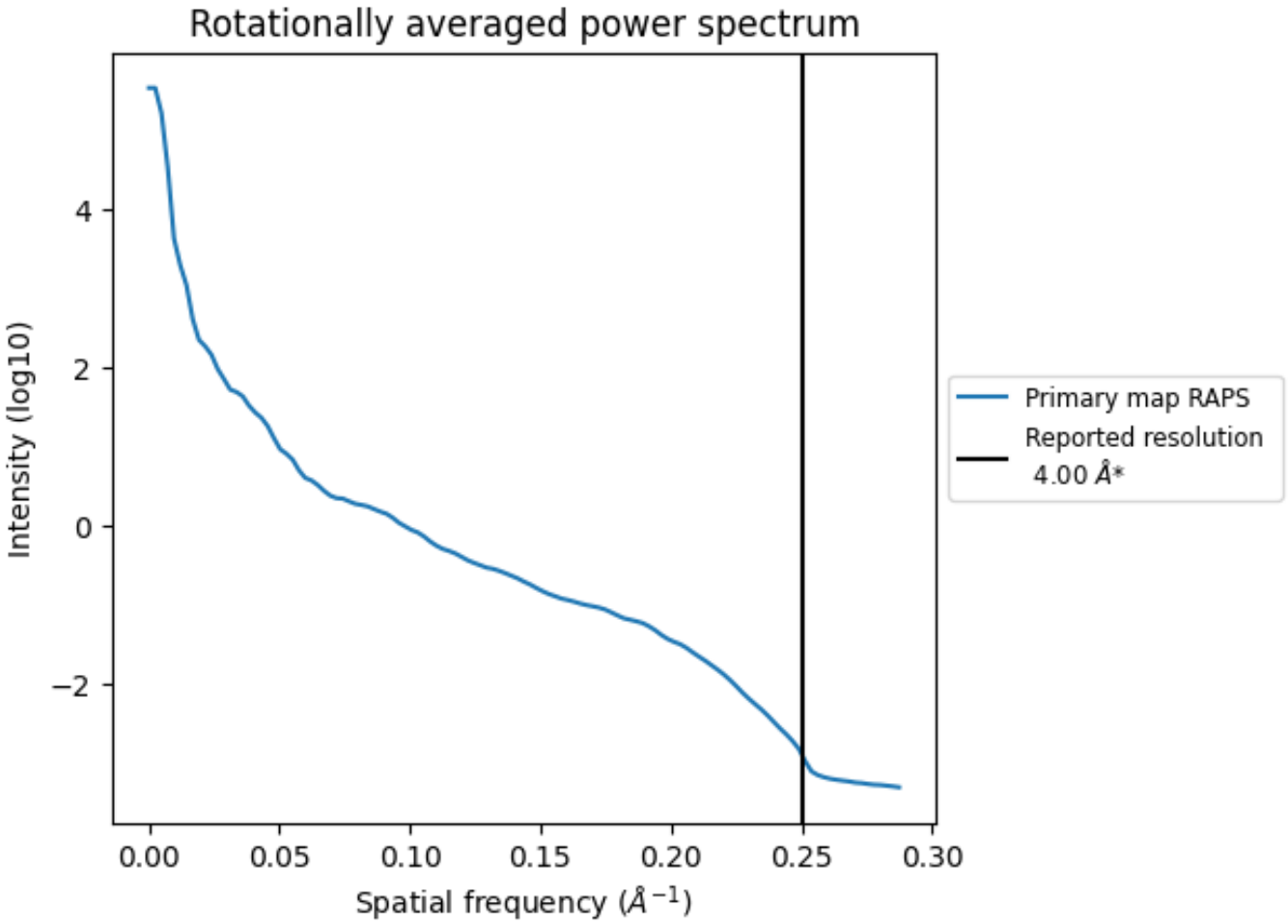
7.2 Volume estimate



The volume at the recommended contour level is 2171 nm^3; this corresponds to an approximate mass of 1962 kDa.

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

7.3 Rotationally averaged power spectrum (i)

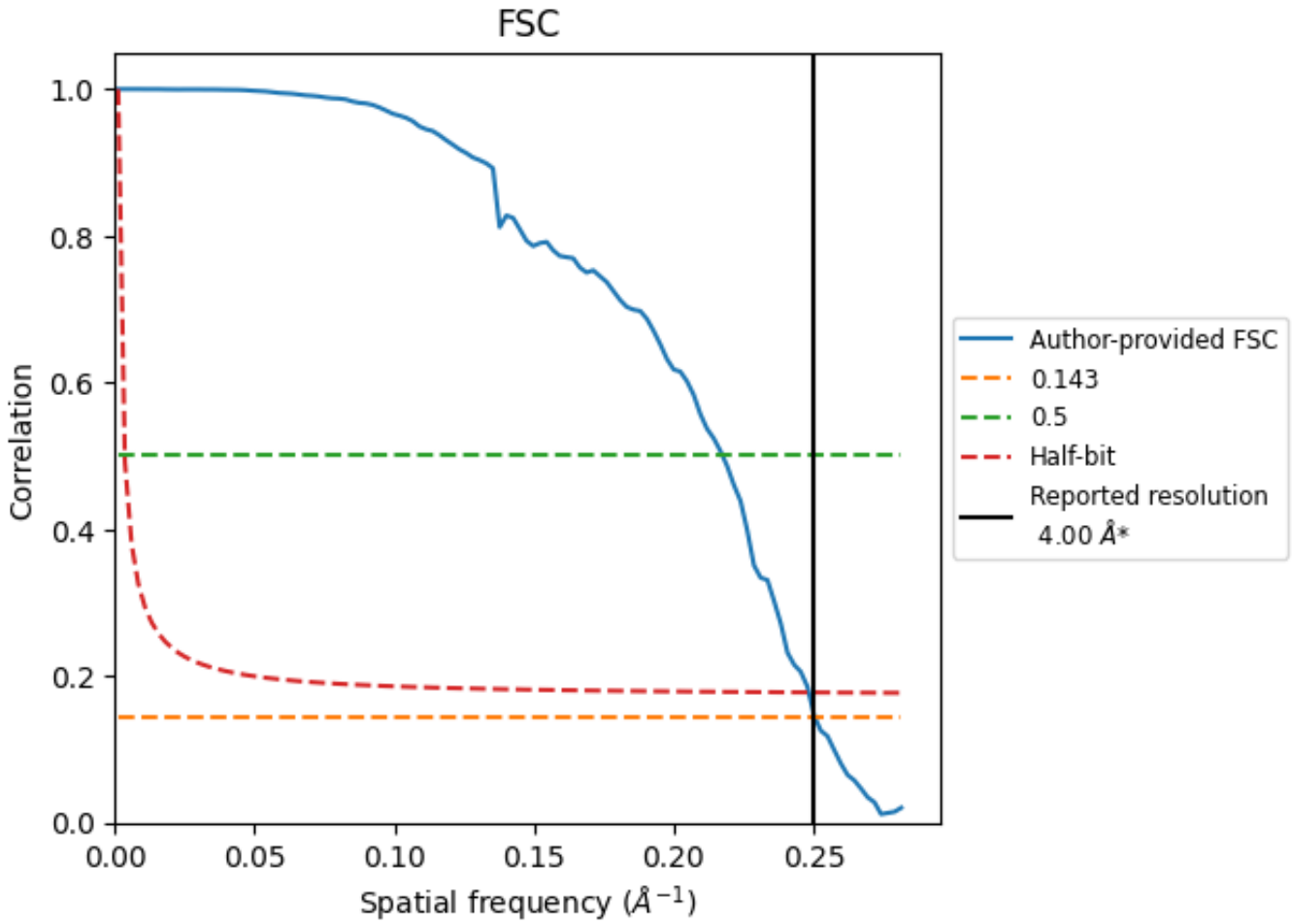


*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

8.2 Resolution estimates (i)

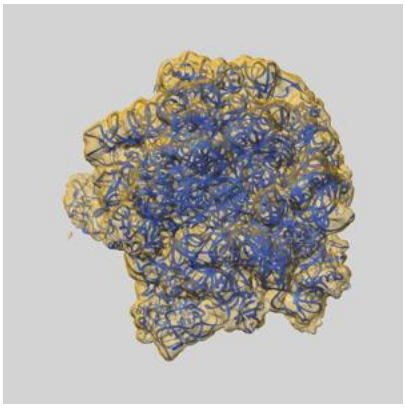
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.99	4.60	4.03
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

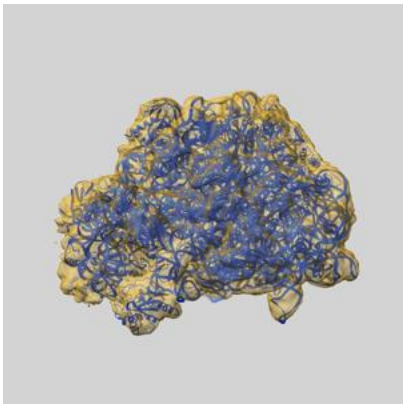
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12219 and PDB model 7BL6. Per-residue inclusion information can be found in section 3 on page 10.

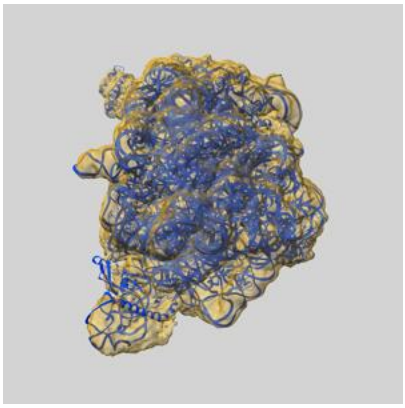
9.1 Map-model overlay



X



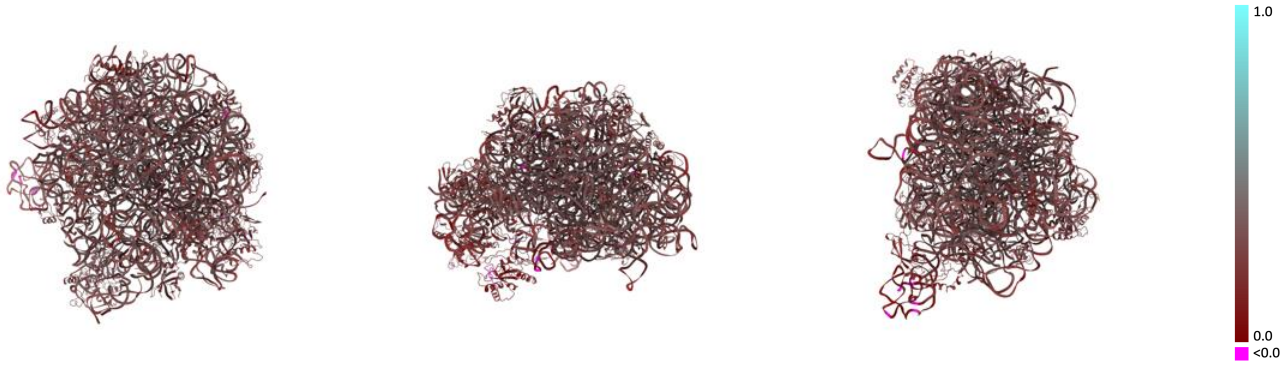
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

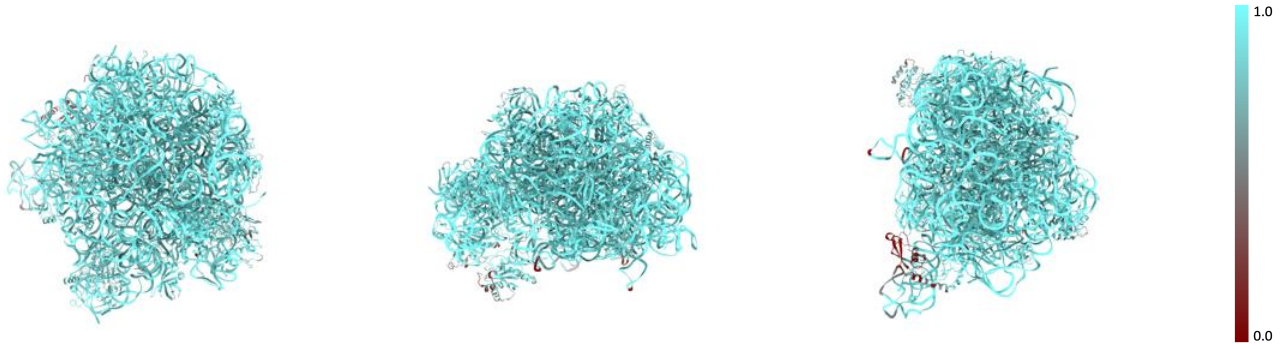
9.2 Q-score mapped to coordinate model (i)



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.

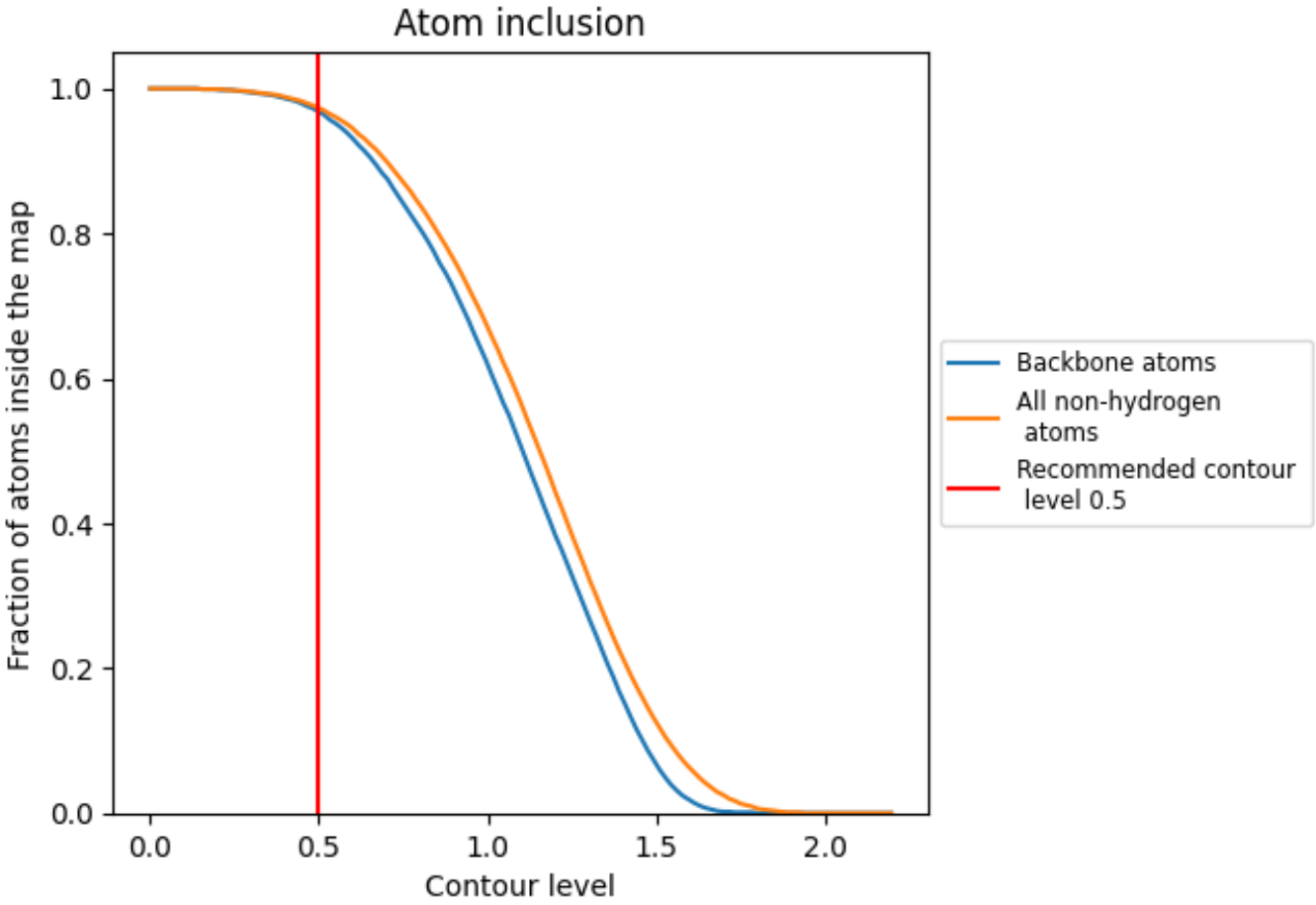
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 97% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9730	0.2890
0	0.9810	0.2670
1	0.9950	0.2680
2	0.9970	0.2870
3	1.0000	0.2860
9	0.8530	0.1990
A	0.9900	0.3010
B	0.9970	0.2850
C	0.9910	0.3020
D	0.9700	0.3000
E	0.9160	0.2710
F	0.8990	0.2090
G	0.9000	0.2490
H	0.5700	0.2020
J	0.9850	0.2910
K	0.9770	0.2810
L	0.9560	0.2820
M	0.9810	0.2930
N	0.9920	0.2700
O	0.9710	0.2530
P	0.9600	0.2810
Q	0.9850	0.2690
R	0.9270	0.2820
S	0.9820	0.2780
T	0.9830	0.2920
U	0.9620	0.2600
V	0.9510	0.2710
W	0.9930	0.2860
X	0.9900	0.2870
Y	0.9500	0.2140
Z	0.9410	0.2580
d	0.6740	0.1790
g	0.9930	0.2860