Full wwPDB EM Validation Report

Apr 22, 2025 – 07:34 AM EDT

PDB ID	:	8VK0 / pdb_00008vk0
EMDB ID	:	EMD-43294
Title	:	Structure of Mycobacterium smegmatis 50S ribosomal subunit bound to HflX:50S-HflX-A
Authors	:	Majumdar, S.; Koripella, R.K.; Sharma, M.R.; Manjari, S.R.; Banavali, N.K.; Agrawal, R.K.
Deposited on	:	2024-01-08
Resolution	:	3.14 Å(reported)
Based on initial models	:	5O61, 6DZI

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 (i) symbol.

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

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

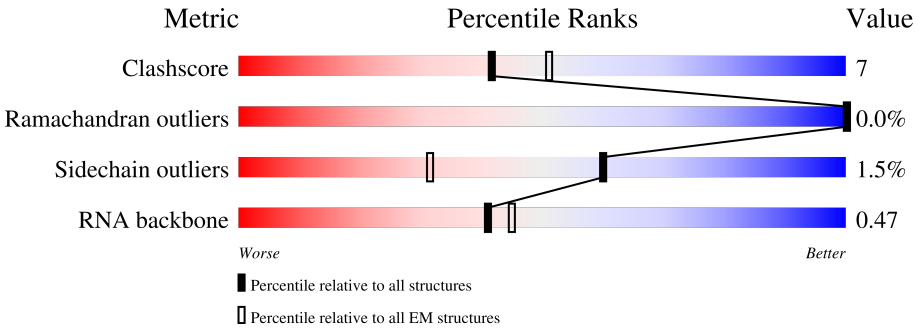
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.14 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	2	61	92% 5% •
2	3	24	83% 12% •
3	4	470	14% 24% 61% 6% 9%
4	A	3120	5% 65% 27% 7% •
5	B	118	• 50% 37% 9% •
6	C	278	• 85% 14% •
7	D	217	91% 8% •

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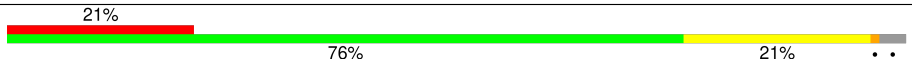
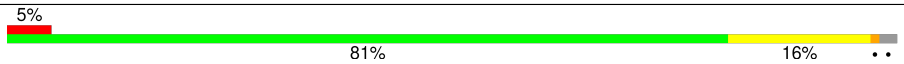
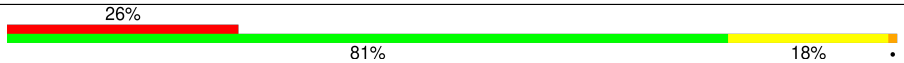
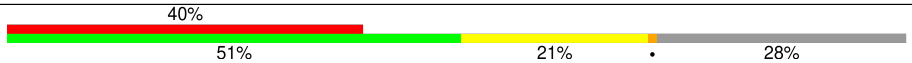
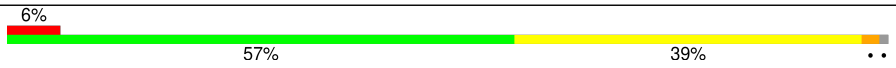
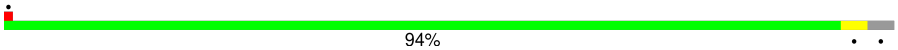
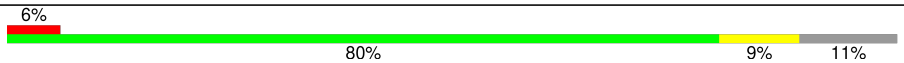
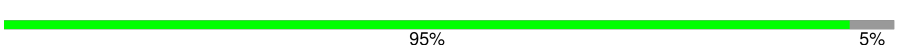
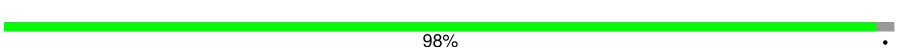
Mol	Chain	Length	Quality of chain
8	E	215	
9	F	187	
10	G	179	
11	H	151	
12	I	175	
13	J	142	
14	K	147	
15	L	122	
16	M	147	
17	N	138	
18	O	199	
19	P	127	
20	Q	113	
21	R	129	
22	S	103	
23	T	153	
24	U	100	
25	V	105	
26	W	215	
27	X	88	
28	Y	64	
29	Z	77	
30	b	57	
31	c	55	
32	d	47	

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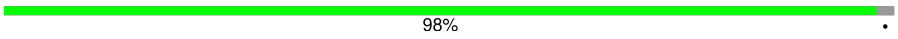
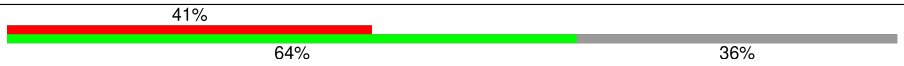
Mol	Chain	Length	Quality of chain
33	e	64	
34	f	37	
35	g	75	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	GCP	4	501	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 100928 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 L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	2	59	Total	C	N	O	0	0
			474	292	95	87		

- Molecule 2 is a protein called 50S Ribosomal Protein L37.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	3	23	Total	C	N	O	0	0
			189	111	50	28		

- Molecule 3 is a protein called GTPase HflX.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	426	Total	C	N	O	S	0	0
			3228	1997	599	625	7		

- Molecule 4 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	3119	Total	C	N	O	P	0	0
			66981	29854	12313	21695	3119		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	118	Total	C	N	O	P	0	0
			2522	1126	468	810	118		

- Molecule 6 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	275	Total	C	N	O	S	0	0
			2110	1298	438	370	4		

- Molecule 7 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	214	Total	C	N	O	S	0	0
			1587	982	310	290	5		

- Molecule 8 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	209	Total	C	N	O	S	0	0
			1569	969	295	303	2		

- Molecule 9 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	182	Total	C	N	O	S	0	0
			1445	907	271	261	6		

- Molecule 10 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	176	Total	C	N	O	S	0	0
			1348	845	249	253	1		

- Molecule 11 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	151	Total	C	N	O	S	0	0
			1018	635	188	194	1		

- Molecule 12 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	126	Total	C	N	O	S	0	0
			918	580	156	180	2		

- Molecule 13 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	133	Total	C	N	O	S	0	0
			990	625	175	187	3		

- Molecule 14 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	146	Total	C	N	O	S	0	0
			1130	722	207	200	1		

- Molecule 15 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	122	Total	C	N	O	S	0	0
			938	586	179	170	3		

- Molecule 16 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	145	Total	C	N	O	S	0	0
			1078	676	205	194	3		

- Molecule 17 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	136	Total	C	N	O	S	0	0
			1092	690	213	187	2		

- Molecule 18 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	118	Total	C	N	O	S	0	0
			928	583	180	163	2		

- Molecule 19 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	P	126	Total	C	N	O	0	0
			956	586	199	171		

- Molecule 20 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	113	Total	C	N	O	S	0	0
			907	570	171	165	1		

- Molecule 21 is a protein called 50S Ribosomal Protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	R	124	Total 988	C 613	N 203	O 172	0	0

- Molecule 22 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	S	100	Total 754	C 478	N 137	O 139	0	0

- Molecule 23 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	T	114	Total 873	C 543	N 171	O 159	0	0

- Molecule 24 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	U	97	Total 756	C 479	N 138	O 139	0	0

- Molecule 25 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	97	Total 732	C 456	N 137	O 137	S 2	0	0

- Molecule 26 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	W	192	Total 1428	C 881	N 255	O 292	0	0

- Molecule 27 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	X	79	Total 586	C 361	N 123	O 102	0	0

- Molecule 28 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	63	Total	C	N	O	S	0	0
			470	283	103	80	4		

- Molecule 29 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	64	Total	C	N	O	S	0	0
			531	324	103	103	1		

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	54	Total	C	N	O	S	0	0
			423	260	93	69	1		

- Molecule 31 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	49	Total	C	N	O	S	0	0
			405	248	82	71	4		

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	46	Total	C	N	O	S	0	0
			377	225	97	54	1		

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	e	63	Total	C	N	O	0	0
			502	302	115	85		

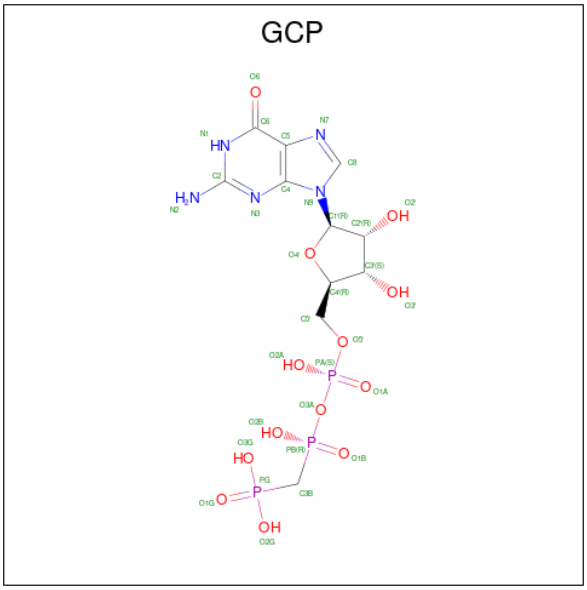
- Molecule 34 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	37	Total	C	N	O	S	0	0
			299	181	66	47	5		

- Molecule 35 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	48	Total	C	N	O	S	0	0
			364	225	63	71	5		

- Molecule 36 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



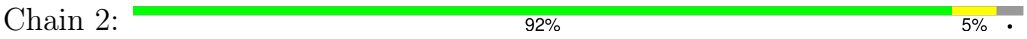
Mol	Chain	Residues	Atoms					AltConf
36	4	1	Total	C	N	O	P	0
			32	11	5	13	3	

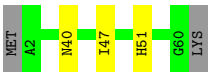
3 Residue-property plots (i)

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 L30

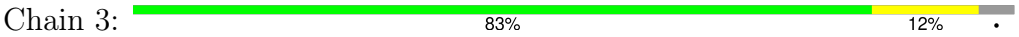
Chain 2:

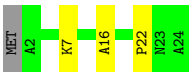




• Molecule 2: 50S Ribosomal Protein L37

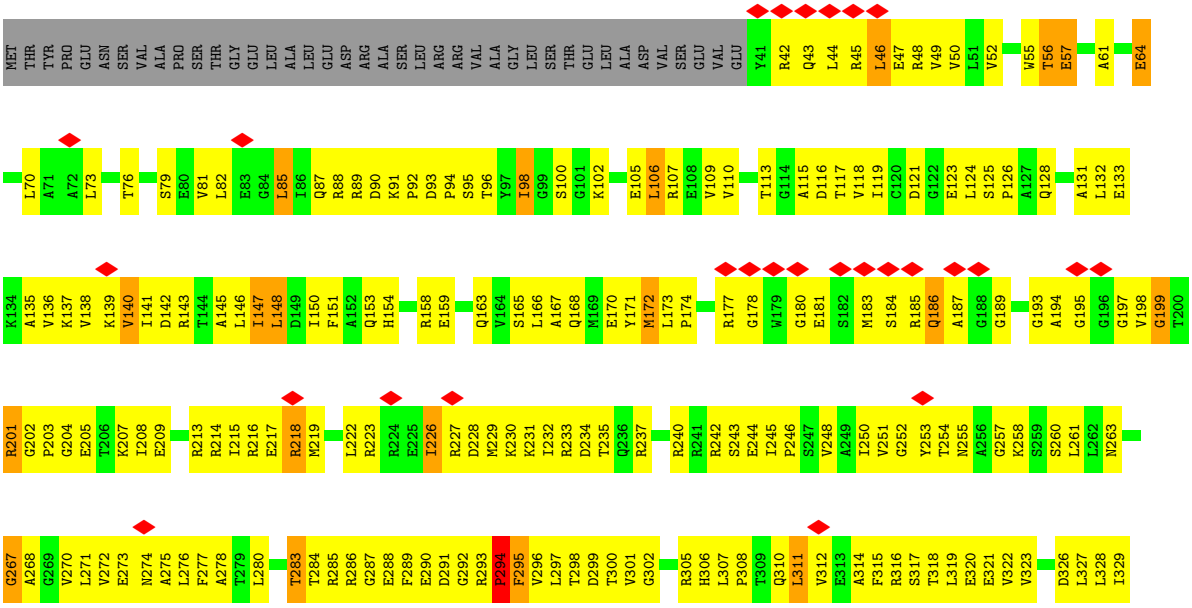
Chain 3:

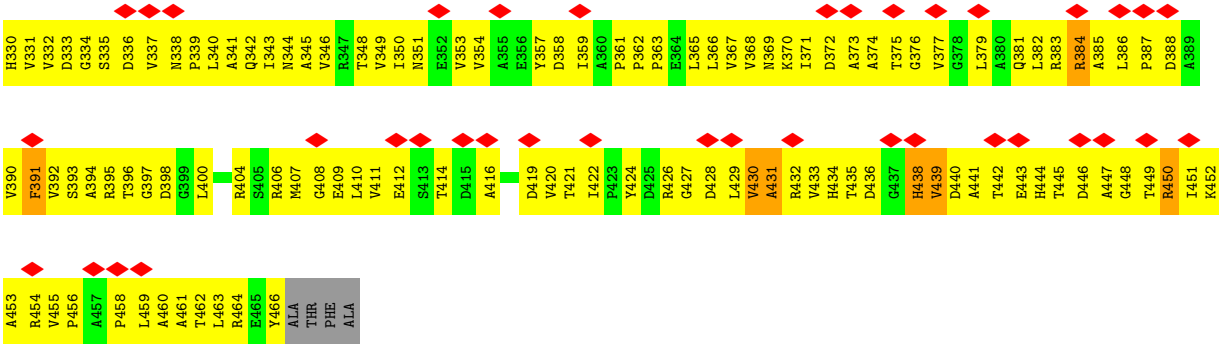




• Molecule 3: GTPase HflX

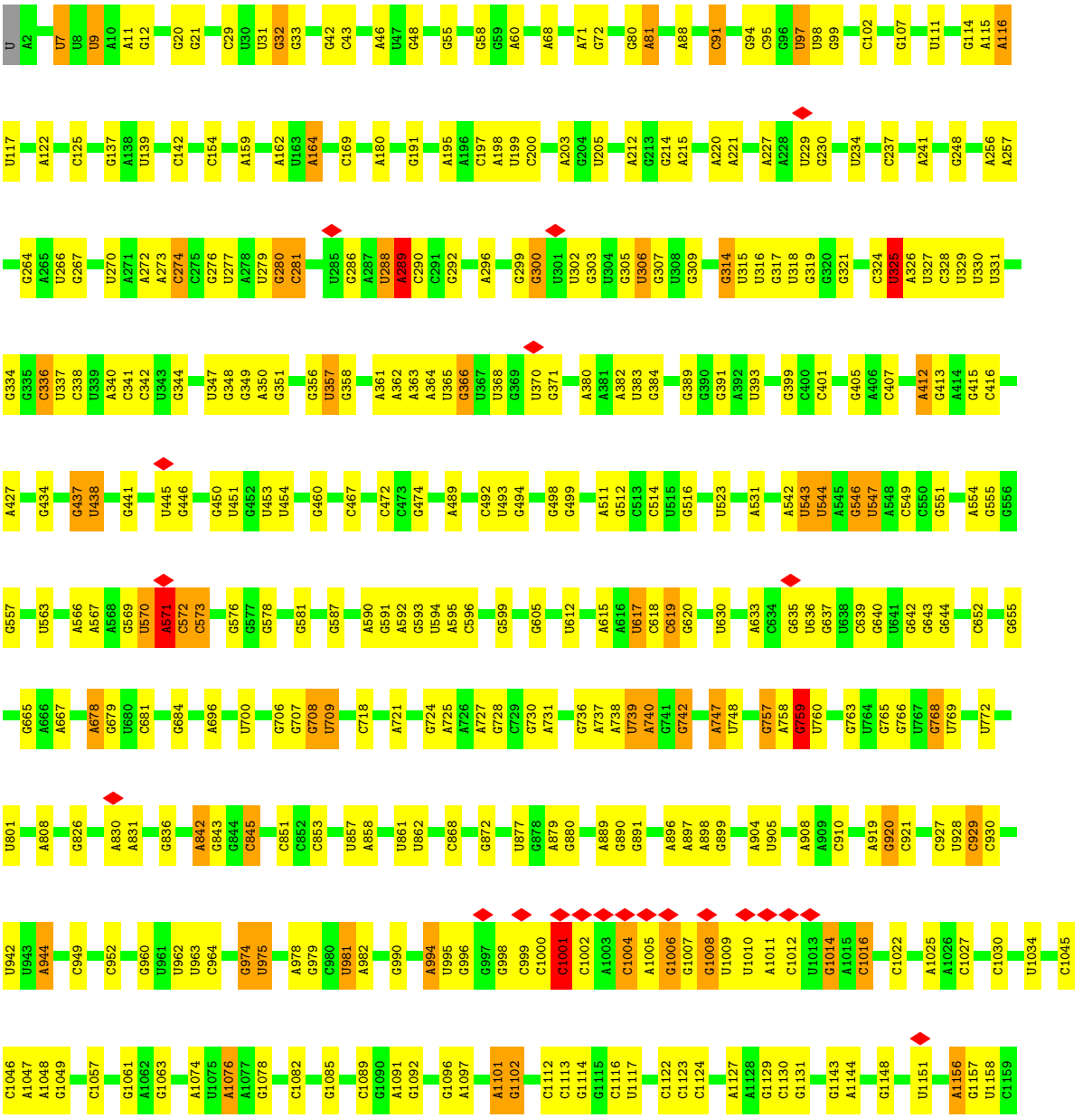
Chain 4:

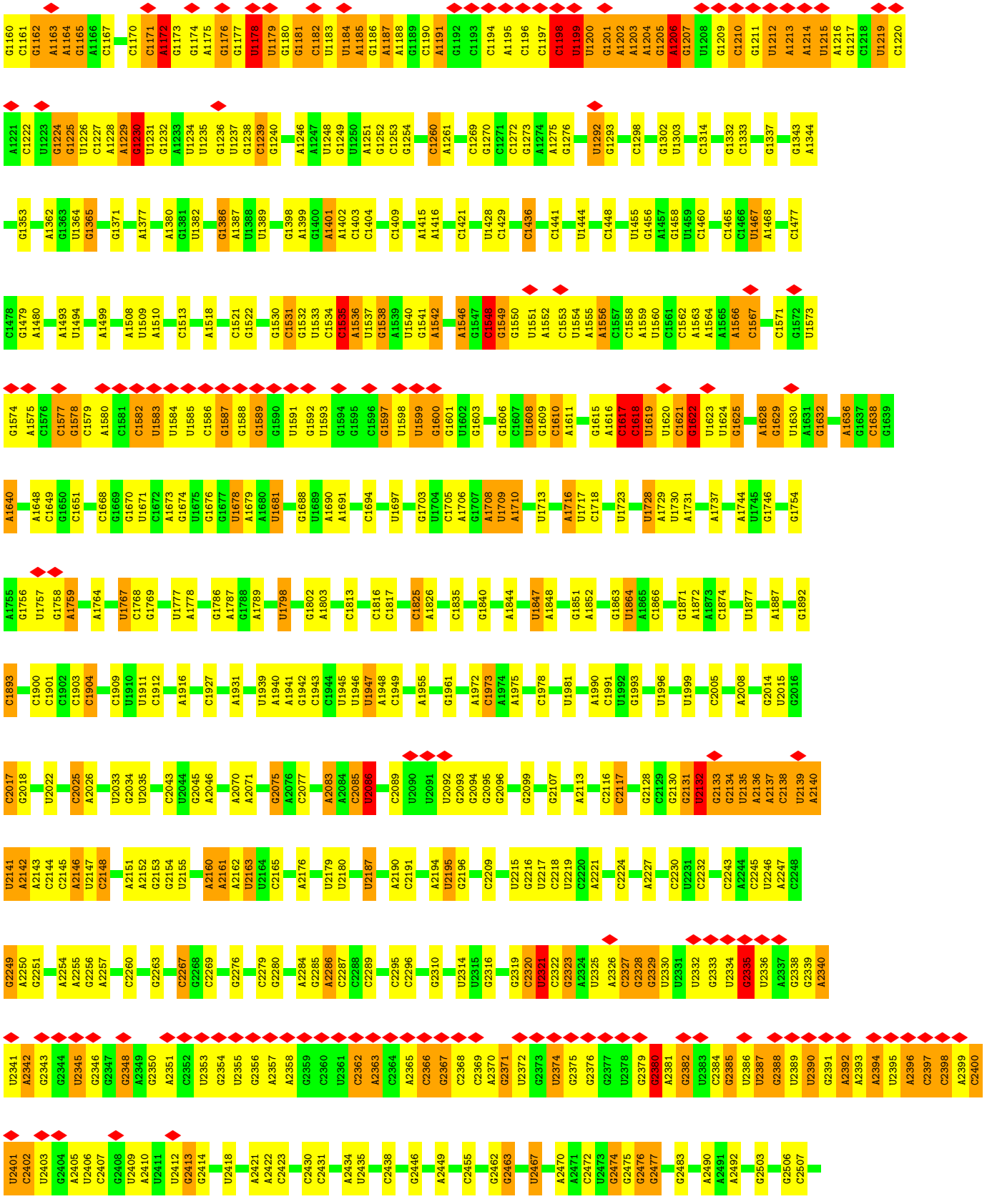


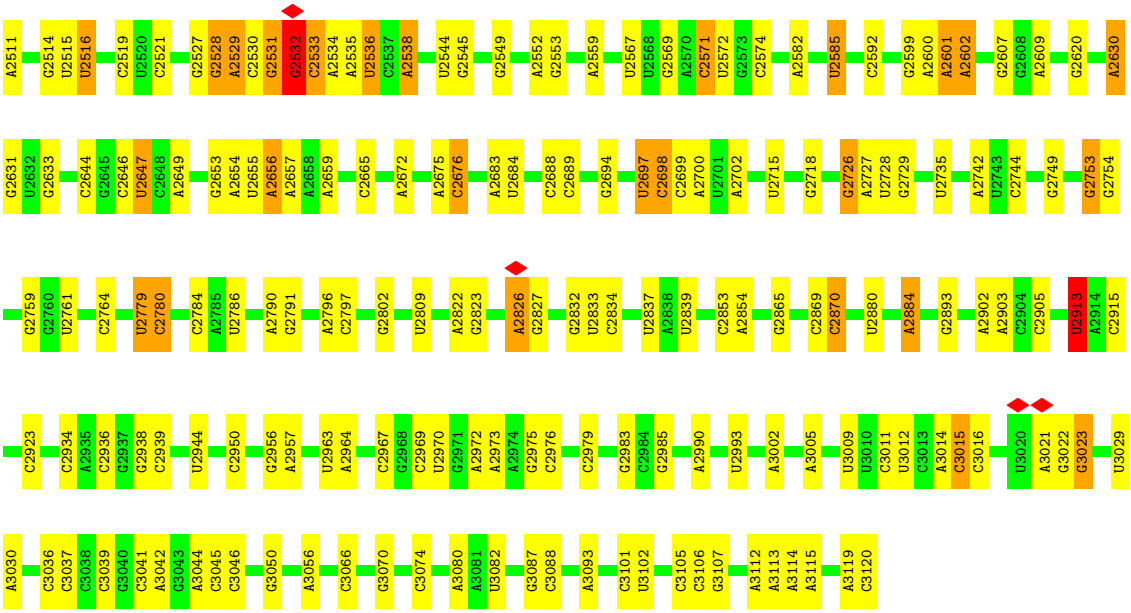


• Molecule 4: 23S ribosomal RNA

Chain A:

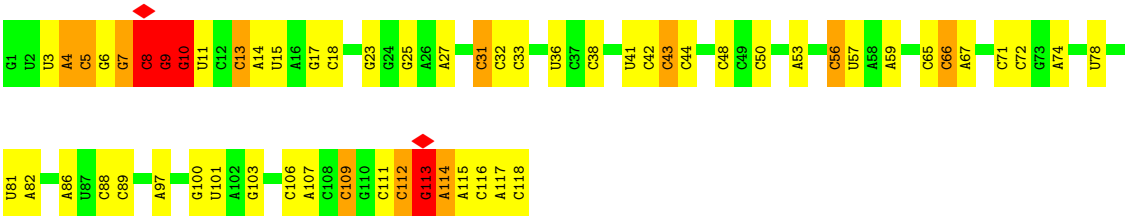



G1160 C1161 G1162 A1163 A1164 G1165 A1166 C1167 C1170 C1171 A1172 G1173 G1174 A1175 G1176 G1177 U1178 U1179 G1180 G1181 C1182 U1183 U1184 A1185 G1186 A1187 A1188 G1189 C1190 A1191 G1192 C1193 C1194 A1195 C1196 C1197 C1198 U1199 U1200 G1201 A1202 A1203 A1204 G1205 A1206 G1207 U1208 G1209 C1210 G1211 U1212 A1213 A1214 U1215 A1216 G1217 C1218 U1219 C1220
A1221 C1222 U1223 G1224 G1225 U1226 C1227 A1228 A1229 G1230 U1231 G1232 A1233 U1234 U1235 G1236 U1237 G1238 C1239 G1240 A1246 A1247 U1248 G1249 U1250 A1251 G1252 C1253 G1254 C1260 A1261 C1269 G1270 C1271 C1272 G1273 A1274 A1275 G1276 U1292 G1293 C1298 G1302 U1303 C1314 G1332 C1333 G1337 G1343 A1344
G1353 A1362 G1363 U1364 G1365 G1371 A1377 A1380 G1381 U1382 G1386 A1387 U1388 U1389 G1398 A1399 G1400 A1401 A1402 C1403 C1404 C1409 A1415 A1416 C1421 U1428 C1429 C1436 C1441 U1444 C1448 U1455 G1456 A1457 G1458 U1459 C1460 C1465 C1466 U1467 A1468 C1477
C1478 G1479 A1480 A1493 U1494 A1499 A1508 U1509 A1510 C1513 A1518 C1521 G1522 G1530 C1531 G1532 U1533 C1534 C1535 A1536 U1537 G1538 A1539 U1540 G1541 A1542 A1546 G1547 C1548 G1549 G1550 U1551 A1552 C1553 U1554 A1555 A1556 C1557 C1558 A1559 U1560 C1561 C1562 A1563 A1564 A1565 A1566 C1567 C1571 G1572 U1573
G1574 A1575 G1576 C1577 G1578 C1579 A1580 C1581 C1582 U1583 U1584 U1585 C1586 G1587 G1588 G1589 G1590 U1591 G1592 U1593 G1594 G1595 C1596 G1597 U1598 U1599 G1600 G1601 U1602 G1603 G1606 C1607 U1608 G1609 C1610 A1611 G1615 A1616 C1617 C1618 U1619 U1620 C1621 G1622 U1623 U1624 G1625 A1628 G1629 U1630 A1631 G1632 A1636 G1637 C1638 G1639
A1640 A1648 C1649 G1650 C1651 C1668 G1669 G1670 U1671 C1672 A1673 G1674 U1675 G1676 G1677 U1678 A1679 A1680 U1681 G1688 U1689 A1690 A1691 C1694 U1697 G1703 U1704 C1705 A1706 G1707 A1708 U1709 A1710 U1713 A1716 U1717 C1718 U1723 U1728 A1729 U1730 A1731 A1737 A1744 U1745 G1746 G1754
A1755 G1756 U1757 G1758 A1759 A1764 U1767 C1768 G1769 U1777 A1778 G1786 A1787 G1788 A1789 U1798 G1802 A1803 C1813 C1816 C1817 C1825 A1826 C1835 G1840 A1844 U1847 A1848 G1851 A1852 G1863 U1864 A1865 C1866 G1871 A1872 A1873 C1874 U1877 A1887 G1892
C1893 C1900 C1901 C1902 C1903 C1904 C1909 U1910 U1911 C1912 A1916 C1927 A1931 U1939 A1940 A1941 G1942 C1943 C1944 U1945 U1946 U1947 A1948 C1949 A1955 G1961 A1972 C1973 A1974 A1975 C1978 U1981 A1990 C1991 U1992 G1993 U1996 U1999 C2005 A2008 G2014 U2015 G2016
C2017 G2018 U2022 C2025 A2026 U2033 G2034 U2035 C2043 U2044 G2045 A2046 A2070 A2071 G2075 A2076 C2077 A2083 A2084 C2085 U2086 C2089 U2090 U2091 U2092 G2093 G2094 G2095 G2096 C2099 G2107 A2113 C2116 C2117 G2128 C2129 G2130 G2131 U2132 G2133 G2134 U2135 A2136 A2137 C2138 U2139 A2140
U2141 A2142 A2143 C2144 C2145 A2146 U2147 C2148 A2151 A2152 G2153 G2154 U2155 A2160 A2161 A2162 U2163 U2164 C2165 A2176 U2179 U2180 U2187 A2190 C2191 A2194 U2195 G2196 C2209 U2215 G2216 U2217 C2218 U2219 C2220 A2221 C2224 A2227 C2230 U2231 C2232 C2243 A2244 C2245 U2246 A2247 C2248
G2249 A2250 G2251 A2254 A2255 G2256 A2257 C2260 G2263 C2267 G2268 C2269 G2276 C2279 G2280 A2284 G2285 A2286 C2287 C2288 C2289 C2295 C2296 G2310 U2314 U2315 G2316 G2319 C2320 U2321 C2322 G2323 A2324 U2325 A2326 C2327 G2328 G2329 U2330 U2331 U2332 G2333 U2334 G2335 U2336 A2337 G2338 G2339 A2340
U2341 A2342 G2343 G2344 U2345 G2346 G2347 G2348 A2349 G2350 A2351 C2352 U2353 G2354 U2355 G2356 A2357 A2358 G2359 C2360 U2361 C2362 A2363 C2364 A2365 C2366 G2367 C2368 C2369 A2370 G2371 U2372 G2373 U2374 G2375 G2376 G2377 U2378 G2379 G2380 A2381 G2382 U2383 C2384 G2385 U2386 U2387 G2388 U2389 U2390 G2391 A2392 A2393 A2394 U2395 A2396 C2397 C2398 A2399 C2400
U2401 C2402 U2403 G2404 A2405 U2406 C2407 G2408 U2409 A2410 U2411 U2412 G2413 G2414 U2418 A2421 A2422 C2423 C2430 C2431 A2434 U2435 C2438 G2446 A2449 C2455 G2462 G2463 U2467 A2470 A2471 C2472 U2473 G2474 G2475 G2476 G2477 G2483 A2490 A2491 A2492 G2503 G2506 C2507



• Molecule 5: 5S ribosomal RNA

Chain B:



• Molecule 6: 50S ribosomal protein L2

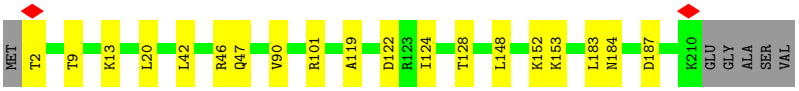
Chain C:

• Molecule 7: 50S ribosomal protein L3

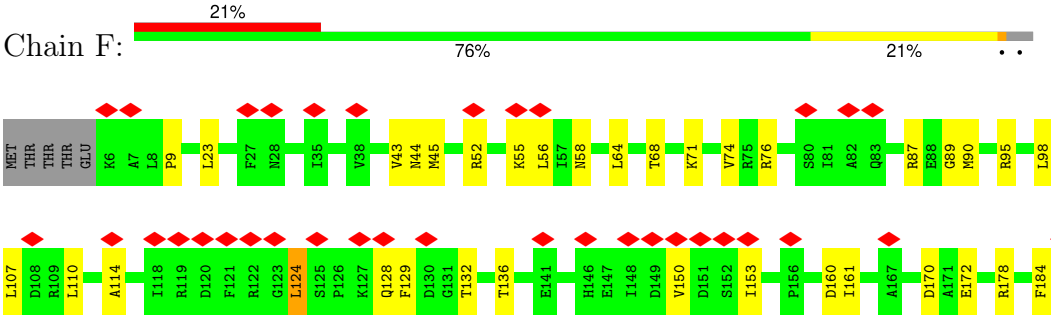
Chain D:

• Molecule 8: 50S Ribosomal Protein L4

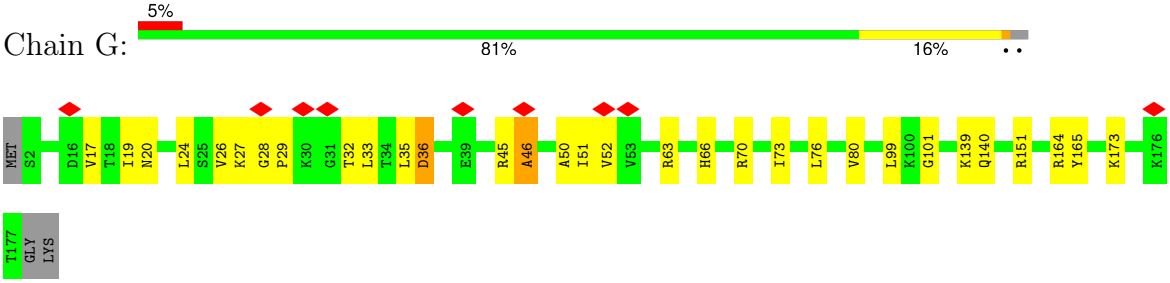
Chain E:



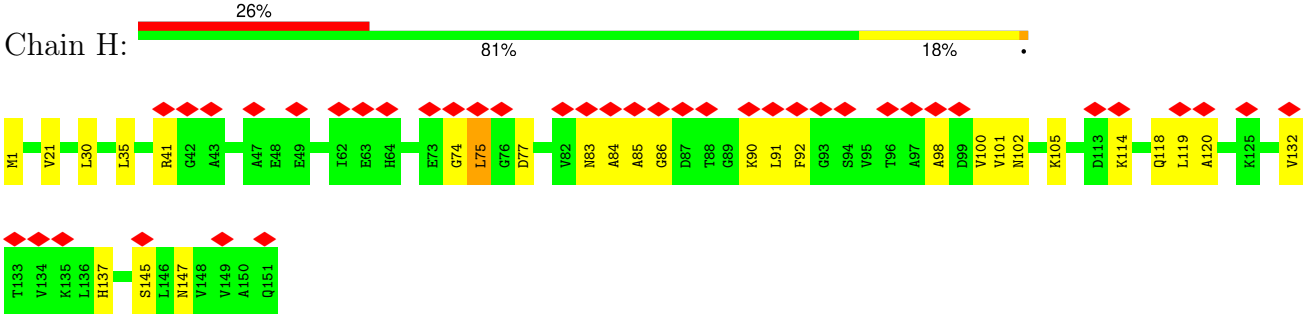
• Molecule 9: 50S Ribosomal Protein L5



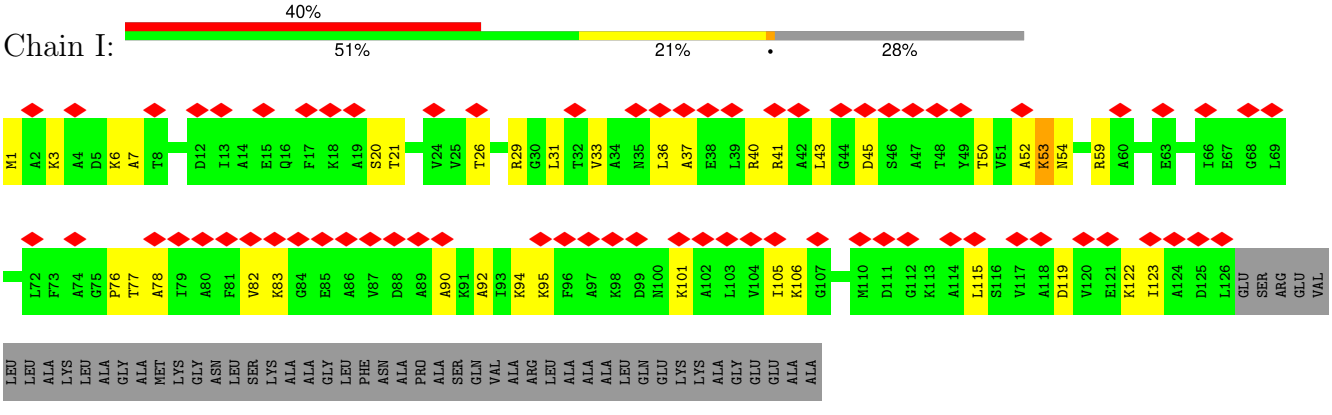
• Molecule 10: 50S ribosomal protein L6



• Molecule 11: 50S ribosomal protein L9

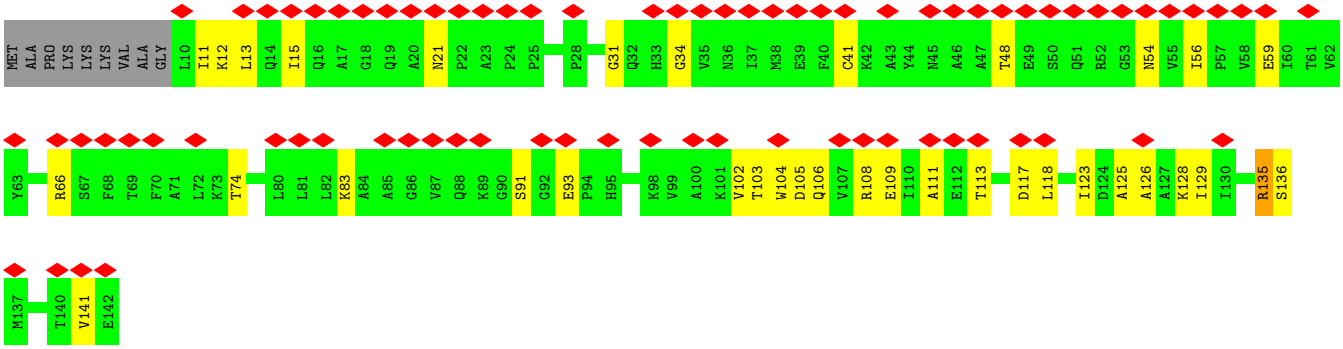


• Molecule 12: 50S ribosomal protein L10



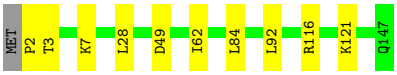
• Molecule 13: 50S ribosomal protein L11

Chain J:



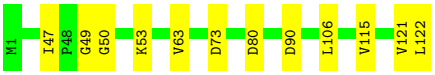
• Molecule 14: 50S Ribosomal Protein L13

Chain K:



• Molecule 15: 50S ribosomal protein L14

Chain L:



• Molecule 16: 50S ribosomal protein L15

Chain M:

• Molecule 17: Large ribosomal subunit protein uL16

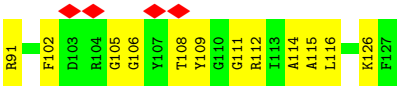
Chain N:

• Molecule 18: 50S ribosomal protein L17

Chain O:

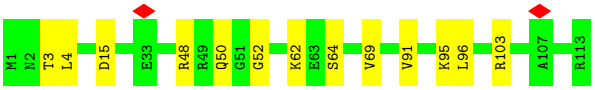
• Molecule 19: 50S Ribosomal Protein L18

Chain P:



• Molecule 20: 50S ribosomal protein L19

Chain Q:

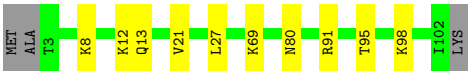


• Molecule 21: 50S Ribosomal Protein L20

Chain R:

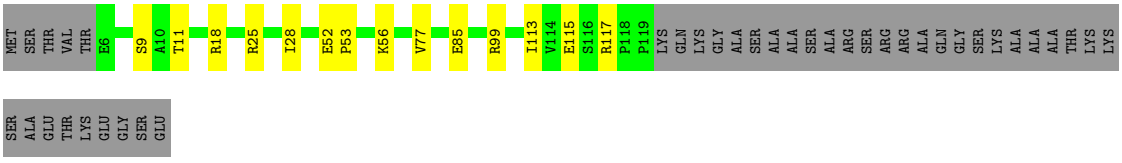
• Molecule 22: 50S Ribosomal Protein L21

Chain S:



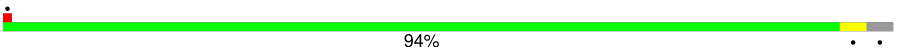
• Molecule 23: 50S Ribosomal Protein L22

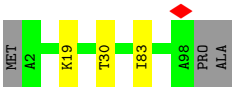
Chain T:



• Molecule 24: 50S Ribosomal Protein L23

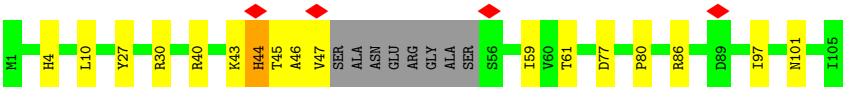
Chain U:





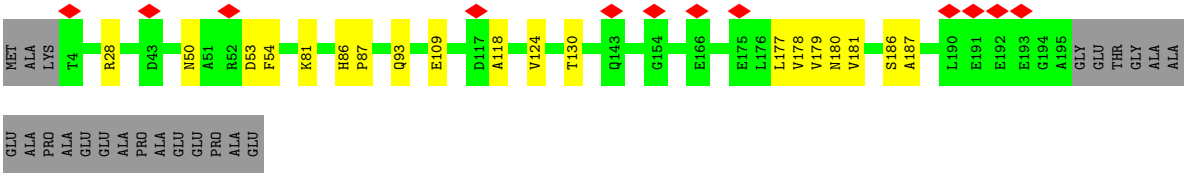
• Molecule 25: 50S ribosomal protein L24

Chain V:



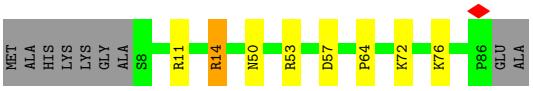
• Molecule 26: 50S ribosomal protein L25

Chain W:



• Molecule 27: 50S ribosomal protein L27

Chain X:

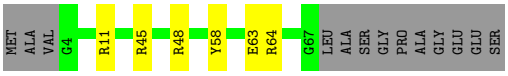


• Molecule 28: 50S Ribosomal Protein L28

Chain Y:

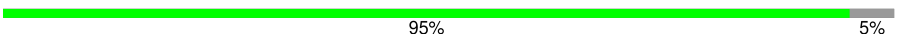
• Molecule 29: 50S ribosomal protein L29

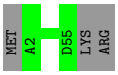
Chain Z:



• Molecule 30: 50S ribosomal protein L32

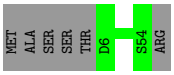
Chain b:





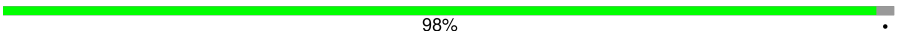
• Molecule 31: 50S Ribosomal Protein L33

Chain c:



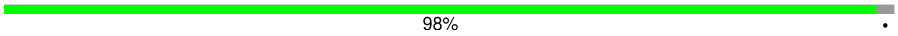
• Molecule 32: 50S ribosomal protein L34

Chain d:



• Molecule 33: 50S ribosomal protein L35

Chain e:

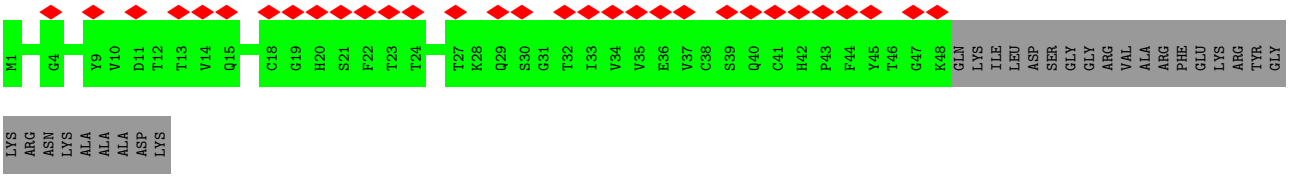


• Molecule 34: 50S ribosomal protein L36

Chain f:

• Molecule 35: 50S Ribosomal Protein L31

Chain g:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	57434	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	51.22	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.771	Depositor
Minimum map value	-0.951	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.19	Depositor
Map size (Å)	433.19998, 433.19998, 433.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.083, 1.083, 1.083	Depositor

5 Model quality

5.1 Standard geometry

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

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	2	0.47	0/477	0.56	0/640
2	3	0.36	0/191	0.49	0/247
3	4	0.51	0/3268	0.67	3/4428 (0.1%)
4	A	0.90	1/75001 (0.0%)	1.18	566/117027 (0.5%)
5	B	0.72	0/2821	1.38	57/4396 (1.3%)
6	C	0.50	0/2153	0.58	0/2895
7	D	0.51	0/1609	0.60	0/2165
8	E	0.47	0/1592	0.61	2/2153 (0.1%)
9	F	0.32	0/1467	0.64	2/1973 (0.1%)
10	G	0.35	0/1369	0.64	0/1848
11	H	0.32	0/1027	0.68	1/1398 (0.1%)
12	I	0.31	0/925	0.64	0/1246
13	J	0.31	0/1006	0.64	0/1364
14	K	0.48	0/1157	0.54	0/1567
15	L	0.51	0/946	0.56	0/1268
16	M	0.44	0/1091	0.56	0/1457
17	N	0.43	0/1118	0.57	0/1506
18	O	0.53	0/945	0.60	0/1267
19	P	0.41	0/966	0.75	1/1298 (0.1%)
20	Q	0.49	0/921	0.62	1/1236 (0.1%)
21	R	0.54	0/1000	0.56	0/1341
22	S	0.47	0/764	0.58	0/1030
23	T	0.50	0/887	0.59	0/1204
24	U	0.50	0/766	0.56	0/1030
25	V	0.44	0/738	0.64	0/987
26	W	0.33	0/1443	0.60	0/1970
27	X	0.47	0/595	0.59	0/798
28	Y	0.47	0/478	0.55	0/641
29	Z	0.44	0/534	0.53	0/713
30	b	0.48	0/427	0.63	0/572
31	c	0.40	0/413	0.48	0/553
32	d	0.49	0/380	0.52	0/500

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	e	0.41	0/507	0.51	0/672
34	f	0.46	0/303	0.54	0/401
35	g	0.34	0/372	0.61	0/503
All	All	0.79	1/109657 (0.0%)	1.07	633/164294 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	F	0	1
10	G	0	2
11	H	0	1
12	I	0	2
13	J	0	1
18	O	0	1
19	P	0	4
26	W	0	1
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	571	A	N9-C4	6.05	1.41	1.37

All (633) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2402	C	N1-C2-O2	14.25	127.45	118.90
4	A	2402	C	N3-C2-O2	-13.03	112.78	121.90
4	A	617	U	C2-N1-C1'	11.10	131.02	117.70
4	A	1567	C	N3-C2-O2	-10.84	114.32	121.90
4	A	1220	C	C2-N1-C1'	10.53	130.38	118.80
4	A	2521	C	C6-N1-C2	-10.42	116.13	120.30
4	A	617	U	N1-C2-O2	10.38	130.07	122.80
4	A	3046	C	C2-N1-C1'	10.37	130.20	118.80
4	A	2402	C	C6-N1-C2	-10.26	116.19	120.30
4	A	1225	G	C6-C5-N7	-10.26	124.25	130.40
4	A	3046	C	N3-C2-O2	-10.19	114.76	121.90
4	A	1225	G	C4-N9-C1'	10.14	139.68	126.50
5	B	5	C	C5-C6-N1	10.06	126.03	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1608	U	C5-C6-N1	10.00	127.70	122.70
4	A	617	U	N3-C2-O2	-9.81	115.33	122.20
4	A	2025	C	N1-C2-O2	9.81	124.78	118.90
4	A	2402	C	C2-N1-C1'	9.78	129.56	118.80
4	A	2117	C	N1-C2-O2	9.64	124.68	118.90
4	A	543	U	N1-C2-O2	9.61	129.53	122.80
4	A	1225	G	N3-C4-N9	9.53	131.72	126.00
5	B	5	C	C6-N1-C2	-9.53	116.49	120.30
4	A	1534	C	N1-C2-O2	9.47	124.58	118.90
4	A	1225	G	C8-N9-C1'	-9.45	114.71	127.00
4	A	2387	U	C2-N1-C1'	9.38	128.95	117.70
4	A	1178	U	N3-C2-O2	-9.36	115.65	122.20
4	A	1567	C	N1-C2-O2	9.26	124.46	118.90
4	A	2025	C	C2-N1-C1'	9.15	128.87	118.80
4	A	1403	C	N1-C2-O2	9.09	124.35	118.90
4	A	1292	U	N3-C2-O2	-9.07	115.85	122.20
4	A	543	U	N3-C2-O2	-8.94	115.94	122.20
4	A	3046	C	C6-N1-C2	-8.94	116.72	120.30
5	B	13	C	N3-C2-O2	-8.92	115.65	121.90
4	A	1225	G	C4-C5-N7	8.89	114.36	110.80
4	A	2521	C	C2-N1-C1'	8.87	128.56	118.80
4	A	905	U	C2-N1-C1'	8.86	128.33	117.70
4	A	1403	C	N3-C2-O2	-8.81	115.73	121.90
4	A	1534	C	C2-N1-C1'	8.80	128.49	118.80
4	A	2025	C	N3-C2-O2	-8.81	115.74	121.90
4	A	1428	U	C2-N1-C1'	8.78	128.24	117.70
4	A	1224	G	N3-C2-N2	8.75	126.03	119.90
4	A	270	U	N1-C2-O2	8.71	128.90	122.80
4	A	1429	C	C2-N1-C1'	8.70	128.37	118.80
4	A	1947	U	C2-N1-C1'	8.70	128.13	117.70
4	A	1947	U	N1-C2-O2	8.69	128.88	122.80
4	A	1292	U	N1-C2-O2	8.69	128.88	122.80
4	A	1428	U	N3-C2-O2	-8.68	116.12	122.20
5	B	13	C	N1-C2-O2	8.66	124.10	118.90
5	B	32	C	C2-N1-C1'	8.64	128.31	118.80
4	A	1428	U	N1-C2-O2	8.59	128.81	122.80
4	A	2521	C	C5-C6-N1	8.54	125.27	121.00
4	A	270	U	N3-C2-O2	-8.46	116.28	122.20
5	B	13	C	C2-N1-C1'	8.46	128.11	118.80
5	B	13	C	C6-N1-C2	-8.40	116.94	120.30
4	A	2117	C	N3-C2-O2	-8.37	116.04	121.90
4	A	1638	C	C2-N1-C1'	8.36	127.99	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1947	U	N3-C2-O2	-8.35	116.36	122.20
4	A	324	C	N1-C2-O2	8.34	123.91	118.90
4	A	383	U	C2-N1-C1'	8.30	127.67	117.70
4	A	472	C	N1-C2-O2	8.29	123.88	118.90
4	A	2375	G	N3-C4-N9	8.29	130.97	126.00
4	A	2387	U	N1-C2-O2	8.28	128.60	122.80
4	A	1161	C	N3-C2-O2	-8.27	116.11	121.90
4	A	288	U	N3-C2-O2	-8.19	116.46	122.20
4	A	1225	G	N9-C4-C5	-8.19	102.13	105.40
4	A	1973	C	N3-C2-O2	-8.16	116.19	121.90
4	A	3046	C	N1-C2-O2	8.14	123.78	118.90
4	A	2402	C	C5-C6-N1	8.11	125.06	121.00
4	A	102	C	C2-N1-C1'	8.04	127.65	118.80
4	A	2944	U	N3-C2-O2	-8.03	116.58	122.20
4	A	2180	U	N1-C2-O2	8.02	128.41	122.80
4	A	1210	C	N1-C2-O2	8.02	123.71	118.90
4	A	905	U	N1-C2-O2	7.98	128.39	122.80
4	A	2387	U	N3-C2-O2	-7.97	116.62	122.20
4	A	2689	C	C2-N1-C1'	7.96	127.56	118.80
4	A	543	U	C2-N1-C1'	7.95	127.24	117.70
5	B	10	G	C8-N9-C4	-7.94	103.23	106.40
4	A	1178	U	N1-C2-O2	7.92	128.35	122.80
4	A	1403	C	C2-N1-C1'	7.89	127.48	118.80
5	B	32	C	N1-C2-O2	7.86	123.62	118.90
4	A	383	U	N3-C2-O2	-7.79	116.75	122.20
4	A	383	U	N1-C2-O2	7.79	128.25	122.80
4	A	1534	C	N3-C2-O2	-7.79	116.45	121.90
4	A	2375	G	C6-C5-N7	-7.78	125.73	130.40
4	A	1535	C	N1-C2-O2	7.74	123.54	118.90
4	A	102	C	C6-N1-C2	-7.70	117.22	120.30
4	A	472	C	C2-N1-C1'	7.66	127.23	118.80
4	A	324	C	C2-N1-C1'	7.62	127.19	118.80
4	A	1579	C	C2-N1-C1'	7.58	127.14	118.80
4	A	288	U	N1-C2-O2	7.54	128.08	122.80
4	A	619	C	C2-N1-C1'	7.53	127.08	118.80
4	A	709	U	C2-N1-C1'	7.51	126.71	117.70
4	A	1161	C	C6-N1-C2	-7.51	117.30	120.30
9	F	98	LEU	CA-CB-CG	7.47	132.49	115.30
4	A	905	U	N3-C2-O2	-7.45	116.98	122.20
4	A	617	U	C6-N1-C1'	-7.45	110.77	121.20
4	A	1694	C	C6-N1-C2	-7.41	117.34	120.30
5	B	5	C	N1-C2-O2	7.40	123.34	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	898	A	C2-N3-C4	7.35	114.28	110.60
5	B	116	C	N1-C2-O2	7.32	123.29	118.90
4	A	1220	C	C6-N1-C1'	-7.31	112.03	120.80
4	A	1597	G	N3-C4-C5	-7.29	124.95	128.60
4	A	1215	U	C2-N1-C1'	7.28	126.44	117.70
4	A	2327	C	N1-C2-O2	7.27	123.26	118.90
5	B	116	C	N3-C2-O2	-7.27	116.81	121.90
4	A	2477	G	C6-C5-N7	-7.26	126.04	130.40
4	A	962	U	C2-N1-C1'	7.25	126.39	117.70
5	B	111	C	N3-C2-O2	-7.24	116.83	121.90
4	A	9	U	N3-C2-O2	-7.24	117.13	122.20
4	A	1847	U	N3-C2-O2	-7.23	117.14	122.20
4	A	1171	C	N1-C2-O2	7.21	123.23	118.90
4	A	1161	C	N1-C2-O2	7.21	123.23	118.90
4	A	2287	C	N1-C2-O2	7.18	123.21	118.90
4	A	3011	C	C6-N1-C2	-7.18	117.43	120.30
4	A	1681	U	C2-N1-C1'	7.18	126.31	117.70
4	A	2647	U	N1-C2-O2	7.15	127.80	122.80
4	A	1567	C	C6-N1-C2	-7.14	117.44	120.30
4	A	1429	C	C6-N1-C2	-7.13	117.45	120.30
4	A	1220	C	C6-N1-C2	-7.09	117.47	120.30
4	A	1170	C	N1-C2-O2	7.05	123.13	118.90
5	B	112	C	C6-N1-C2	-7.04	117.48	120.30
4	A	2180	U	N3-C2-O2	-7.03	117.28	122.20
4	A	472	C	N3-C2-O2	-7.02	116.98	121.90
4	A	709	U	N3-C2-O2	-7.00	117.30	122.20
4	A	949	C	C6-N1-C2	-6.98	117.51	120.30
4	A	1591	U	C2-N1-C1'	6.98	126.07	117.70
4	A	571	A	C2-N3-C4	6.96	114.08	110.60
4	A	2320	C	O4'-C1'-N1	6.96	113.77	108.20
4	A	1210	C	C2-N1-C1'	6.95	126.44	118.80
4	A	2287	C	N3-C2-O2	-6.93	117.05	121.90
4	A	1421	C	C6-N1-C2	-6.92	117.53	120.30
4	A	1534	C	C6-N1-C2	-6.92	117.53	120.30
4	A	2944	U	N1-C2-O2	6.92	127.64	122.80
5	B	72	C	C2-N1-C1'	6.88	126.37	118.80
4	A	1333	C	C2-N1-C1'	6.86	126.35	118.80
4	A	2287	C	C6-N1-C2	-6.84	117.56	120.30
4	A	1239	C	C6-N1-C2	-6.83	117.57	120.30
4	A	2025	C	C6-N1-C1'	-6.82	112.62	120.80
4	A	1477	C	C5-C6-N1	6.81	124.41	121.00
4	A	974	G	P-O3'-C3'	6.81	127.87	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1123	C	C6-N1-C2	-6.80	117.58	120.30
4	A	1292	U	C2-N1-C1'	6.80	125.86	117.70
4	A	2435	U	N3-C2-O2	-6.80	117.44	122.20
19	P	38	LEU	CA-CB-CG	6.79	130.92	115.30
4	A	1224	G	N1-C2-N2	-6.78	110.10	116.20
4	A	2362	C	N1-C2-O2	6.78	122.97	118.90
4	A	619	C	N1-C2-O2	6.78	122.97	118.90
4	A	853	C	C2-N1-C1'	6.76	126.24	118.80
4	A	2321	U	C5-C6-N1	6.76	126.08	122.70
4	A	2647	U	C2-N1-C1'	6.75	125.79	117.70
4	A	1429	C	C5-C6-N1	6.74	124.37	121.00
4	A	9	U	C2-N1-C1'	6.73	125.78	117.70
4	A	1597	G	C4-N9-C1'	6.71	135.23	126.50
5	B	32	C	C6-N1-C2	-6.70	117.62	120.30
4	A	1045	C	C2-N1-C1'	6.70	126.17	118.80
4	A	169	C	C2-N1-C1'	6.70	126.17	118.80
4	A	324	C	C5-C6-N1	6.69	124.34	121.00
4	A	700	U	N3-C2-O2	-6.68	117.53	122.20
5	B	31	C	C2-N1-C1'	6.68	126.15	118.80
4	A	1421	C	C5-C6-N1	6.67	124.34	121.00
4	A	1260	C	C2-N1-C1'	6.67	126.13	118.80
3	4	199	GLY	N-CA-C	-6.66	96.44	113.10
4	A	1210	C	N3-C2-O2	-6.66	117.24	121.90
4	A	2880	U	N1-C2-O2	6.66	127.47	122.80
4	A	2321	U	O5'-P-OP1	-6.66	99.70	105.70
4	A	740	A	O4'-C1'-N9	6.66	113.53	108.20
4	A	102	C	C5-C6-N1	6.64	124.32	121.00
4	A	929	C	C5-C6-N1	6.64	124.32	121.00
5	B	10	G	O4'-C1'-N9	6.64	113.51	108.20
4	A	1535	C	N3-C2-O2	-6.64	117.25	121.90
4	A	2780	C	C6-N1-C2	-6.63	117.65	120.30
4	A	2993	U	N3-C2-O2	-6.63	117.56	122.20
4	A	1597	G	N3-C4-N9	6.63	129.98	126.00
4	A	324	C	C6-N1-C2	-6.62	117.65	120.30
4	A	1681	U	N1-C2-O2	6.61	127.43	122.80
4	A	2375	G	C4-N9-C1'	6.61	135.09	126.50
4	A	2870	C	C6-N1-C2	-6.61	117.66	120.30
4	A	2521	C	N1-C2-O2	6.60	122.86	118.90
4	A	274	C	C2-N1-C1'	6.60	126.06	118.80
4	A	1220	C	C5-C6-N1	6.60	124.30	121.00
4	A	2398	C	C6-N1-C2	-6.57	117.67	120.30
4	A	1587	G	N3-C4-C5	-6.57	125.31	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1441	C	N1-C2-O2	6.57	122.84	118.90
4	A	1535	C	C6-N1-C2	-6.55	117.68	120.30
4	A	1694	C	C2-N1-C1'	6.54	125.99	118.80
4	A	2325	U	N3-C2-O2	-6.54	117.62	122.20
4	A	929	C	C6-N1-C2	-6.53	117.69	120.30
4	A	2005	C	C6-N1-C2	-6.53	117.69	120.30
4	A	709	U	N1-C2-O2	6.52	127.36	122.80
4	A	2267	C	C6-N1-C2	-6.52	117.69	120.30
4	A	1638	C	N1-C2-O2	6.51	122.81	118.90
4	A	2296	C	C6-N1-C2	-6.51	117.70	120.30
4	A	2375	G	N9-C4-C5	-6.51	102.80	105.40
4	A	2327	C	N3-C2-O2	-6.50	117.35	121.90
4	A	1429	C	N1-C2-O2	6.48	122.79	118.90
4	A	2870	C	C5-C6-N1	6.48	124.24	121.00
4	A	2697	U	O4'-C1'-N1	6.47	113.38	108.20
4	A	1694	C	C5-C6-N1	6.46	124.23	121.00
4	A	3011	C	C5-C6-N1	6.46	124.23	121.00
5	B	6	G	N3-C4-N9	6.45	129.87	126.00
4	A	547	U	N1-C2-O2	6.44	127.31	122.80
4	A	325	U	N3-C2-O2	-6.44	117.69	122.20
5	B	32	C	N3-C2-O2	-6.44	117.39	121.90
4	A	3046	C	C6-N1-C1'	-6.44	113.07	120.80
4	A	325	U	C2-N1-C1'	6.43	125.42	117.70
4	A	1220	C	N1-C2-O2	6.43	122.76	118.90
4	A	2375	G	C8-N9-C1'	-6.42	118.65	127.00
4	A	29	C	C2-N1-C1'	6.41	125.85	118.80
4	A	2345	U	P-O3'-C3'	6.40	127.38	119.70
4	A	1239	C	C5-C6-N1	6.39	124.20	121.00
4	A	191	G	C4-N9-C1'	6.38	134.79	126.50
4	A	325	U	N1-C2-O2	6.36	127.25	122.80
4	A	1260	C	C6-N1-C2	-6.35	117.76	120.30
4	A	3036	C	N1-C2-O2	6.34	122.71	118.90
4	A	619	C	N3-C2-O2	-6.34	117.46	121.90
4	A	1102	G	N3-C4-C5	-6.33	125.44	128.60
4	A	111	U	C2-N1-C1'	6.32	125.29	117.70
4	A	1587	G	C4-N9-C1'	6.30	134.69	126.50
4	A	2232	C	C6-N1-C2	-6.29	117.78	120.30
5	B	31	C	N1-C2-O2	6.28	122.67	118.90
4	A	1567	C	C2-N1-C1'	6.26	125.69	118.80
4	A	277	U	N3-C2-O2	-6.26	117.82	122.20
5	B	7	G	N3-C4-N9	-6.25	122.25	126.00
4	A	1061	G	C4-N9-C1'	6.25	134.62	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1535	C	C2-N1-C1'	6.24	125.67	118.80
4	A	2477	G	N1-C2-N3	6.24	127.65	123.90
4	A	270	U	C2-N1-C1'	6.24	125.19	117.70
4	A	324	C	N3-C2-O2	-6.24	117.53	121.90
4	A	2005	C	C5-C6-N1	6.23	124.12	121.00
4	A	2430	C	C2-N1-C1'	6.21	125.64	118.80
11	H	75	LEU	CA-CB-CG	6.21	129.59	115.30
4	A	3011	C	C2-N1-C1'	6.20	125.62	118.80
4	A	1206	A	OP2-P-O3'	6.18	118.79	105.20
4	A	2477	G	N7-C8-N9	6.18	116.19	113.10
4	A	2880	U	N3-C2-O2	-6.17	117.88	122.20
4	A	197	C	C5-C6-N1	6.17	124.08	121.00
4	A	1617	C	C6-N1-C2	-6.17	117.83	120.30
4	A	288	U	C5-C6-N1	6.16	125.78	122.70
5	B	6	G	C4-N9-C1'	6.16	134.51	126.50
4	A	102	C	N1-C2-O2	6.16	122.59	118.90
4	A	2698	C	N1-C2-O2	6.16	122.59	118.90
4	A	1006	G	N1-C6-O6	-6.14	116.22	119.90
4	A	1448	C	C6-N1-C2	-6.13	117.85	120.30
4	A	2375	G	C4-C5-N7	6.12	113.25	110.80
4	A	2689	C	C6-N1-C2	-6.12	117.85	120.30
4	A	2647	U	N3-C2-O2	-6.12	117.92	122.20
4	A	1225	G	N7-C8-N9	6.11	116.16	113.10
4	A	2295	C	C5-C6-N1	6.11	124.05	121.00
4	A	1638	C	C5-C6-N1	6.10	124.05	121.00
4	A	2779	U	P-O3'-C3'	6.10	127.03	119.70
4	A	2387	U	C6-N1-C1'	-6.10	112.66	121.20
4	A	2699	C	C6-N1-C2	-6.10	117.86	120.30
4	A	1276	G	N3-C4-N9	6.10	129.66	126.00
5	B	88	C	C2-N1-C1'	6.09	125.50	118.80
4	A	2327	C	C6-N1-C2	-6.08	117.87	120.30
4	A	288	U	C6-N1-C2	-6.07	117.36	121.00
4	A	1903	C	C2-N1-C1'	6.07	125.47	118.80
4	A	962	U	N3-C2-O2	-6.05	117.96	122.20
4	A	277	U	N1-C2-O2	6.05	127.04	122.80
4	A	2684	U	N3-C2-O2	-6.05	117.97	122.20
4	A	1681	U	N3-C2-O2	-6.04	117.97	122.20
4	A	2366	C	N3-C2-O2	-6.04	117.67	121.90
4	A	1183	U	C2-N1-C1'	6.04	124.95	117.70
4	A	1276	G	C4-N9-C1'	6.04	134.35	126.50
4	A	2409	U	C2-N1-C1'	6.04	124.94	117.70
5	B	31	C	C6-N1-C2	-6.04	117.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1638	C	C6-N1-C2	-6.03	117.89	120.30
4	A	1171	C	N3-C2-O2	-6.03	117.68	121.90
4	A	454	U	C2-N1-C1'	6.02	124.92	117.70
4	A	2698	C	C2-N1-C1'	6.02	125.42	118.80
4	A	1403	C	C6-N1-C2	-6.01	117.90	120.30
4	A	962	U	N1-C2-O2	6.00	127.00	122.80
4	A	1973	C	C6-N1-C1'	6.00	128.00	120.80
4	A	289	A	C2-N3-C4	6.00	113.60	110.60
4	A	1947	U	P-O3'-C3'	5.97	126.87	119.70
4	A	1531	C	C5-C6-N1	5.97	123.99	121.00
4	A	2477	G	C4-N9-C1'	5.97	134.26	126.50
4	A	2689	C	C5-C6-N1	5.97	123.99	121.00
4	A	999	C	N3-C2-O2	-5.96	117.72	121.90
4	A	1225	G	N3-C2-N2	5.96	124.08	119.90
4	A	964	C	C6-N1-C2	-5.96	117.92	120.30
4	A	1230	G	C5-C6-O6	5.96	132.17	128.60
4	A	2086	U	C2-N1-C1'	5.95	124.84	117.70
4	A	2075	G	O4'-C1'-N9	5.95	112.96	108.20
4	A	1817	C	C5-C6-N1	5.95	123.97	121.00
4	A	1651	C	C6-N1-C2	-5.95	117.92	120.30
4	A	759	G	N3-C4-C5	5.94	131.57	128.60
4	A	845	C	C6-N1-C2	-5.94	117.92	120.30
4	A	2780	C	C5-C6-N1	5.94	123.97	121.00
4	A	2335	G	N3-C4-C5	-5.94	125.63	128.60
4	A	2335	G	N3-C4-N9	5.94	129.56	126.00
4	A	2993	U	N1-C2-O2	5.92	126.95	122.80
4	A	1172	A	O4'-C1'-N9	5.92	112.94	108.20
4	A	1477	C	C6-N1-C2	-5.92	117.93	120.30
4	A	1165	G	C8-N9-C4	-5.92	104.03	106.40
4	A	1170	C	C5-C6-N1	5.92	123.96	121.00
4	A	1123	C	C5-C6-N1	5.91	123.96	121.00
4	A	191	G	C8-N9-C1'	-5.91	119.32	127.00
4	A	630	U	N3-C2-O2	-5.91	118.06	122.20
5	B	6	G	C8-N9-C1'	-5.91	119.32	127.00
4	A	2780	C	N1-C2-O2	5.90	122.44	118.90
4	A	2571	C	C2-N1-C1'	5.89	125.28	118.80
4	A	571	A	N3-C4-C5	-5.89	122.67	126.80
4	A	1978	C	N1-C2-O2	5.89	122.44	118.90
4	A	1816	C	C2-N1-C1'	5.89	125.28	118.80
4	A	1817	C	C6-N1-C2	-5.88	117.95	120.30
4	A	1123	C	C2-N1-C1'	5.88	125.27	118.80
4	A	357	U	P-O3'-C3'	5.88	126.75	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1030	C	C2-N1-C1'	5.88	125.27	118.80
4	A	2430	C	C6-N1-C2	-5.88	117.95	120.30
5	B	72	C	N1-C2-O2	5.88	122.43	118.90
4	A	1082	C	C5-C6-N1	5.87	123.93	121.00
4	A	1448	C	C5-C6-N1	5.87	123.94	121.00
4	A	2243	C	C2-N1-C1'	5.87	125.26	118.80
4	A	2455	C	C6-N1-C2	-5.87	117.95	120.30
4	A	1458	G	C4-N9-C1'	5.86	134.12	126.50
4	A	2688	C	C5-C6-N1	5.86	123.93	121.00
5	B	8	C	C5-C6-N1	5.86	123.93	121.00
4	A	407	C	C6-N1-C2	-5.86	117.96	120.30
4	A	2477	G	N1-C2-N2	-5.85	110.93	116.20
4	A	1608	U	C6-N1-C2	-5.85	117.49	121.00
4	A	1816	C	C6-N1-C2	-5.84	117.96	120.30
5	B	10	G	N7-C8-N9	5.84	116.02	113.10
4	A	29	C	C5-C6-N1	5.84	123.92	121.00
4	A	2077	C	C6-N1-C2	-5.84	117.97	120.30
5	B	72	C	C5-C6-N1	5.84	123.92	121.00
4	A	905	U	C6-N1-C1'	-5.83	113.03	121.20
4	A	599	G	O4'-C1'-N9	5.83	112.86	108.20
4	A	1767	U	C5-C6-N1	5.83	125.61	122.70
4	A	472	C	C6-N1-C2	-5.83	117.97	120.30
4	A	234	U	N3-C2-O2	-5.82	118.12	122.20
4	A	1597	G	C2-N3-C4	5.82	114.81	111.90
4	A	205	U	N1-C2-O2	5.81	126.86	122.80
4	A	547	U	C2-N1-C1'	5.81	124.67	117.70
4	A	1678	U	C2-N1-C1'	5.80	124.66	117.70
4	A	1816	C	C5-C6-N1	5.80	123.90	121.00
4	A	205	U	N3-C2-O2	-5.79	118.15	122.20
4	A	139	U	C2-N1-C1'	5.79	124.64	117.70
4	A	3015	C	C2-N1-C1'	5.79	125.16	118.80
4	A	1276	G	C8-N9-C1'	-5.78	119.48	127.00
4	A	1333	C	C5-C6-N1	5.78	123.89	121.00
4	A	2086	U	N1-C2-O2	5.78	126.85	122.80
4	A	9	U	N1-C2-O2	5.78	126.84	122.80
4	A	237	C	N1-C2-O2	5.78	122.37	118.90
4	A	336	C	P-O3'-C3'	5.75	126.61	119.70
3	4	294	PRO	N-CA-C	5.75	127.06	112.10
5	B	5	C	C2-N3-C4	5.75	122.77	119.90
5	B	56	C	C6-N1-C2	-5.74	118.00	120.30
4	A	1991	C	C6-N1-C2	-5.73	118.01	120.30
4	A	2423	C	C6-N1-C2	-5.73	118.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	32	C	C6-N1-C1'	-5.73	113.93	120.80
4	A	2295	C	C6-N1-C2	-5.73	118.01	120.30
4	A	2934	C	C6-N1-C2	-5.72	118.01	120.30
4	A	2085	C	C2-N1-C1'	5.72	125.09	118.80
4	A	2409	U	N1-C2-O2	5.72	126.80	122.80
5	B	114	A	O4'-C1'-N9	5.72	112.78	108.20
4	A	1467	U	N3-C2-O2	-5.71	118.20	122.20
4	A	2230	C	C5-C6-N1	5.71	123.86	121.00
5	B	7	G	N3-C4-C5	5.71	131.46	128.60
4	A	1428	U	C6-N1-C1'	-5.71	113.21	121.20
4	A	1638	C	C6-N1-C1'	-5.70	113.96	120.80
4	A	2521	C	N3-C2-O2	-5.70	117.91	121.90
5	B	18	C	C2-N1-C1'	5.70	125.07	118.80
4	A	1045	C	N3-C2-O2	-5.70	117.91	121.90
4	A	1531	C	C6-N1-C2	-5.69	118.02	120.30
4	A	1579	C	C5-C6-N1	5.69	123.84	121.00
4	A	2287	C	C2-N1-C1'	5.69	125.06	118.80
4	A	2979	C	N1-C2-O2	5.69	122.31	118.90
4	A	1224	G	N9-C4-C5	-5.68	103.13	105.40
4	A	1534	C	C6-N1-C1'	-5.68	113.98	120.80
4	A	2913	U	N3-C2-O2	-5.67	118.23	122.20
4	A	630	U	N1-C2-O2	5.67	126.77	122.80
4	A	2322	C	C6-N1-C2	-5.67	118.03	120.30
4	A	3037	C	C6-N1-C2	-5.67	118.03	120.30
4	A	438	U	N3-C2-O2	-5.67	118.23	122.20
4	A	2325	U	N1-C2-O2	5.67	126.77	122.80
4	A	1549	G	O4'-C1'-N9	5.66	112.73	108.20
4	A	547	U	N3-C2-O2	-5.65	118.24	122.20
4	A	454	U	C5-C6-N1	5.65	125.53	122.70
5	B	5	C	C2-N1-C1'	5.65	125.02	118.80
4	A	91	C	C2-N1-C1'	5.65	125.01	118.80
4	A	974	G	OP2-P-O3'	5.65	117.62	105.20
4	A	1996	U	C2-N1-C1'	5.64	124.47	117.70
4	A	1061	G	C8-N9-C1'	-5.64	119.66	127.00
4	A	1597	G	C8-N9-C1'	-5.64	119.67	127.00
4	A	2117	C	C2-N1-C1'	5.63	125.00	118.80
4	A	2979	C	C2-N1-C1'	5.63	124.99	118.80
4	A	1429	C	C6-N1-C1'	-5.62	114.06	120.80
4	A	2409	U	N3-C2-O2	-5.62	118.27	122.20
4	A	514	C	C6-N1-C2	-5.61	118.06	120.30
4	A	1610	C	C2-N1-C1'	5.61	124.97	118.80
5	B	65	C	C2-N1-C1'	5.61	124.97	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	274	C	C6-N1-C2	-5.60	118.06	120.30
4	A	1183	U	N3-C2-O2	-5.60	118.28	122.20
4	A	2366	C	N1-C2-O2	5.60	122.26	118.90
5	B	72	C	C6-N1-C2	-5.59	118.06	120.30
4	A	975	U	C2-N1-C1'	5.59	124.41	117.70
4	A	2975	G	N1-C6-O6	-5.59	116.55	119.90
4	A	1874	C	C6-N1-C2	-5.58	118.07	120.30
4	A	2698	C	N3-C2-O2	-5.57	118.00	121.90
4	A	2684	U	N1-C2-O2	5.57	126.70	122.80
4	A	2869	C	C2-N1-C1'	5.57	124.92	118.80
4	A	97	U	P-O3'-C3'	5.56	126.37	119.70
4	A	681	C	C5-C6-N1	5.56	123.78	121.00
4	A	277	U	C2-N1-C1'	5.56	124.37	117.70
4	A	1292	U	P-O3'-C3'	5.56	126.37	119.70
4	A	3045	C	C6-N1-C2	-5.54	118.08	120.30
4	A	1579	C	N1-C2-O2	5.54	122.22	118.90
4	A	191	G	O4'-C1'-N9	5.54	112.63	108.20
4	A	1214	A	O4'-C1'-N9	5.54	112.63	108.20
4	A	1333	C	N1-C2-O2	5.53	122.22	118.90
4	A	237	C	C2-N1-C1'	5.53	124.88	118.80
4	A	1224	G	C8-N9-C1'	-5.53	119.82	127.00
4	A	2402	C	C6-N1-C1'	-5.52	114.17	120.80
4	A	1386	G	C8-N9-C4	-5.52	104.19	106.40
4	A	2532	G	C4-N9-C1'	5.52	133.67	126.50
5	B	9	G	C5-N7-C8	-5.51	101.54	104.30
4	A	3036	C	N3-C2-O2	-5.50	118.05	121.90
4	A	2689	C	N1-C2-O2	5.50	122.20	118.90
4	A	288	U	C2-N1-C1'	5.50	124.29	117.70
4	A	2656	A	P-O3'-C3'	5.49	126.29	119.70
4	A	1082	C	C6-N1-C2	-5.49	118.11	120.30
4	A	1170	C	C6-N1-C2	-5.49	118.11	120.30
4	A	2467	U	N3-C2-O2	-5.49	118.36	122.20
4	A	571	A	N3-C4-N9	5.48	131.79	127.40
4	A	1587	G	N3-C4-N9	5.48	129.29	126.00
4	A	1610	C	N1-C2-O2	5.48	122.19	118.90
5	B	8	C	C6-N1-C2	-5.48	118.11	120.30
4	A	29	C	N1-C2-O2	5.47	122.18	118.90
4	A	1182	C	C5-C6-N1	5.47	123.73	121.00
4	A	43	C	C2-N1-C1'	5.47	124.81	118.80
5	B	32	C	C5-C6-N1	5.47	123.73	121.00
4	A	1260	C	N3-C2-O2	-5.46	118.08	121.90
5	B	111	C	C6-N1-C2	-5.46	118.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	842	A	P-O3'-C3'	5.46	126.26	119.70
5	B	66	C	N1-C2-O2	5.46	122.18	118.90
4	A	1554	U	N3-C2-O2	-5.46	118.38	122.20
4	A	1204	A	C4-N9-C1'	5.46	136.12	126.30
4	A	1235	U	OP2-P-O3'	5.46	117.20	105.20
4	A	2165	C	N1-C2-O2	5.45	122.17	118.90
4	A	2438	C	N1-C2-O2	5.45	122.17	118.90
4	A	2688	C	C2-N1-C1'	5.45	124.80	118.80
4	A	169	C	C6-N1-C2	-5.45	118.12	120.30
4	A	1571	C	C2-N1-C1'	5.44	124.79	118.80
4	A	1230	G	P-O3'-C3'	5.43	126.22	119.70
4	A	549	C	C6-N1-C2	-5.42	118.13	120.30
4	A	2269	C	C6-N1-C2	-5.42	118.13	120.30
4	A	2944	U	C2-N1-C1'	5.42	124.20	117.70
4	A	930	C	C6-N1-C2	-5.41	118.14	120.30
8	E	148	LEU	CA-CB-CG	5.41	127.75	115.30
4	A	1117	U	N3-C2-O2	-5.41	118.42	122.20
4	A	1993	G	C4-N9-C1'	5.41	133.53	126.50
4	A	2435	U	C2-N1-C1'	5.40	124.19	117.70
4	A	2155	U	C2-N1-C1'	5.40	124.18	117.70
4	A	1183	U	N1-C2-O2	5.40	126.58	122.80
4	A	1901	C	C5-C6-N1	5.40	123.70	121.00
4	A	1947	U	C6-N1-C1'	-5.40	113.64	121.20
4	A	1171	C	C6-N1-C2	-5.40	118.14	120.30
4	A	1927	C	C2-N1-C1'	5.40	124.74	118.80
5	B	113	G	O4'-C1'-N9	5.40	112.52	108.20
4	A	981	U	P-O3'-C3'	5.39	126.17	119.70
4	A	1276	G	C6-C5-N7	-5.39	127.17	130.40
4	A	237	C	C6-N1-C2	-5.38	118.15	120.30
4	A	617	U	C5-C6-N1	5.38	125.39	122.70
4	A	1554	U	N1-C2-O2	5.38	126.57	122.80
5	B	116	C	C6-N1-C2	-5.38	118.15	120.30
5	B	56	C	N3-C2-O2	-5.37	118.14	121.90
4	A	2209	C	C5-C6-N1	5.37	123.69	121.00
4	A	199	U	N3-C2-O2	-5.36	118.45	122.20
4	A	3036	C	C6-N1-C2	-5.36	118.16	120.30
4	A	921	C	C6-N1-C2	-5.36	118.16	120.30
4	A	2375	G	C5-C6-O6	-5.36	125.39	128.60
4	A	1909	C	C6-N1-C2	-5.35	118.16	120.30
4	A	2320	C	P-O3'-C3'	5.34	126.11	119.70
4	A	199	U	N1-C2-O2	5.34	126.54	122.80
4	A	2418	U	N1-C2-O2	5.34	126.54	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1458	G	C8-N9-C1'	-5.34	120.06	127.00
4	A	963	U	N3-C2-O2	-5.33	118.47	122.20
4	A	1697	U	N3-C2-O2	-5.33	118.47	122.20
4	A	2117	C	C6-N1-C2	-5.33	118.17	120.30
4	A	619	C	C6-N1-C1'	-5.33	114.40	120.80
4	A	383	U	C6-N1-C1'	-5.33	113.74	121.20
4	A	2644	C	C6-N1-C2	-5.33	118.17	120.30
4	A	1292	U	C6-N1-C2	-5.32	117.81	121.00
4	A	2688	C	C6-N1-C2	-5.32	118.17	120.30
4	A	237	C	C5-C6-N1	5.31	123.66	121.00
4	A	2869	C	N3-C2-O2	-5.31	118.18	121.90
5	B	31	C	C5-C6-N1	5.31	123.65	121.00
9	F	124	LEU	CA-CB-CG	5.31	127.50	115.30
4	A	1124	C	C6-N1-C2	-5.30	118.18	120.30
4	A	1509	U	C6-N1-C1'	5.30	128.63	121.20
4	A	1978	C	N3-C2-O2	-5.30	118.19	121.90
4	A	1467	U	N1-C2-O2	5.30	126.51	122.80
4	A	2472	C	C5-C6-N1	5.29	123.65	121.00
5	B	113	G	C4-N9-C1'	-5.29	119.62	126.50
4	A	851	C	C5-C6-N1	5.29	123.64	121.00
4	A	2085	C	C5-C6-N1	5.28	123.64	121.00
5	B	9	G	N7-C8-N9	5.28	115.74	113.10
4	A	1382	U	C2-N1-C1'	5.28	124.03	117.70
4	A	523	U	N1-C2-O2	5.28	126.49	122.80
4	A	1298	C	C5-C6-N1	5.27	123.64	121.00
4	A	1579	C	C6-N1-C2	-5.27	118.19	120.30
4	A	910	C	C6-N1-C2	-5.27	118.19	120.30
4	A	3036	C	C2-N1-C1'	5.27	124.60	118.80
5	B	31	C	N3-C2-O2	-5.27	118.21	121.90
4	A	514	C	C5-C6-N1	5.27	123.64	121.00
4	A	2689	C	C6-N1-C1'	-5.27	114.48	120.80
4	A	2923	C	C5-C6-N1	5.27	123.63	121.00
4	A	845	C	C5-C6-N1	5.27	123.63	121.00
4	A	2269	C	C5-C6-N1	5.26	123.63	121.00
4	A	1199	U	P-O3'-C3'	5.26	126.01	119.70
4	A	2319	G	N3-C4-N9	5.26	129.16	126.00
4	A	2380	G	OP1-P-O3'	5.26	116.77	105.20
4	A	2880	U	C5-C6-N1	5.26	125.33	122.70
5	B	112	C	C5-C6-N1	5.25	123.63	121.00
4	A	1798	U	N1-C2-O2	5.25	126.47	122.80
4	A	2397	C	P-O3'-C3'	5.25	126.00	119.70
4	A	2585	U	N3-C2-O2	-5.25	118.53	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1298	C	C6-N1-C2	-5.24	118.20	120.30
5	B	10	G	P-O3'-C3'	5.24	125.99	119.70
4	A	1202	A	C4-N9-C1'	5.24	135.72	126.30
4	A	1904	C	C2-N1-C1'	5.24	124.56	118.80
4	A	1057	C	C6-N1-C2	-5.23	118.21	120.30
4	A	1900	C	C6-N1-C2	-5.23	118.21	120.30
4	A	2322	C	C5-C6-N1	5.23	123.61	121.00
4	A	1260	C	N1-C2-O2	5.23	122.04	118.90
4	A	1531	C	C2-N1-C1'	5.23	124.55	118.80
20	Q	15	ASP	CB-CG-OD1	5.23	123.00	118.30
4	A	111	U	C5-C6-N1	5.22	125.31	122.70
4	A	1102	G	C4-N9-C1'	5.22	133.29	126.50
4	A	2472	C	C2-N1-C1'	5.22	124.54	118.80
4	A	1947	U	C5-C6-N1	5.21	125.31	122.70
4	A	328	C	N1-C2-O2	5.21	122.03	118.90
4	A	1215	U	N1-C2-O2	5.21	126.45	122.80
4	A	853	C	C6-N1-C2	-5.21	118.22	120.30
4	A	3074	C	C5-C6-N1	5.21	123.60	121.00
4	A	1798	U	N3-C2-O2	-5.20	118.56	122.20
4	A	1973	C	C6-N1-C2	-5.20	118.22	120.30
4	A	2362	C	C5-C6-N1	5.19	123.60	121.00
4	A	1939	U	C5-C6-N1	5.19	125.30	122.70
4	A	2335	G	C4-N9-C1'	5.19	133.25	126.50
4	A	1409	C	C6-N1-C2	-5.19	118.22	120.30
4	A	1579	C	C6-N1-C1'	-5.19	114.58	120.80
4	A	2780	C	C2-N1-C1'	5.19	124.51	118.80
4	A	2430	C	C5-C6-N1	5.19	123.59	121.00
4	A	2532	G	N3-C4-N9	5.19	129.11	126.00
4	A	898	A	C4-N9-C1'	5.18	135.62	126.30
4	A	2477	G	C2-N3-C4	-5.18	109.31	111.90
4	A	1441	C	C2-N3-C4	5.17	122.49	119.90
4	A	543	U	C6-N1-C1'	-5.17	113.96	121.20
4	A	2939	C	C5-C6-N1	5.17	123.58	121.00
4	A	1622	G	N3-C4-C5	-5.16	126.02	128.60
4	A	43	C	C6-N1-C2	-5.16	118.24	120.30
4	A	546	G	O4'-C1'-N9	5.16	112.33	108.20
4	A	3037	C	C2-N1-C1'	5.16	124.47	118.80
4	A	1548	C	C5-C6-N1	5.16	123.58	121.00
4	A	1016	C	N1-C2-O2	5.15	121.99	118.90
4	A	1403	C	C6-N1-C1'	-5.15	114.62	120.80
4	A	1610	C	C6-N1-C2	-5.15	118.24	120.30
5	B	4	A	C8-N9-C4	-5.15	103.74	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1045	C	C6-N1-C2	-5.14	118.24	120.30
4	A	1224	G	C4-N9-C1'	5.14	133.19	126.50
4	A	154	C	C6-N1-C2	-5.14	118.24	120.30
4	A	197	C	C2-N1-C1'	5.14	124.46	118.80
8	E	122	ASP	CB-CG-OD2	5.14	122.93	118.30
4	A	2585	U	N1-C2-O2	5.14	126.40	122.80
4	A	1513	C	C2-N1-C1'	5.14	124.45	118.80
4	A	742	G	N3-C4-N9	5.13	129.08	126.00
4	A	2592	C	C6-N1-C2	-5.13	118.25	120.30
4	A	1640	A	C4-N9-C1'	5.13	135.53	126.30
4	A	853	C	N1-C2-O2	5.12	121.97	118.90
4	A	999	C	C6-N1-C2	-5.12	118.25	120.30
4	A	1441	C	C5-C6-N1	5.12	123.56	121.00
4	A	2022	U	N3-C2-O2	-5.12	118.62	122.20
4	A	2260	C	N1-C2-O2	5.12	121.97	118.90
4	A	498	G	C6-C5-N7	-5.12	127.33	130.40
4	A	1198	C	C6-N1-C2	-5.11	118.25	120.30
4	A	1874	C	C5-C6-N1	5.11	123.56	121.00
4	A	2418	U	N3-C2-O2	-5.11	118.62	122.20
4	A	709	U	C6-N1-C1'	-5.11	114.05	121.20
4	A	514	C	C2-N1-C1'	5.11	124.42	118.80
4	A	1521	C	C6-N1-C2	-5.10	118.26	120.30
4	A	2699	C	C5-C6-N1	5.10	123.55	121.00
4	A	2880	U	C2-N1-C1'	5.10	123.82	117.70
4	A	2884	A	C2-N3-C4	5.10	113.15	110.60
4	A	7	U	N1-C2-O2	5.10	126.37	122.80
4	A	571	A	O4'-C1'-N9	5.09	112.28	108.20
4	A	2218	C	C6-N1-C2	-5.09	118.26	120.30
4	A	472	C	C6-N1-C1'	-5.09	114.69	120.80
4	A	1001	C	C5-C6-N1	5.09	123.55	121.00
4	A	2571	C	N1-C2-O2	5.09	121.95	118.90
4	A	1171	C	C2-N3-C4	5.08	122.44	119.90
4	A	2761	U	N3-C2-O2	-5.08	118.64	122.20
4	A	757	G	O4'-C1'-N9	5.08	112.26	108.20
4	A	205	U	C2-N1-C1'	5.07	123.79	117.70
4	A	3046	C	O4'-C1'-N1	5.07	112.26	108.20
4	A	2514	G	N3-C4-N9	5.07	129.04	126.00
4	A	142	C	C6-N1-C2	-5.07	118.27	120.30
4	A	952	C	C6-N1-C2	-5.07	118.27	120.30
4	A	2328	G	P-O3'-C3'	5.07	125.78	119.70
4	A	3023	G	C8-N9-C4	-5.06	104.38	106.40
4	A	1225	G	C5-N7-C8	-5.06	101.77	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2289	C	C5-C6-N1	5.06	123.53	121.00
4	A	1045	C	N1-C2-O2	5.05	121.93	118.90
4	A	2155	U	N3-C2-O2	-5.05	118.66	122.20
4	A	2418	U	C2-N1-C1'	5.05	123.76	117.70
4	A	1102	G	N3-C4-N9	5.05	129.03	126.00
4	A	1460	C	C2-N1-C1'	5.05	124.35	118.80
4	A	1618	C	C6-N1-C2	-5.05	118.28	120.30
4	A	467	C	C6-N1-C2	-5.04	118.28	120.30
4	A	1382	U	N3-C2-O2	-5.04	118.67	122.20
4	A	2633	G	N3-C4-N9	5.04	129.03	126.00
5	B	38	C	N1-C2-O2	5.04	121.92	118.90
4	A	1893	C	C5-C6-N1	5.04	123.52	121.00
4	A	1610	C	N3-C2-O2	-5.04	118.37	121.90
3	4	267	GLY	N-CA-C	-5.04	100.51	113.10
5	B	111	C	N1-C2-O2	5.04	121.92	118.90
4	A	1887	A	C2-N3-C4	5.03	113.12	110.60
4	A	2077	C	C5-C6-N1	5.03	123.52	121.00
4	A	2939	C	C6-N1-C2	-5.03	118.29	120.30
4	A	2249	G	N3-C4-N9	5.03	129.02	126.00
4	A	281	C	C6-N1-C2	-5.03	118.29	120.30
4	A	630	U	C2-N1-C1'	5.02	123.73	117.70
4	A	2698	C	C6-N1-C2	-5.02	118.29	120.30
4	A	2086	U	C5-C6-N1	5.02	125.21	122.70
4	A	2267	C	C5-C6-N1	5.01	123.51	121.00
4	A	366	G	N3-C4-N9	5.01	129.00	126.00
4	A	2132	U	N3-C2-O2	-5.01	118.69	122.20
4	A	1697	U	C2-N1-C1'	5.01	123.71	117.70
4	A	1993	G	C8-N9-C1'	-5.01	120.49	127.00
5	B	10	G	OP1-P-O3'	5.01	116.21	105.20
4	A	836	G	C4-N9-C1'	5.00	133.01	126.50
4	A	3016	C	N1-C2-O2	5.00	121.90	118.90
4	A	1034	U	N1-C2-O2	5.00	126.30	122.80

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	F	68	THR	Peptide
10	G	46	ALA	Peptide
10	G	52	VAL	Peptide
11	H	137	HIS	Peptide
12	I	52	ALA	Peptide

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Mol	Chain	Res	Type	Group
12	I	53	LYS	Peptide
13	J	54	ASN	Peptide
18	O	57	LYS	Peptide
19	P	102	PHE	Peptide
19	P	25	LEU	Peptide
19	P	5	PRO	Peptide
19	P	80	HIS	Peptide
26	W	118	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	474	0	500	2	0
2	3	189	0	205	3	0
3	4	3228	0	3284	515	0
4	A	66981	0	33700	293	0
5	B	2522	0	1285	20	0
6	C	2110	0	2165	28	0
7	D	1587	0	1630	12	0
8	E	1569	0	1607	13	0
9	F	1445	0	1476	23	0
10	G	1348	0	1399	20	0
11	H	1018	0	988	19	0
12	I	918	0	959	29	0
13	J	990	0	1021	26	0
14	K	1130	0	1167	8	0
15	L	938	0	1000	7	0
16	M	1078	0	1151	8	0
17	N	1092	0	1128	9	0
18	O	928	0	972	5	0
19	P	956	0	991	42	0
20	Q	907	0	938	8	0
21	R	988	0	1038	11	0
22	S	754	0	802	7	0
23	T	873	0	909	8	0
24	U	756	0	802	2	0
25	V	732	0	782	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	W	1428	0	1443	11	0
27	X	586	0	601	7	0
28	Y	470	0	482	4	0
29	Z	531	0	541	3	0
30	b	423	0	463	0	0
31	c	405	0	411	0	0
32	d	377	0	411	0	0
33	e	502	0	541	0	0
34	f	299	0	324	0	0
35	g	364	0	352	0	0
36	4	32	0	14	15	0
All	All	100928	0	67482	1038	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 7.

All (1038) 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)
3:4:445:THR:CG2	3:4:450:ARG:HB2	1.86	1.06
3:4:202:GLY:HA3	4:A:2676:C:C4'	1.86	1.05
3:4:354:VAL:HG11	3:4:361:PRO:HG3	1.38	1.04
3:4:426:ARG:HG3	3:4:429:LEU:HB2	1.38	1.04
3:4:85:LEU:HD11	3:4:106:LEU:HD21	1.40	1.02
3:4:261:LEU:HD11	3:4:392:VAL:HG11	1.40	1.00
3:4:202:GLY:HA3	4:A:2676:C:H4'	1.40	0.99
3:4:102:LYS:HG2	4:A:2132:U:H5'	1.43	0.98
3:4:85:LEU:CD1	3:4:106:LEU:HD21	1.95	0.97
3:4:395:ARG:HH21	36:4:501:GCP:C2	1.79	0.96
3:4:288:GLU:HG3	3:4:292:GLY:HA2	1.46	0.94
3:4:288:GLU:CG	3:4:292:GLY:HA2	1.97	0.94
3:4:177:ARG:HA	3:4:183:MET:SD	2.08	0.94
3:4:48:ARG:HB3	3:4:115:ALA:HA	1.50	0.93
3:4:250:ILE:CD1	3:4:258:LYS:HA	1.98	0.93
3:4:373:ALA:CB	36:4:501:GCP:HN1	1.82	0.92
4:A:1209:G:H1	4:A:1219:U:H3	1.18	0.91
3:4:42:ARG:HH12	3:4:44:LEU:HB2	1.35	0.91
3:4:181:GLU:HA	3:4:184:SER:CB	2.00	0.90
3:4:445:THR:HG23	3:4:450:ARG:HB2	1.50	0.90
4:A:2329:G:H1	4:A:2406:U:H3	1.17	0.90
3:4:173:LEU:HD13	3:4:215:ILE:HG21	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:379:LEU:HG	3:4:383:ARG:HD2	1.55	0.88
3:4:187:ALA:HA	4:A:2826:A:C5	2.08	0.88
3:4:354:VAL:HG13	3:4:359:ILE:HG13	1.56	0.87
3:4:181:GLU:HA	3:4:184:SER:HB2	1.53	0.87
3:4:186:GLN:HB3	3:4:207:LYS:HZ3	1.37	0.87
3:4:384:ARG:HG2	3:4:385:ALA:N	1.90	0.87
3:4:227:ARG:NE	3:4:227:ARG:HA	1.90	0.85
3:4:286:ARG:HB2	4:A:2697:U:O2'	1.76	0.85
3:4:434:HIS:HB3	4:A:1185:A:H1'	1.59	0.85
3:4:426:ARG:HA	3:4:429:LEU:HD23	1.56	0.85
3:4:383:ARG:HH21	3:4:391:PHE:HE1	1.24	0.85
19:P:50:GLN:HA	19:P:63:ALA:HB3	1.59	0.84
3:4:82:LEU:HD13	3:4:113:THR:HB	1.59	0.84
3:4:371:ILE:HA	3:4:374:ALA:HB2	1.60	0.83
3:4:271:LEU:HD22	3:4:278:ALA:HB1	1.61	0.83
3:4:350:ILE:O	3:4:353:VAL:HG22	1.79	0.82
3:4:373:ALA:HB3	36:4:501:GCP:HN1	1.39	0.82
3:4:432:ARG:HB3	3:4:436:ASP:HB2	1.61	0.82
3:4:85:LEU:HD21	3:4:106:LEU:CD1	2.09	0.82
3:4:228:ASP:O	3:4:231:LYS:HG2	1.80	0.82
3:4:46:LEU:HD12	3:4:117:THR:CG2	2.09	0.82
3:4:294:PRO:HB3	3:4:296:VAL:HG23	1.62	0.81
3:4:445:THR:HG21	3:4:450:ARG:HB2	1.61	0.81
3:4:250:ILE:HD11	3:4:258:LYS:HA	1.64	0.80
3:4:326:ASP:HB3	3:4:412:GLU:OE1	1.81	0.80
3:4:461:ALA:HB3	3:4:463:LEU:HD13	1.62	0.80
3:4:187:ALA:HA	4:A:2826:A:C4	2.16	0.80
3:4:253:TYR:HE1	3:4:332:VAL:HG12	1.45	0.80
3:4:227:ARG:HA	3:4:227:ARG:HE	1.46	0.79
3:4:250:ILE:HD13	3:4:258:LYS:HA	1.63	0.79
3:4:251:VAL:HG22	3:4:252:GLY:H	1.47	0.79
4:A:2140:A:H5'	4:A:2141:U:C5	2.18	0.79
4:A:2367:G:N2	4:A:2370:A:C5	2.50	0.79
3:4:49:VAL:HG12	3:4:117:THR:OG1	1.83	0.79
3:4:294:PRO:O	3:4:295:PHE:C	2.19	0.79
3:4:327:LEU:C	3:4:328:LEU:HD12	2.04	0.78
3:4:293:ARG:HH22	3:4:414:THR:HA	1.47	0.78
3:4:372:ASP:C	3:4:374:ALA:H	1.86	0.78
3:4:395:ARG:NH2	36:4:501:GCP:N3	2.30	0.78
3:4:420:VAL:HA	3:4:466:TYR:HD1	1.47	0.78
3:4:426:ARG:HE	3:4:430:VAL:HG13	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1566:A:H61	4:A:1606:G:N2	1.83	0.77
3:4:271:LEU:CD2	3:4:278:ALA:HB1	2.15	0.76
4:A:2367:G:C2	4:A:2370:A:N7	2.53	0.76
3:4:42:ARG:NH1	3:4:44:LEU:HB2	1.99	0.76
3:4:107:ARG:O	3:4:110:VAL:HG12	1.84	0.76
3:4:381:GLN:O	3:4:384:ARG:HD3	1.86	0.76
3:4:420:VAL:HG22	3:4:421:THR:N	2.02	0.75
3:4:456:PRO:HB2	3:4:459:LEU:HD23	1.69	0.75
3:4:382:LEU:HB3	3:4:386:LEU:HD12	1.68	0.75
12:I:37:ALA:O	12:I:41:ARG:HB3	1.87	0.74
3:4:371:ILE:HG22	3:4:372:ASP:H	1.52	0.74
3:4:344:ASN:O	3:4:348:THR:HG23	1.86	0.74
3:4:250:ILE:HG22	3:4:298:THR:O	1.88	0.74
3:4:257:GLY:O	36:4:501:GCP:O3A	2.05	0.74
3:4:443:GLU:HG2	3:4:452:LYS:HD3	1.69	0.73
3:4:366:LEU:HD11	3:4:387:PRO:HD2	1.69	0.73
3:4:173:LEU:HD13	3:4:215:ILE:CG2	2.19	0.73
3:4:379:LEU:O	3:4:383:ARG:HG3	1.88	0.72
3:4:223:ARG:HA	3:4:226:ILE:HD11	1.71	0.72
3:4:420:VAL:HG22	3:4:421:THR:H	1.52	0.72
3:4:443:GLU:HG2	3:4:452:LYS:CD	2.18	0.72
3:4:300:THR:HB	3:4:318:THR:HG23	1.70	0.72
3:4:395:ARG:HG2	3:4:396:THR:H	1.54	0.72
3:4:45:ARG:O	3:4:46:LEU:HD13	1.88	0.72
3:4:288:GLU:CB	3:4:292:GLY:HA2	2.19	0.72
3:4:383:ARG:HB3	3:4:383:ARG:NH1	2.03	0.72
3:4:339:PRO:HG2	3:4:382:LEU:HD21	1.72	0.72
3:4:147:ILE:HD11	3:4:151:PHE:CE2	2.24	0.72
3:4:422:ILE:HG23	3:4:429:LEU:HG	1.71	0.72
19:P:42:ARG:HH11	19:P:109:TYR:H	1.38	0.72
3:4:153:GLN:HG3	3:4:154:HIS:HD2	1.56	0.71
3:4:424:TYR:CZ	3:4:447:ALA:HA	2.24	0.71
3:4:251:VAL:HG22	3:4:252:GLY:N	2.04	0.71
3:4:87:GLN:HG3	4:A:2133:G:H5”	1.71	0.71
3:4:213:ARG:O	3:4:217:GLU:HG3	1.90	0.71
3:4:288:GLU:HG3	3:4:292:GLY:CA	2.20	0.71
3:4:366:LEU:HD23	3:4:366:LEU:H	1.56	0.71
3:4:87:GLN:NE2	4:A:2133:G:H8	1.89	0.70
3:4:102:LYS:O	3:4:106:LEU:HD23	1.90	0.70
3:4:181:GLU:HA	3:4:184:SER:HB3	1.73	0.70
4:A:1566:A:N6	4:A:1606:G:H21	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1158:U:H3	4:A:1232:G:H1	1.37	0.70
3:4:199:GLY:C	3:4:201:ARG:H	1.94	0.70
19:P:73:ILE:HG13	19:P:75:GLY:H	1.56	0.70
3:4:102:LYS:HD3	4:A:2133:G:O5'	1.91	0.70
3:4:426:ARG:C	3:4:428:ASP:H	1.93	0.70
3:4:45:ARG:C	3:4:46:LEU:HD22	2.11	0.70
3:4:50:VAL:CG2	3:4:118:VAL:HG22	2.22	0.69
3:4:373:ALA:HB3	36:4:501:GCP:N1	2.08	0.69
3:4:263:ASN:HD21	3:4:270:VAL:H	1.41	0.69
3:4:147:ILE:HG21	3:4:308:PRO:HG3	1.74	0.69
7:D:63:ILE:HG22	7:D:65:PRO:HD2	1.73	0.69
3:4:199:GLY:CA	3:4:201:ARG:HD2	2.23	0.69
3:4:340:LEU:H	3:4:340:LEU:HD22	1.58	0.68
4:A:2413:G:H2'	4:A:2414:G:H8	1.58	0.68
3:4:430:VAL:O	3:4:431:ALA:C	2.31	0.68
5:B:112:C:H3'	5:B:113:G:H4'	1.73	0.68
4:A:365:U:H3	4:A:437:G:H1	1.41	0.68
3:4:260:SER:OG	3:4:394:ALA:HB1	1.94	0.68
3:4:311:LEU:HD23	3:4:312:VAL:H	1.58	0.68
3:4:327:LEU:HD23	3:4:328:LEU:N	2.09	0.68
3:4:46:LEU:HD12	3:4:117:THR:HG21	1.76	0.67
3:4:349:VAL:O	3:4:353:VAL:HG13	1.94	0.67
3:4:371:ILE:HB	3:4:391:PHE:HA	1.75	0.67
3:4:199:GLY:HA2	3:4:201:ARG:CZ	2.24	0.67
3:4:436:ASP:HB3	3:4:439:VAL:HG13	1.76	0.67
3:4:271:LEU:HD23	3:4:273:GLU:H	1.57	0.67
3:4:432:ARG:HA	3:4:435:THR:HG23	1.75	0.67
9:F:124:LEU:HB2	9:F:185:LYS:HG2	1.74	0.67
3:4:432:ARG:HB3	3:4:436:ASP:CB	2.24	0.67
25:V:43:LYS:HB3	25:V:59:ILE:HA	1.77	0.67
4:A:2140:A:H5'	4:A:2141:U:H5	1.59	0.67
3:4:202:GLY:N	3:4:203:PRO:HD2	2.10	0.66
3:4:288:GLU:HB2	3:4:292:GLY:HA2	1.78	0.66
3:4:455:VAL:HB	3:4:460:ALA:HB3	1.75	0.66
3:4:422:ILE:HG21	3:4:426:ARG:NH1	2.10	0.66
3:4:370:LYS:O	3:4:374:ALA:HA	1.96	0.66
3:4:372:ASP:C	3:4:374:ALA:N	2.49	0.66
4:A:2367:G:C2	4:A:2370:A:C5	2.84	0.66
3:4:307:LEU:HD13	3:4:312:VAL:HG21	1.76	0.66
3:4:271:LEU:HD21	3:4:273:GLU:HB2	1.78	0.66
4:A:1209:G:N1	4:A:1219:U:N3	2.39	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:84:ALA:HA	11:H:91:LEU:HA	1.78	0.66
4:A:2474:G:H5"	4:A:2474:G:N3	2.11	0.65
3:4:461:ALA:HB3	3:4:463:LEU:CD1	2.26	0.65
3:4:445:THR:HG21	3:4:450:ARG:CB	2.27	0.65
4:A:1636:A:H62	4:A:1802:G:H21	1.45	0.65
3:4:85:LEU:HD21	3:4:106:LEU:HD13	1.77	0.65
3:4:371:ILE:HG22	3:4:372:ASP:N	2.11	0.65
3:4:148:LEU:HD12	3:4:148:LEU:O	1.96	0.65
3:4:432:ARG:HH21	3:4:459:LEU:HA	1.62	0.65
4:A:2134:G:N2	4:A:2146:A:O2'	2.29	0.65
4:A:2335:G:N7	4:A:2392:A:N6	2.45	0.65
3:4:379:LEU:CG	3:4:383:ARG:HD2	2.28	0.64
3:4:186:GLN:HB3	3:4:207:LYS:NZ	2.10	0.64
3:4:237:ARG:O	3:4:237:ARG:HG3	1.97	0.64
3:4:199:GLY:HA3	3:4:201:ARG:HD2	1.79	0.64
4:A:347:U:H2'	4:A:348:G:H8	1.63	0.64
4:A:2034:G:OP1	6:C:88:ARG:NH2	2.30	0.64
3:4:202:GLY:O	3:4:203:PRO:C	2.35	0.64
3:4:445:THR:HG21	3:4:450:ARG:HG3	1.80	0.63
11:H:118:GLN:HG3	11:H:120:ALA:H	1.63	0.63
3:4:374:ALA:C	3:4:376:GLY:H	2.00	0.63
3:4:426:ARG:NE	3:4:430:VAL:HG13	2.14	0.63
4:A:2136:A:N6	4:A:2139:U:C4	2.67	0.63
3:4:443:GLU:CG	3:4:452:LYS:HD3	2.28	0.63
13:J:135:ARG:NH1	13:J:136:SER:OG	2.32	0.63
3:4:424:TYR:OH	3:4:447:ALA:HA	1.97	0.63
9:F:150:VAL:HA	9:F:153:ILE:HD12	1.81	0.62
4:A:2137:A:H4'	4:A:2142:A:N1	2.13	0.62
3:4:323:VAL:HG21	3:4:357:TYR:CD1	2.34	0.62
3:4:46:LEU:O	3:4:47:GLU:HB2	1.99	0.62
3:4:263:ASN:OD1	3:4:270:VAL:HG22	1.99	0.62
4:A:747:A:N6	4:A:768:G:O2'	2.33	0.62
3:4:424:TYR:HB3	13:J:31:GLY:O	2.00	0.62
4:A:2363:A:H61	4:A:2374:U:H3	1.47	0.62
3:4:165:SER:HA	3:4:168:GLN:HG3	1.82	0.61
3:4:171:TYR:HB2	3:4:310:GLN:OE1	1.99	0.61
4:A:572:C:H2'	25:V:46:ALA:HA	1.82	0.61
3:4:442:THR:HG23	3:4:442:THR:O	2.00	0.61
12:I:1:MET:SD	12:I:6:LYS:NZ	2.73	0.61
19:P:39:VAL:O	19:P:49:VAL:HG13	2.00	0.61
4:A:2137:A:O3'	4:A:2138:C:H4'	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:85:LEU:HD21	3:4:106:LEU:HD11	1.82	0.61
3:4:408:GLY:O	3:4:411:VAL:HG22	2.00	0.61
4:A:1273:G:OP2	21:R:58:ARG:NH1	2.33	0.61
4:A:1599:U:H5"	4:A:1600:G:H8	1.66	0.61
4:A:1825:C:N4	4:A:1840:G:OP2	2.32	0.61
3:4:76:THR:CG2	3:4:150:ILE:HD11	2.31	0.61
3:4:319:LEU:O	3:4:322:VAL:HG12	2.01	0.61
19:P:42:ARG:NH1	19:P:109:TYR:O	2.34	0.61
3:4:245:ILE:CG2	3:4:294:PRO:HG2	2.30	0.61
3:4:444:HIS:CD2	3:4:445:THR:H	2.18	0.61
3:4:148:LEU:HA	3:4:311:LEU:HD13	1.83	0.61
6:C:136:ILE:HG21	6:C:142:ILE:HD11	1.82	0.61
3:4:147:ILE:O	3:4:150:ILE:HG22	2.01	0.61
4:A:570:U:O4'	25:V:44:HIS:NE2	2.34	0.61
3:4:383:ARG:HB3	3:4:383:ARG:HH11	1.64	0.60
4:A:325:U:O2	4:A:450:G:C2	2.54	0.60
18:O:10:LEU:HB2	18:O:17:GLN:HG3	1.84	0.60
3:4:50:VAL:HG23	3:4:118:VAL:HG22	1.83	0.60
3:4:117:THR:HA	3:4:139:LYS:HB2	1.82	0.60
4:A:1187:A:O2'	4:A:1191:A:N1	2.33	0.60
4:A:1611:A:H2	6:C:134:ARG:HH21	1.47	0.60
3:4:371:ILE:HD12	3:4:390:VAL:O	2.00	0.60
3:4:443:GLU:HG2	3:4:452:LYS:CG	2.31	0.60
4:A:1863:G:H5"	4:A:1864:U:H5'	1.83	0.60
4:A:2014:G:HO2'	6:C:257:THR:HG1	1.44	0.60
3:4:340:LEU:HD22	3:4:340:LEU:N	2.16	0.60
3:4:354:VAL:HG13	3:4:359:ILE:CG1	2.29	0.60
4:A:2160:A:H61	4:A:2187:U:H3	1.48	0.60
26:W:28:ARG:NH1	26:W:93:GLN:O	2.34	0.60
4:A:2245:C:OP1	21:R:25:ARG:NH1	2.35	0.60
28:Y:17:SER:HB3	28:Y:27:ARG:HD2	1.83	0.60
3:4:353:VAL:CG2	3:4:354:VAL:N	2.65	0.60
3:4:366:LEU:HD21	3:4:387:PRO:HB2	1.82	0.60
19:P:43:SER:HB2	19:P:47:ILE:HG22	1.84	0.60
19:P:84:VAL:HG13	19:P:116:LEU:HD13	1.83	0.60
4:A:1156:A:H2'	4:A:1157:G:C8	2.37	0.60
18:O:11:GLY:O	18:O:16:HIS:ND1	2.34	0.60
4:A:587:G:N1	4:A:590:A:OP2	2.35	0.59
3:4:167:ALA:O	3:4:170:GLU:HG2	2.03	0.59
3:4:199:GLY:C	3:4:201:ARG:N	2.55	0.59
7:D:7:LEU:H	7:D:34:ASN:HD21	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:51:ILE:HD11	10:G:73:ILE:HD12	1.84	0.59
3:4:294:PRO:O	3:4:296:VAL:N	2.35	0.59
3:4:180:GLY:O	3:4:184:SER:HB2	2.01	0.59
15:L:115:VAL:HG13	15:L:121:VAL:HG21	1.84	0.59
4:A:1001:C:N4	4:A:1004:C:OP2	2.34	0.59
3:4:291:ASP:OD2	3:4:438:HIS:HB3	2.01	0.59
3:4:392:VAL:HG13	3:4:400:LEU:CD2	2.32	0.59
3:4:426:ARG:HA	3:4:429:LEU:CD2	2.30	0.59
4:A:861:U:O4	7:D:142:GLN:NE2	2.35	0.59
5:B:9:G:H5'	5:B:10:G:H2'	1.84	0.59
12:I:20:SER:OG	12:I:21:THR:N	2.36	0.59
3:4:153:GLN:HG3	3:4:154:HIS:CD2	2.37	0.59
3:4:219:MET:O	3:4:223:ARG:HG3	2.03	0.59
6:C:163:ILE:HG22	6:C:178:PRO:HD3	1.82	0.59
2:3:22:PRO:HB3	4:A:1102:G:H2'	1.84	0.59
3:4:436:ASP:HB3	3:4:439:VAL:HG22	1.85	0.59
4:A:896:A:OP1	6:C:218:ARG:NH2	2.35	0.59
4:A:1582:C:N4	4:A:1589:G:O6	2.35	0.59
5:B:50:C:H5"	19:P:78:LYS:HB3	1.84	0.59
3:4:46:LEU:HD12	3:4:117:THR:HG22	1.84	0.58
3:4:243:SER:O	3:4:244:GLU:C	2.40	0.58
3:4:295:PHE:CG	3:4:295:PHE:O	2.55	0.58
4:A:1555:A:N6	4:A:1617:C:O2	2.36	0.58
4:A:2131:G:O6	4:A:2148:C:N4	2.36	0.58
4:A:1198:C:H41	4:A:1205:G:H5"	1.68	0.58
6:C:66:ASP:OD1	6:C:103:ARG:NH1	2.36	0.58
4:A:1209:G:O6	4:A:1219:U:C4	2.56	0.58
29:Z:45:ARG:HH12	29:Z:48:ARG:HH21	1.52	0.58
3:4:420:VAL:HG23	3:4:466:TYR:HA	1.84	0.58
4:A:325:U:O2	4:A:450:G:N2	2.36	0.58
3:4:202:GLY:HA3	4:A:2676:C:O4'	2.02	0.58
3:4:327:LEU:HA	3:4:363:PRO:O	2.03	0.58
4:A:2385:G:OP1	4:A:2396:A:N6	2.36	0.58
3:4:106:LEU:HA	3:4:109:VAL:HG22	1.85	0.58
3:4:150:ILE:HG23	3:4:151:PHE:HD2	1.69	0.58
3:4:293:ARG:NH2	3:4:414:THR:HA	2.19	0.58
4:A:1177:G:H21	13:J:113:THR:HB	1.68	0.58
13:J:13:LEU:HD13	13:J:15:ILE:HG22	1.86	0.58
3:4:311:LEU:HD23	3:4:312:VAL:N	2.19	0.57
3:4:329:ILE:O	3:4:329:ILE:HG22	2.04	0.57
3:4:432:ARG:HE	3:4:459:LEU:HD12	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:289:A:N6	4:A:300:G:O6	2.37	0.57
3:4:443:GLU:HG2	3:4:452:LYS:HG3	1.86	0.57
3:4:353:VAL:HG23	3:4:354:VAL:N	2.20	0.57
4:A:2135:U:C5	4:A:2137:A:C8	2.92	0.57
4:A:2967:C:O2'	10:G:151:ARG:NH1	2.37	0.57
19:P:42:ARG:H	19:P:106:GLY:HA3	1.70	0.57
17:N:65:TRP:HB2	17:N:105:GLU:HB2	1.87	0.57
3:4:100:SER:OG	4:A:2131:G:H4'	2.05	0.57
3:4:283:THR:HG23	3:4:299:ASP:HB3	1.86	0.57
3:4:107:ARG:HD3	3:4:135:ALA:O	2.04	0.57
3:4:242:ARG:O	3:4:243:SER:C	2.43	0.57
3:4:123:GLU:C	3:4:124:LEU:HD12	2.24	0.57
3:4:367:VAL:CG1	3:4:392:VAL:HG21	2.35	0.57
4:A:730:G:H2'	16:M:113:LEU:HD13	1.87	0.57
4:A:2286:A:H2	4:A:2727:A:H62	1.52	0.57
4:A:2390:U:O2	4:A:2392:A:N6	2.38	0.57
4:A:2532:G:H3'	4:A:2533:C:H2'	1.85	0.57
9:F:55:LYS:HA	9:F:58:ASN:HD22	1.70	0.57
13:J:74:THR:HG23	13:J:83:LYS:HD3	1.86	0.57
4:A:759:G:H1	27:X:64:PRO:HB3	1.69	0.57
6:C:108:PRO:HD2	6:C:111:LEU:HD22	1.87	0.57
29:Z:11:ARG:NH1	29:Z:63:GLU:OE1	2.38	0.57
4:A:1272:C:OP1	21:R:92:ARG:NH2	2.37	0.56
9:F:129:PHE:HE1	9:F:136:THR:H	1.54	0.56
3:4:267:GLY:O	3:4:268:ALA:HB3	2.05	0.56
3:4:371:ILE:O	3:4:372:ASP:HB2	2.04	0.56
3:4:379:LEU:HD21	3:4:391:PHE:CE2	2.39	0.56
4:A:1541:G:OP2	4:A:1629:G:N2	2.39	0.56
4:A:2335:G:OP2	4:A:2338:G:N1	2.37	0.56
17:N:35:GLN:OE1	17:N:130:ARG:NH2	2.39	0.56
3:4:47:GLU:HA	3:4:79:SER:CA	2.35	0.56
3:4:438:HIS:O	3:4:439:VAL:C	2.42	0.56
3:4:443:GLU:O	3:4:451:ILE:HD13	2.05	0.56
4:A:1172:A:N3	12:I:29:ARG:NH1	2.53	0.56
4:A:1398:G:N2	4:A:1401:A:OP2	2.37	0.56
3:4:263:ASN:ND2	3:4:270:VAL:H	2.02	0.56
4:A:2015:U:OP2	6:C:272:ARG:NH2	2.38	0.56
4:A:2802:G:H21	7:D:135:GLN:HE21	1.54	0.56
5:B:7:G:O2'	19:P:37:ARG:NH2	2.39	0.56
3:4:436:ASP:HB3	3:4:439:VAL:CG1	2.35	0.56
3:4:61:ALA:HA	3:4:64:GLU:OE2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2476:G:H2'	4:A:2477:G:H8	1.70	0.56
5:B:43:C:H5'	9:F:71:LYS:HD2	1.86	0.56
3:4:132:LEU:O	3:4:136:VAL:HG22	2.06	0.56
3:4:393:SER:O	36:4:501:GCP:N7	2.39	0.56
4:A:1556:A:H2	4:A:1615:G:H22	1.52	0.56
13:J:34:GLY:O	13:J:66:ARG:NH1	2.39	0.56
4:A:2043:C:O2'	4:A:2195:U:OP2	2.24	0.56
3:4:47:GLU:HA	3:4:79:SER:HA	1.88	0.56
4:A:1112:C:O2	22:S:12:LYS:NZ	2.37	0.56
4:A:2367:G:N3	4:A:2370:A:N7	2.54	0.56
19:P:46:HIS:NE2	19:P:65:SER:O	2.39	0.56
3:4:47:GLU:HA	3:4:79:SER:HB3	1.87	0.56
3:4:327:LEU:HD21	3:4:329:ILE:CD1	2.35	0.56
4:A:2035:U:OP2	6:C:157:ARG:NH1	2.39	0.56
3:4:43:GLN:HA	3:4:43:GLN:NE2	2.20	0.55
3:4:183:MET:HA	3:4:186:GLN:HB2	1.86	0.55
4:A:365:U:O2	4:A:437:G:N2	2.37	0.55
4:A:1224:G:O2'	12:I:54:ASN:ND2	2.40	0.55
5:B:112:C:N4	5:B:113:G:N3	2.54	0.55
19:P:50:GLN:HA	19:P:63:ALA:CB	2.34	0.55
3:4:420:VAL:CG2	3:4:466:TYR:HA	2.36	0.55
3:4:76:THR:HG21	3:4:150:ILE:HD11	1.88	0.55
3:4:393:SER:C	3:4:395:ARG:H	2.10	0.55
3:4:426:ARG:C	3:4:428:ASP:N	2.59	0.55
15:L:50:GLY:O	15:L:53:LYS:NZ	2.39	0.55
4:A:573:C:H41	25:V:47:VAL:HB	1.72	0.55
4:A:652:C:O2'	21:R:48:ARG:NH1	2.40	0.55
10:G:29:PRO:HD3	10:G:80:VAL:HA	1.89	0.55
4:A:1209:G:O6	4:A:1219:U:O4	2.24	0.55
4:A:1540:U:O2	4:A:1632:G:O6	2.25	0.55
3:4:202:GLY:O	3:4:204:GLY:N	2.40	0.55
3:4:246:PRO:CD	3:4:293:ARG:HB3	2.37	0.55
4:A:2136:A:N3	4:A:2136:A:H2'	2.22	0.55
3:4:167:ALA:HB2	3:4:311:LEU:HA	1.89	0.55
3:4:187:ALA:CA	4:A:2826:A:C5	2.86	0.55
3:4:333:ASP:OD2	3:4:336:ASP:HB2	2.07	0.55
3:4:432:ARG:HA	3:4:435:THR:O	2.07	0.55
4:A:1181:G:N2	13:J:136:SER:O	2.39	0.55
4:A:1455:U:OP1	24:U:19:LYS:NZ	2.39	0.55
4:A:3102:U:O2	18:O:45:ARG:NH2	2.39	0.55
15:L:63:VAL:HG12	15:L:106:LEU:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:370:LYS:HE3	36:4:501:GCP:H1'	1.89	0.55
4:A:615:A:OP2	14:K:116:ARG:NH1	2.40	0.55
3:4:441:ALA:H	3:4:453:ALA:CB	2.20	0.55
3:4:422:ILE:O	3:4:448:GLY:HA3	2.07	0.55
3:4:444:HIS:CG	3:4:445:THR:H	2.25	0.55
4:A:1710:A:N6	4:A:1716:A:N7	2.54	0.55
3:4:253:TYR:CD1	3:4:342:GLN:HB3	2.42	0.54
4:A:889:A:OP1	6:C:48:ARG:NH1	2.40	0.54
4:A:3066:C:H5"	20:Q:52:GLY:HA3	1.89	0.54
4:A:1122:C:H2'	4:A:1129:G:H2'	1.89	0.54
4:A:2538:A:OP1	9:F:95:ARG:NH2	2.40	0.54
3:4:340:LEU:H	3:4:340:LEU:CD2	2.20	0.54
3:4:445:THR:HG21	3:4:450:ARG:CG	2.37	0.54
4:A:1562:C:H2'	4:A:1563:A:C8	2.41	0.54
3:4:444:HIS:CG	3:4:445:THR:N	2.74	0.54
4:A:2137:A:H3'	4:A:2137:A:N3	2.21	0.54
12:I:3:LYS:O	12:I:7:ALA:HB3	2.08	0.54
3:4:271:LEU:CD2	3:4:273:GLU:H	2.21	0.54
4:A:2323:G:O6	4:A:2412:U:C4	2.61	0.54
4:A:3070:G:O2'	4:A:3087:G:N2	2.41	0.54
19:P:22:HIS:HA	19:P:105:GLY:HA2	1.88	0.54
3:4:159:GLU:HG3	3:4:229:MET:SD	2.47	0.54
3:4:430:VAL:O	3:4:432:ARG:N	2.40	0.54
19:P:40:VAL:HG23	19:P:106:GLY:H	1.73	0.54
20:Q:48:ARG:HD2	20:Q:50:GLN:HB2	1.88	0.54
3:4:292:GLY:O	3:4:293:ARG:C	2.43	0.54
16:M:91:GLY:H	16:M:122:VAL:HG23	1.73	0.54
23:T:25:ARG:HA	23:T:28:ILE:HG12	1.89	0.54
3:4:251:VAL:CG2	3:4:252:GLY:H	2.20	0.54
3:4:374:ALA:C	3:4:376:GLY:N	2.62	0.54
4:A:1552:A:O2'	4:A:1618:C:N4	2.40	0.54
3:4:148:LEU:HD12	3:4:148:LEU:C	2.27	0.54
3:4:294:PRO:CB	3:4:296:VAL:HG23	2.34	0.54
3:4:323:VAL:HG21	3:4:357:TYR:CE1	2.43	0.54
4:A:1181:G:O2'	13:J:91:SER:O	2.26	0.54
4:A:1199:U:OP1	4:A:1201:G:N2	2.41	0.54
3:4:436:ASP:CB	3:4:439:VAL:HG13	2.37	0.54
4:A:1560:U:O2	6:C:134:ARG:NH2	2.41	0.54
4:A:2754:G:N7	10:G:173:LYS:NZ	2.47	0.54
5:B:78:U:OP1	26:W:28:ARG:NH2	2.41	0.54
3:4:136:VAL:O	3:4:137:LYS:HB2	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:163:GLN:HB3	3:4:314:ALA:HB3	1.90	0.53
15:L:90:ASP:OD2	15:L:90:ASP:N	2.40	0.53
3:4:339:PRO:CG	3:4:382:LEU:HD21	2.38	0.53
3:4:420:VAL:HG23	3:4:466:TYR:CA	2.38	0.53
3:4:463:LEU:HD12	3:4:463:LEU:H	1.73	0.53
4:A:708:G:N2	8:E:187:ASP:OD1	2.41	0.53
3:4:246:PRO:HD3	3:4:293:ARG:HB3	1.90	0.53
3:4:463:LEU:CD1	3:4:463:LEU:H	2.22	0.53
4:A:2219:U:OP1	7:D:133:ARG:NH2	2.42	0.53
20:Q:62:LYS:HE2	20:Q:64:SER:HB3	1.90	0.53
3:4:173:LEU:HB3	3:4:174:PRO:HD3	1.90	0.53
27:X:11:ARG:O	27:X:14:ARG:NH1	2.38	0.53
3:4:263:ASN:HD21	3:4:270:VAL:N	2.04	0.53
3:4:426:ARG:HG2	3:4:427:GLY:N	2.24	0.53
4:A:571:A:OP1	4:A:572:C:N4	2.34	0.53
4:A:1535:C:H3'	4:A:1536:A:H8	1.73	0.53
11:H:98:ALA:O	11:H:102:ASN:ND2	2.41	0.53
26:W:186:SER:OG	26:W:187:ALA:N	2.41	0.53
3:4:214:ARG:O	3:4:218:ARG:HD3	2.09	0.53
5:B:48:C:OP2	19:P:14:ARG:NH1	2.42	0.53
8:E:119:ALA:HB2	8:E:124:ILE:HD12	1.90	0.53
9:F:103:MET:HG3	9:F:107:LEU:HD12	1.91	0.53
19:P:50:GLN:CA	19:P:63:ALA:HB3	2.37	0.53
3:4:87:GLN:HE21	4:A:2133:G:H8	1.55	0.53
3:4:377:VAL:C	3:4:379:LEU:H	2.12	0.53
4:A:1436:C:O2'	23:T:18:ARG:NH2	2.42	0.53
4:A:2536:U:O2	9:F:44:ASN:ND2	2.42	0.53
3:4:280:LEU:HD12	3:4:315:PHE:CZ	2.44	0.53
3:4:368:VAL:HB	3:4:371:ILE:HD11	1.91	0.53
3:4:136:VAL:HG23	3:4:138:VAL:H	1.73	0.52
3:4:202:GLY:N	3:4:203:PRO:CD	2.72	0.52
4:A:2380:G:N2	4:A:2382:G:OP2	2.43	0.52
4:A:1113:C:O2	14:K:3:THR:OG1	2.25	0.52
11:H:77:ASP:HB2	11:H:147:ASN:HB2	1.90	0.52
4:A:1337:G:OP2	22:S:91:ARG:NH1	2.42	0.52
3:4:213:ARG:HB3	3:4:214:ARG:HH21	1.74	0.52
3:4:365:LEU:HD11	3:4:388:ASP:CB	2.40	0.52
3:4:416:ALA:O	3:4:454:ARG:HB2	2.08	0.52
4:A:2519:C:OP2	19:P:24:ARG:NH2	2.43	0.52
15:L:47:ILE:HG22	15:L:49:GLY:H	1.74	0.52
3:4:73:LEU:HG	3:4:146:LEU:CD2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:73:LEU:HG	3:4:146:LEU:HG	1.91	0.52
3:4:369:ASN:C	3:4:371:ILE:H	2.13	0.52
19:P:41:ASN:ND2	19:P:48:HIS:O	2.43	0.52
13:J:125:ALA:O	13:J:129:ILE:HB	2.09	0.52
3:4:215:ILE:O	3:4:219:MET:HG3	2.10	0.52
3:4:85:LEU:HD13	3:4:106:LEU:HD21	1.89	0.52
3:4:330:HIS:NE2	3:4:346:VAL:HB	2.25	0.52
3:4:348:THR:O	3:4:351:ASN:HB2	2.10	0.52
4:A:349:G:H2'	4:A:350:A:H8	1.75	0.52
3:4:124:LEU:HD12	3:4:124:LEU:N	2.25	0.52
3:4:180:GLY:HA2	3:4:183:MET:HG2	1.91	0.52
3:4:328:LEU:HD12	3:4:328:LEU:N	2.24	0.52
3:4:432:ARG:NE	3:4:459:LEU:HD12	2.24	0.52
4:A:306:U:OP2	11:H:41:ARG:NH1	2.43	0.52
4:A:724:G:N2	4:A:727:A:OP2	2.36	0.52
3:4:132:LEU:HG	3:4:140:VAL:HG11	1.91	0.52
4:A:1076:A:N6	17:N:83:MET:HE1	2.24	0.52
7:D:144:VAL:HA	7:D:147:ARG:HG3	1.92	0.52
13:J:111:ALA:HB2	13:J:126:ALA:HB2	1.91	0.52
3:4:102:LYS:HD3	4:A:2133:G:P	2.50	0.51
3:4:227:ARG:HE	3:4:227:ARG:CA	2.20	0.51
13:J:21:ASN:ND2	13:J:41:CYS:SG	2.82	0.51
26:W:178:VAL:HG12	26:W:179:VAL:HG23	1.91	0.51
3:4:82:LEU:HD12	3:4:115:ALA:HB2	1.92	0.51
3:4:222:LEU:CD2	3:4:226:ILE:HG23	2.40	0.51
3:4:248:VAL:HG21	3:4:295:PHE:CD1	2.45	0.51
4:A:2726:G:H5"	4:A:2727:A:H5"	1.91	0.51
6:C:146:GLU:HB2	6:C:189:CYS:HB3	1.93	0.51
3:4:151:PHE:CE1	3:4:315:PHE:CE2	2.99	0.51
12:I:76:PRO:O	12:I:106:LYS:NZ	2.33	0.51
16:M:94:GLY:N	16:M:97:GLU:OE1	2.43	0.51
3:4:106:LEU:O	3:4:109:VAL:HG22	2.11	0.51
3:4:280:LEU:HD12	3:4:315:PHE:HZ	1.74	0.51
3:4:456:PRO:HB2	3:4:458:PRO:HD2	1.92	0.51
3:4:55:TRP:CG	3:4:55:TRP:O	2.64	0.51
3:4:119:ILE:N	3:4:119:ILE:HD12	2.24	0.51
4:A:2142:A:H2'	4:A:2143:A:O4'	2.10	0.51
25:V:10:LEU:HD13	25:V:80:PRO:HG3	1.92	0.51
3:4:48:ARG:HB2	3:4:116:ASP:OD1	2.11	0.51
3:4:335:SER:HB3	3:4:375:THR:OG1	2.11	0.51
3:4:420:VAL:HA	3:4:466:TYR:CD1	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:47:GLU:HA	3:4:79:SER:CB	2.40	0.51
3:4:49:VAL:HG22	3:4:81:VAL:HA	1.91	0.51
3:4:223:ARG:HA	3:4:226:ILE:CD1	2.41	0.51
4:A:1212:U:H4'	4:A:1215:U:H5	1.76	0.51
4:A:1546:A:N6	4:A:1625:G:O6	2.44	0.51
4:A:2983:G:N2	10:G:140:GLN:OE1	2.43	0.51
12:I:3:LYS:O	12:I:7:ALA:CB	2.59	0.51
3:4:180:GLY:CA	3:4:183:MET:HG2	2.40	0.51
4:A:2138:C:H4'	4:A:2142:A:C2	2.46	0.51
3:4:76:THR:O	3:4:76:THR:HG22	2.10	0.51
3:4:261:LEU:HD11	3:4:392:VAL:CG1	2.29	0.51
4:A:2476:G:H2'	4:A:2477:G:C8	2.45	0.51
3:4:70:LEU:HD22	3:4:121:ASP:HB3	1.92	0.50
3:4:178:GLY:C	3:4:180:GLY:H	2.14	0.50
3:4:392:VAL:HG13	3:4:400:LEU:HD23	1.92	0.50
4:A:1566:A:N6	4:A:1606:G:N2	2.47	0.50
3:4:430:VAL:HG12	3:4:434:HIS:HD2	1.75	0.50
3:4:456:PRO:HD2	3:4:459:LEU:HB2	1.94	0.50
3:4:148:LEU:HD11	3:4:168:GLN:HB3	1.92	0.50
3:4:436:ASP:HB3	3:4:439:VAL:CG2	2.41	0.50
3:4:458:PRO:HG2	3:4:459:LEU:HD22	1.93	0.50
13:J:48:THR:HB	13:J:56:ILE:HD13	1.94	0.50
4:A:2176:A:N3	4:A:2784:C:O2'	2.39	0.50
5:B:101:U:O3'	26:W:81:LYS:NZ	2.45	0.50
12:I:33:VAL:O	12:I:37:ALA:N	2.39	0.50
19:P:49:VAL:HG12	19:P:50:GLN:N	2.26	0.50
3:4:456:PRO:CB	3:4:459:LEU:HD23	2.38	0.50
4:A:2323:G:O6	4:A:2412:U:O4	2.30	0.50
4:A:2528:G:N2	9:F:160:ASP:OD2	2.45	0.50
3:4:46:LEU:HD22	3:4:46:LEU:N	2.26	0.50
3:4:95:SER:O	3:4:131:ALA:HB3	2.11	0.50
3:4:193:GLY:O	3:4:194:ALA:C	2.49	0.50
3:4:294:PRO:C	3:4:296:VAL:N	2.62	0.50
3:4:371:ILE:CA	3:4:374:ALA:HB2	2.35	0.50
3:4:420:VAL:CG2	3:4:421:THR:N	2.72	0.50
3:4:452:LYS:NZ	3:4:452:LYS:HB3	2.26	0.50
17:N:84:GLY:O	17:N:85:SER:OG	2.28	0.50
3:4:419:ASP:HA	3:4:452:LYS:HA	1.93	0.50
3:4:424:TYR:CE2	3:4:447:ALA:HA	2.47	0.50
4:A:1209:G:N2	4:A:1219:U:O2	2.40	0.50
4:A:2086:U:H3	4:A:2096:G:H1	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:84:ASN:HB2	16:M:118:LEU:HD12	1.94	0.50
3:4:89:ARG:HD3	3:4:91:LYS:O	2.11	0.49
3:4:284:THR:O	3:4:285:ARG:HD3	2.12	0.49
25:V:86:ARG:HB2	25:V:97:ILE:HD12	1.94	0.49
3:4:331:VAL:HA	3:4:367:VAL:O	2.12	0.49
3:4:392:VAL:HG13	3:4:400:LEU:HD21	1.94	0.49
7:D:14:THR:OG1	7:D:15:GLN:N	2.44	0.49
10:G:36:ASP:OD1	10:G:36:ASP:N	2.46	0.49
3:4:173:LEU:N	3:4:174:PRO:CD	2.75	0.49
3:4:187:ALA:C	3:4:189:GLY:H	2.15	0.49
4:A:2086:U:O4	4:A:2096:G:O6	2.30	0.49
3:4:201:ARG:NH2	4:A:2286:A:N7	2.60	0.49
4:A:1176:G:HO2'	4:A:1178:U:H3	1.59	0.49
3:4:110:VAL:HG21	3:4:138:VAL:HG21	1.94	0.49
3:4:222:LEU:HD23	3:4:226:ILE:HG23	1.95	0.49
3:4:382:LEU:O	3:4:386:LEU:HB2	2.13	0.49
8:E:184:ASN:OD1	8:E:184:ASN:N	2.45	0.49
12:I:77:THR:OG1	12:I:106:LYS:NZ	2.45	0.49
3:4:230:LYS:HD3	3:4:233:ARG:HH21	1.77	0.49
4:A:1209:G:N1	4:A:1219:U:C2	2.77	0.49
4:A:1548:C:H42	4:A:1621:C:H5	1.60	0.49
4:A:2400:C:H3'	4:A:2401:U:H4'	1.95	0.49
10:G:35:LEU:HD22	10:G:76:LEU:HD22	1.95	0.49
3:4:250:ILE:HD13	3:4:258:LYS:CA	2.40	0.49
3:4:350:ILE:O	3:4:354:VAL:HG23	2.12	0.49
3:4:432:ARG:O	3:4:433:VAL:C	2.51	0.49
19:P:43:SER:CB	19:P:47:ILE:HG22	2.41	0.49
3:4:166:LEU:HD22	3:4:226:ILE:CD1	2.43	0.49
4:A:920:G:N2	4:A:944:A:OP1	2.44	0.49
7:D:7:LEU:HB2	7:D:34:ASN:HD21	1.78	0.49
14:K:49:ASP:OD1	14:K:121:LYS:NZ	2.44	0.49
3:4:87:GLN:HG2	3:4:88:ARG:H	1.78	0.49
3:4:88:ARG:HG2	4:A:2137:A:N6	2.28	0.49
3:4:173:LEU:CD1	3:4:215:ILE:HG21	2.34	0.49
3:4:181:GLU:C	3:4:184:SER:H	2.16	0.49
4:A:347:U:H2'	4:A:348:G:C8	2.47	0.49
4:A:2137:A:H4'	4:A:2142:A:C2	2.47	0.49
4:A:2224:C:O2'	4:A:2913:U:OP2	2.30	0.49
27:X:53:ARG:NH1	27:X:57:ASP:OD1	2.46	0.49
3:4:125:SER:OG	3:4:128:GLN:HG3	2.13	0.49
3:4:158:ARG:HD2	3:4:158:ARG:C	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:233:ARG:O	3:4:237:ARG:HG2	2.13	0.49
4:A:2329:G:O6	4:A:2406:U:O4	2.30	0.49
3:4:288:GLU:HG2	3:4:289:PHE:O	2.13	0.48
3:4:295:PHE:O	3:4:295:PHE:CD1	2.66	0.48
4:A:1184:U:O5'	4:A:1187:A:N6	2.45	0.48
4:A:2161:A:O2'	4:A:2163:U:OP2	2.24	0.48
23:T:77:VAL:HG21	23:T:117:ARG:HD2	1.95	0.48
3:4:45:ARG:CZ	3:4:45:ARG:HB3	2.43	0.48
3:4:251:VAL:CG2	3:4:252:GLY:N	2.74	0.48
4:A:2141:U:O2'	4:A:2142:A:H5"	2.12	0.48
6:C:143:HIS:ND1	6:C:194:GLY:O	2.30	0.48
12:I:53:LYS:O	12:I:54:ASN:ND2	2.45	0.48
23:T:9:SER:HB3	23:T:115:GLU:HG2	1.94	0.48
3:4:199:GLY:O	3:4:201:ARG:N	2.47	0.48
3:4:213:ARG:CB	3:4:214:ARG:HH21	2.26	0.48
11:H:101:VAL:HG22	11:H:114:LYS:HB2	1.96	0.48
12:I:115:LEU:HD11	12:I:119:ASP:HB3	1.94	0.48
3:4:187:ALA:CB	4:A:2826:A:C5	2.97	0.48
3:4:223:ARG:O	3:4:226:ILE:HG12	2.13	0.48
3:4:395:ARG:HG2	3:4:396:THR:N	2.26	0.48
3:4:463:LEU:HD12	3:4:463:LEU:N	2.29	0.48
4:A:1163:A:OP1	4:A:1229:A:N6	2.46	0.48
4:A:2530:C:H3'	4:A:2531:G:H2'	1.94	0.48
22:S:27:LEU:HB2	22:S:95:THR:HG21	1.95	0.48
3:4:142:ASP:OD1	3:4:142:ASP:N	2.46	0.48
3:4:287:GLY:O	3:4:294:PRO:O	2.32	0.48
6:C:182:ILE:HB	6:C:269:VAL:HB	1.95	0.48
11:H:118:GLN:HE21	11:H:120:ALA:HB3	1.79	0.48
12:I:119:ASP:HA	12:I:122:LYS:HD2	1.95	0.48
19:P:79:ALA:HB3	19:P:115:ALA:HB3	1.95	0.48
3:4:185:ARG:C	3:4:187:ALA:H	2.17	0.48
3:4:397:GLY:O	3:4:398:ASP:C	2.50	0.48
4:A:1157:G:N2	4:A:1234:U:O2	2.47	0.48
4:A:1160:G:H1	4:A:1230:G:H22	1.61	0.48
11:H:85:ALA:N	11:H:90:LYS:O	2.46	0.48
4:A:356:G:H21	4:A:362:A:H62	1.62	0.48
4:A:1548:C:C2	4:A:1622:G:H1'	2.49	0.48
5:B:44:C:O3'	9:F:102:ARG:NH2	2.46	0.48
9:F:45:MET:HG3	9:F:64:LEU:HD22	1.95	0.48
3:4:102:LYS:CG	4:A:2132:U:H5'	2.31	0.48
3:4:151:PHE:HE2	3:4:277:PHE:CG	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:329:ILE:HA	3:4:365:LEU:O	2.14	0.48
3:4:395:ARG:NH2	36:4:501:GCP:C2	2.62	0.48
4:A:2463:G:OP1	6:C:244:ARG:NH2	2.43	0.48
15:L:122:LEU:HD13	20:Q:69:VAL:HG11	1.95	0.48
3:4:49:VAL:CG2	3:4:81:VAL:HA	2.43	0.48
3:4:90:ASP:HB3	4:A:2137:A:C2	2.48	0.48
3:4:147:ILE:CD1	3:4:151:PHE:CE2	2.95	0.48
4:A:81:A:OP1	25:V:4:HIS:NE2	2.47	0.48
19:P:64:SER:OG	19:P:65:SER:N	2.47	0.48
3:4:76:THR:HG22	3:4:150:ILE:HD11	1.96	0.48
11:H:1:MET:N	11:H:21:VAL:O	2.44	0.48
11:H:100:VAL:HG23	11:H:114:LYS:HG3	1.96	0.48
26:W:50:ASN:ND2	26:W:53:ASP:OD1	2.41	0.48
4:A:1537:U:H2'	4:A:1538:G:H8	1.78	0.47
4:A:1542:A:N1	4:A:1628:A:O2'	2.41	0.47
10:G:17:VAL:HG12	10:G:26:VAL:HG22	1.96	0.47
11:H:75:LEU:O	11:H:145:SER:OG	2.31	0.47
4:A:1116:C:OP2	21:R:58:ARG:NH2	2.47	0.47
4:A:1200:U:HO2'	12:I:50:THR:HG1	1.60	0.47
4:A:3014:A:H62	4:A:3113:A:H2	1.62	0.47
24:U:30:THR:HG23	24:U:83:ILE:HG12	1.96	0.47
12:I:45:ASP:OD2	12:I:45:ASP:N	2.46	0.47
20:Q:91:VAL:HG11	20:Q:96:LEU:HD21	1.95	0.47
3:4:436:ASP:CB	3:4:439:VAL:CG1	2.92	0.47
17:N:43:THR:OG1	17:N:44:ASN:N	2.41	0.47
3:4:151:PHE:CE1	3:4:315:PHE:CZ	3.03	0.47
3:4:426:ARG:NH2	3:4:433:VAL:HG11	2.30	0.47
3:4:455:VAL:CB	3:4:460:ALA:HB3	2.44	0.47
4:A:164:A:OP2	11:H:118:GLN:NE2	2.47	0.47
4:A:2367:G:N2	4:A:2370:A:C4	2.83	0.47
6:C:181:GLU:HG2	6:C:271:ARG:HA	1.96	0.47
13:J:12:LYS:HE2	13:J:59:GLU:HB2	1.97	0.47
21:R:26:GLY:O	21:R:30:ARG:NH1	2.48	0.47
3:4:231:LYS:O	3:4:235:THR:HG22	2.15	0.47
4:A:1198:C:H2'	13:J:128:LYS:HD2	1.96	0.47
4:A:2137:A:HO2'	4:A:2138:C:P	2.37	0.47
13:J:103:THR:OG1	13:J:104:TRP:N	2.46	0.47
3:4:258:LYS:HD3	36:4:501:GCP:O1B	2.15	0.47
3:4:432:ARG:HG2	3:4:459:LEU:HD12	1.95	0.47
4:A:551:G:N2	4:A:554:A:OP2	2.42	0.47
4:A:808:A:O2'	4:A:1468:A:N3	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2764:C:O2'	4:A:2964:A:N3	2.42	0.47
22:S:21:VAL:HG22	22:S:98:LYS:HG3	1.96	0.47
3:4:102:LYS:N	4:A:2132:U:OP1	2.41	0.47
4:A:994:A:N6	4:A:1014:G:O2'	2.46	0.47
4:A:2340:A:O2'	4:A:2342:A:OP1	2.32	0.47
9:F:124:LEU:HG	9:F:184:PHE:HA	1.96	0.47
10:G:99:LEU:HG	10:G:101:GLY:H	1.80	0.47
3:4:449:THR:OG1	3:4:451:ILE:HG12	2.15	0.47
4:A:1198:C:N4	4:A:1206:A:OP2	2.48	0.47
4:A:2371:G:O2'	4:A:2372:U:O4'	2.29	0.47
4:A:1365:G:O6	16:M:21:ARG:NH2	2.46	0.46
3:4:208:ILE:HG23	3:4:209:GLU:N	2.30	0.46
3:4:395:ARG:CG	3:4:396:THR:H	2.23	0.46
4:A:678:A:H5'	8:E:90:VAL:HG13	1.95	0.46
4:A:2367:G:C2	4:A:2370:A:C8	3.03	0.46
21:R:125:SER:O	21:R:125:SER:OG	2.32	0.46
3:4:433:VAL:O	3:4:439:VAL:HB	2.15	0.46
4:A:32:G:H1'	4:A:542:A:C4	2.50	0.46
4:A:1162:G:OP2	4:A:1164:A:N6	2.40	0.46
4:A:2136:A:N6	4:A:2139:U:O4	2.48	0.46
4:A:2385:G:H5"	4:A:2396:A:H61	1.80	0.46
10:G:51:ILE:HD12	10:G:70:ARG:HA	1.96	0.46
23:T:52:GLU:HG2	23:T:53:PRO:HD3	1.97	0.46
25:V:43:LYS:O	25:V:43:LYS:NZ	2.36	0.46
3:4:46:LEU:HA	3:4:116:ASP:OD2	2.15	0.46
4:A:256:A:H2'	4:A:257:A:H8	1.80	0.46
4:A:544:U:O2	4:A:547:U:O2'	2.26	0.46
19:P:49:VAL:O	19:P:50:GLN:HB3	2.15	0.46
19:P:49:VAL:O	19:P:64:SER:HA	2.16	0.46
19:P:68:ALA:O	19:P:71:ARG:NH1	2.49	0.46
3:4:253:TYR:CE1	3:4:332:VAL:HG12	2.37	0.46
4:A:1364:U:C4	16:M:21:ARG:HD3	2.51	0.46
18:O:106:ASP:OD2	18:O:106:ASP:N	2.48	0.46
19:P:52:VAL:HG13	19:P:59:THR:HG22	1.97	0.46
4:A:1269:C:O2'	21:R:121:VAL:O	2.29	0.46
4:A:1562:C:H2'	4:A:1563:A:H8	1.80	0.46
20:Q:48:ARG:HB2	20:Q:95:LYS:HD3	1.97	0.46
21:R:73:ASP:O	21:R:114:ARG:NH2	2.49	0.46
25:V:27:TYR:HB2	25:V:30:ARG:HB2	1.98	0.46
27:X:76:LYS:HB3	27:X:76:LYS:HE3	1.72	0.46
28:Y:21:SER:O	28:Y:21:SER:OG	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:163:GLN:HB3	3:4:314:ALA:CB	2.45	0.46
3:4:232:ILE:HA	3:4:235:THR:HG22	1.97	0.46
3:4:438:HIS:CE1	3:4:456:PRO:HG3	2.51	0.46
4:A:1577:C:H2'	4:A:1578:G:H8	1.81	0.46
4:A:2527:G:O2'	9:F:128:GLN:O	2.33	0.46
7:D:10:LYS:HB3	7:D:198:ILE:HD11	1.98	0.46
10:G:19:ILE:HG12	10:G:24:LEU:HD13	1.97	0.46
19:P:62:ALA:HB3	19:P:91:ARG:HH12	1.81	0.46
3:4:147:ILE:O	3:4:147:ILE:HD12	2.15	0.46
3:4:240:ARG:HG2	4:A:2697:U:O2	2.16	0.46
3:4:393:SER:O	36:4:501:GCP:O6	2.34	0.46
11:H:74:GLY:HA3	11:H:105:LYS:HE3	1.96	0.46
3:4:172:MET:O	3:4:172:MET:SD	2.74	0.46
9:F:132:THR:HG22	9:F:170:ASP:HA	1.98	0.46
3:4:361:PRO:HA	3:4:362:PRO:HD3	1.84	0.46
3:4:430:VAL:HG12	3:4:434:HIS:CD2	2.51	0.46
3:4:445:THR:OG1	3:4:449:THR:HA	2.16	0.46
4:A:531:A:H2'	8:E:46:ARG:HH12	1.81	0.45
4:A:2008:A:N6	4:A:2045:G:O2'	2.42	0.45
13:J:106:GLN:HB3	13:J:109:GLU:HB3	1.97	0.45
25:V:44:HIS:H	25:V:59:ILE:HG12	1.80	0.45
3:4:289:PHE:HD1	3:4:290:GLU:H	1.64	0.45
3:4:332:VAL:HG11	3:4:343:ILE:HG12	1.97	0.45
4:A:1209:G:C6	4:A:1219:U:N3	2.84	0.45
5:B:9:G:O6	5:B:109:C:N4	2.49	0.45
12:I:20:SER:HA	12:I:83:LYS:HD3	1.99	0.45
19:P:67:GLU:OE2	19:P:91:ARG:NH1	2.49	0.45
2:3:16:ALA:O	4:A:1096:G:N2	2.37	0.45
3:4:201:ARG:HG3	4:A:2675:A:H2	1.80	0.45
3:4:426:ARG:HG3	3:4:429:LEU:CB	2.28	0.45
4:A:1705:C:H2'	4:A:1706:A:H8	1.80	0.45
12:I:82:VAL:HG11	12:I:90:ALA:HB2	1.97	0.45
19:P:39:VAL:O	19:P:49:VAL:CG1	2.64	0.45
3:4:89:ARG:HG2	3:4:91:LYS:H	1.81	0.45
3:4:370:LYS:HD3	36:4:501:GCP:C4	2.45	0.45
3:4:460:ALA:O	3:4:463:LEU:HD13	2.16	0.45
14:K:28:LEU:HD22	14:K:62:ILE:HD11	1.98	0.45
3:4:48:ARG:HD2	3:4:82:LEU:HD11	1.98	0.45
3:4:102:LYS:HG2	4:A:2132:U:OP1	2.16	0.45
3:4:301:VAL:HG12	3:4:302:GLY:N	2.32	0.45
2:3:7:LYS:NZ	4:A:1252:G:OP2	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:125:SER:HB2	3:4:126:PRO:CD	2.47	0.45
3:4:305:ARG:HG2	3:4:306:HIS:CD2	2.52	0.45
3:4:430:VAL:O	3:4:433:VAL:N	2.50	0.45
22:S:8:LYS:HG2	22:S:13:GLN:HG2	1.99	0.45
4:A:2137:A:O4'	4:A:2143:A:N6	2.50	0.45
4:A:2323:G:C6	4:A:2412:U:N3	2.84	0.45
19:P:47:ILE:HG21	19:P:112:ARG:HD3	1.99	0.45
3:4:151:PHE:CD1	3:4:311:LEU:HD12	2.52	0.45
3:4:327:LEU:HD21	3:4:329:ILE:HD13	1.98	0.45
3:4:391:PHE:CD1	3:4:391:PHE:N	2.83	0.45
4:A:380:A:N3	4:A:401:C:O2'	2.41	0.45
6:C:240:THR:OG1	6:C:241:SER:N	2.50	0.45
3:4:317:SER:O	3:4:321:GLU:HG2	2.16	0.45
4:A:368:U:H3	4:A:434:G:H1	1.64	0.45
4:A:1194:C:C2	13:J:93:GLU:HG2	2.52	0.45
4:A:1198:C:C2	13:J:128:LYS:HE3	2.52	0.45
4:A:1582:C:N4	4:A:1583:U:O2	2.50	0.45
4:A:2321:U:O4	4:A:2414:G:O6	2.35	0.45
9:F:76:ARG:HD3	9:F:89:GLY:HA2	1.99	0.45
19:P:26:ARG:NH2	19:P:54:ASP:OD2	2.38	0.45
21:R:68:ALA:O	21:R:72:ASN:ND2	2.48	0.45
3:4:89:ARG:CD	3:4:92:PRO:HA	2.47	0.45
3:4:93:ASP:OD2	3:4:94:PRO:HD2	2.17	0.45
3:4:416:ALA:HB1	3:4:455:VAL:N	2.32	0.45
9:F:110:LEU:HA	9:F:114:ALA:HB3	1.99	0.45
13:J:102:VAL:HB	13:J:141:VAL:HG13	1.99	0.45
25:V:45:THR:OG1	25:V:46:ALA:N	2.49	0.45
3:4:199:GLY:C	3:4:201:ARG:HD2	2.37	0.44
3:4:323:VAL:HG11	3:4:357:TYR:HD1	1.82	0.44
4:A:2348:G:N2	4:A:2394:A:OP2	2.49	0.44
4:A:3012:U:O2'	4:A:3030:A:N3	2.42	0.44
13:J:105:ASP:OD1	13:J:105:ASP:N	2.45	0.44
3:4:167:ALA:HA	3:4:170:GLU:OE2	2.18	0.44
3:4:271:LEU:HD21	3:4:273:GLU:CB	2.45	0.44
4:A:858:A:O2'	4:A:1877:U:OP1	2.35	0.44
4:A:1022:C:O2'	17:N:101:ARG:NH2	2.49	0.44
5:B:112:C:C4	5:B:113:G:H1'	2.53	0.44
8:E:47:GLN:HE21	8:E:47:GLN:HB3	1.61	0.44
25:V:77:ASP:OD1	25:V:101:ASN:ND2	2.50	0.44
27:X:72:LYS:HD3	27:X:72:LYS:HA	1.70	0.44
3:4:254:THR:OG1	36:4:501:GCP:O1G	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:440:ASP:O	3:4:441:ALA:HB3	2.17	0.44
4:A:1179:U:C2	13:J:11:ILE:HD11	2.53	0.44
12:I:40:ARG:HD2	13:J:123:ILE:HD13	1.99	0.44
3:4:326:ASP:CB	3:4:412:GLU:OE1	2.57	0.44
4:A:576:G:O2'	23:T:56:LYS:NZ	2.34	0.44
4:A:718:C:O2'	4:A:772:U:OP1	2.31	0.44
10:G:27:LYS:HA	10:G:32:THR:HG22	1.98	0.44
11:H:30:LEU:HD13	11:H:35:LEU:HB2	1.98	0.44
12:I:3:LYS:HG3	12:I:7:ALA:HB2	1.98	0.44
13:J:128:LYS:HD2	13:J:128:LYS:HA	1.71	0.44
22:S:69:LYS:HD2	22:S:91:ARG:HG2	2.00	0.44
3:4:186:GLN:HG3	3:4:207:LYS:HZ1	1.83	0.44
3:4:383:ARG:NE	3:4:391:PHE:CZ	2.85	0.44
4:A:279:U:H2'	4:A:280:G:H8	1.83	0.44
4:A:499:G:OP2	4:A:2630:A:O2'	2.33	0.44
5:B:15:U:OP2	5:B:71:C:O2'	2.34	0.44
6:C:85:ASP:OD2	6:C:88:ARG:NH1	2.47	0.44
12:I:6:LYS:HE2	12:I:6:LYS:HB3	1.82	0.44
3:4:383:ARG:HH11	3:4:383:ARG:CB	2.31	0.44
3:4:441:ALA:H	3:4:453:ALA:HB2	1.82	0.44
4:A:1249:G:H4'	14:K:84:LEU:HD22	1.99	0.44
4:A:1314:C:H1'	21:R:4:VAL:HG12	1.99	0.44
5:B:8:C:H2'	5:B:9:G:H4'	1.98	0.44
10:G:20:ASN:OD1	10:G:20:ASN:N	2.50	0.44
19:P:126:LYS:HE2	19:P:126:LYS:HB3	1.80	0.44
3:4:305:ARG:NH1	3:4:345:ALA:HB2	2.32	0.44
3:4:393:SER:O	3:4:394:ALA:HB3	2.17	0.44
4:A:1210:C:H3'	4:A:1211:G:C8	2.52	0.44
4:A:1541:G:HO2'	4:A:1632:G:N2	2.16	0.44
10:G:28:GLY:HA2	10:G:80:VAL:HG22	1.99	0.44
3:4:96:THR:O	3:4:98:ILE:N	2.49	0.44
3:4:165:SER:HA	3:4:168:GLN:CG	2.48	0.44
3:4:193:GLY:CA	4:A:2809:U:H1'	2.48	0.44
3:4:367:VAL:HG22	3:4:388:ASP:OD2	2.18	0.44
3:4:393:SER:C	3:4:395:ARG:N	2.71	0.44
12:I:43:LEU:HB3	12:I:92:ALA:HB1	1.99	0.44
19:P:49:VAL:O	19:P:64:SER:CA	2.66	0.44
3:4:243:SER:O	3:4:245:ILE:HG23	2.18	0.44
3:4:248:VAL:HG23	3:4:297:LEU:HD13	2.00	0.44
3:4:371:ILE:O	3:4:373:ALA:N	2.51	0.44
4:A:998:G:H1	4:A:1009:U:H3	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1708:A:H1'	4:A:1709:U:H5'	2.00	0.44
17:N:10:ARG:HG2	17:N:90:PRO:HG2	2.00	0.44
3:4:50:VAL:HG23	3:4:50:VAL:O	2.18	0.43
3:4:204:GLY:O	3:4:205:GLU:HG3	2.17	0.43
3:4:456:PRO:HG2	3:4:459:LEU:HD23	1.98	0.43
4:A:1185:A:OP1	4:A:1187:A:N6	2.50	0.43
4:A:1537:U:H2'	4:A:1538:G:C8	2.53	0.43
9:F:178:ARG:NH2	9:F:186:GLU:OE2	2.48	0.43
3:4:300:THR:CB	3:4:318:THR:HG23	2.44	0.43
3:4:369:ASN:OD1	3:4:370:LYS:HG2	2.17	0.43
4:A:1302:G:N2	4:A:1303:U:O4	2.48	0.43
4:A:2143:A:N6	4:A:2144:C:N4	2.66	0.43
4:A:2249:G:H2'	4:A:2250:A:C8	2.54	0.43
11:H:83:ASN:HB3	11:H:92:PHE:HB2	2.01	0.43
19:P:37:ARG:NE	19:P:54:ASP:OD2	2.51	0.43
23:T:11:THR:HG22	23:T:113:ILE:HG12	2.01	0.43
3:4:230:LYS:HE2	3:4:234:ASP:OD1	2.18	0.43
3:4:272:VAL:CG2	36:4:501:GCP:H5'2	2.48	0.43
3:4:327:LEU:HD12	3:4:410:LEU:HB2	2.00	0.43
3:4:381:GLN:HG2	3:4:384:ARG:HD3	2.00	0.43
3:4:426:ARG:O	3:4:428:ASP:N	2.51	0.43
3:4:432:ARG:HB3	3:4:436:ASP:CG	2.38	0.43
3:4:443:GLU:CD	3:4:452:LYS:HD3	2.39	0.43
4:A:1210:C:H3'	4:A:1211:G:H8	1.84	0.43
4:A:2070:A:H2'	4:A:2071:A:C8	2.53	0.43
5:B:9:G:N1	5:B:109:C:N3	2.66	0.43
6:C:37:LEU:HG	6:C:62:TYR:HB2	1.98	0.43
9:F:9:PRO:HG3	9:F:104:TRP:HA	2.00	0.43
12:I:31:LEU:HD13	12:I:36:LEU:HD21	1.98	0.43
12:I:94:LYS:HE2	12:I:105:ILE:HD13	1.99	0.43
12:I:95:LYS:HA	12:I:95:LYS:HD3	1.82	0.43
15:L:80:ASP:OD2	20:Q:103:ARG:NH1	2.51	0.43
3:4:167:ALA:HA	3:4:170:GLU:HG2	2.00	0.43
3:4:195:GLY:C	3:4:197:GLY:N	2.69	0.43
3:4:328:LEU:CD1	3:4:362:PRO:HB2	2.48	0.43
3:4:272:VAL:O	3:4:272:VAL:HG22	2.18	0.43
4:A:114:G:OP2	4:A:116:A:O2'	2.29	0.43
4:A:738:A:H4'	4:A:739:U:H5	1.82	0.43
4:A:1207:G:N7	13:J:118:LEU:HG	2.33	0.43
4:A:2143:A:C6	4:A:2144:C:C4	3.06	0.43
17:N:51:ARG:HD3	17:N:66:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:87:GLN:NE2	4:A:2133:G:C8	2.77	0.43
3:4:110:VAL:HG21	3:4:138:VAL:CG2	2.48	0.43
3:4:348:THR:HA	3:4:351:ASN:ND2	2.33	0.43
3:4:393:SER:O	3:4:395:ARG:N	2.44	0.43
4:A:325:U:C2	4:A:450:G:N1	2.86	0.43
4:A:1558:C:H2'	4:A:1559:A:C8	2.53	0.43
11:H:86:GLY:HA3	11:H:90:LYS:HB3	2.00	0.43
3:4:357:TYR:N	3:4:357:TYR:CD2	2.86	0.43
3:4:371:ILE:CG2	3:4:372:ASP:N	2.80	0.43
3:4:436:ASP:CB	3:4:439:VAL:HG22	2.49	0.43
3:4:441:ALA:H	3:4:453:ALA:HB1	1.83	0.43
4:A:2735:U:O2'	7:D:148:PRO:O	2.29	0.43
26:W:124:VAL:HG22	26:W:181:VAL:HG22	2.00	0.43
3:4:105:GLU:OE1	3:4:105:GLU:HA	2.18	0.43
3:4:420:VAL:CG2	3:4:421:THR:H	2.25	0.43
4:A:314:G:O2'	4:A:321:G:O2'	2.36	0.43
4:A:546:G:O2'	4:A:557:G:O6	2.32	0.43
4:A:2017:C:OP2	6:C:183:ARG:NH2	2.40	0.43
8:E:13:LYS:HB3	8:E:13:LYS:HE3	1.88	0.43
10:G:164:ARG:HG3	10:G:165:TYR:H	1.84	0.43
26:W:50:ASN:O	26:W:54:PHE:HB2	2.19	0.43
3:4:228:ASP:C	3:4:230:LYS:N	2.70	0.43
3:4:254:THR:O	3:4:255:ASN:HB2	2.19	0.43
3:4:289:PHE:CD2	3:4:404:ARG:HG2	2.54	0.43
4:A:1172:A:H62	4:A:1203:A:N6	2.17	0.43
4:A:2138:C:N4	4:A:2141:U:O4	2.52	0.43
8:E:183:LEU:HD23	8:E:183:LEU:HA	1.87	0.43
19:P:76:ASP:HB3	19:P:80:HIS:HA	2.01	0.43
3:4:85:LEU:HD21	3:4:106:LEU:CD2	2.49	0.43
3:4:316:ARG:O	3:4:320:GLU:HG3	2.18	0.43
3:4:426:ARG:CG	3:4:427:GLY:N	2.81	0.43
5:B:81:U:H2'	5:B:82:A:C8	2.53	0.43
10:G:46:ALA:HB3	10:G:50:ALA:HB3	2.00	0.43
19:P:41:ASN:N	19:P:49:VAL:HG22	2.34	0.43
3:4:46:LEU:O	3:4:47:GLU:CB	2.65	0.42
3:4:295:PHE:CE1	3:4:407:MET:SD	3.13	0.42
4:A:21:G:O2'	23:T:85:GLU:O	2.31	0.42
4:A:1668:C:O2'	4:A:1764:A:N3	2.42	0.42
12:I:115:LEU:HD21	12:I:123:ILE:HD12	2.01	0.42
3:4:305:ARG:HH22	3:4:341:ALA:C	2.22	0.42
3:4:435:THR:HG23	3:4:435:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2552:A:H2'	4:A:2553:G:C8	2.54	0.42
4:A:2970:U:H4'	10:G:139:LYS:HB2	2.02	0.42
3:4:82:LEU:CD1	3:4:113:THR:HB	2.40	0.42
4:A:759:G:N1	27:X:64:PRO:HB3	2.34	0.42
4:A:2083:A:N6	4:A:2099:G:O2'	2.51	0.42
4:A:2135:U:C5	4:A:2137:A:H8	2.37	0.42
4:A:2323:G:N1	4:A:2412:U:N3	2.68	0.42
4:A:2340:A:N6	4:A:2388:G:O6	2.44	0.42
4:A:2515:U:H2'	4:A:2516:U:C6	2.53	0.42
8:E:2:THR:OG1	8:E:20:LEU:O	2.37	0.42
22:S:80:ASN:OD1	22:S:80:ASN:N	2.51	0.42
27:X:50:ASN:HD22	27:X:50:ASN:HA	1.67	0.42
3:4:357:TYR:N	3:4:357:TYR:HD2	2.17	0.42
3:4:426:ARG:HE	3:4:430:VAL:CG1	2.25	0.42
3:4:434:HIS:CB	4:A:1185:A:H1'	2.37	0.42
4:A:2116:C:H2'	4:A:2117:C:H6	1.84	0.42
4:A:2529:A:H2'	4:A:2530:C:C6	2.54	0.42
3:4:133:GLU:O	3:4:137:LYS:HA	2.19	0.42
3:4:199:GLY:CA	3:4:201:ARG:CZ	2.97	0.42
4:A:2973:A:H4'	10:G:63:ARG:HG2	2.01	0.42
9:F:56:LEU:HD13	9:F:56:LEU:HA	1.88	0.42
11:H:77:ASP:N	11:H:77:ASP:OD1	2.52	0.42
11:H:100:VAL:HG12	11:H:119:LEU:HD12	2.01	0.42
19:P:44:ALA:O	19:P:112:ARG:NH1	2.52	0.42
19:P:79:ALA:O	19:P:81:SER:N	2.53	0.42
3:4:118:VAL:C	3:4:119:ILE:HD12	2.39	0.42
3:4:124:LEU:HD13	3:4:142:ASP:HB3	2.00	0.42
3:4:443:GLU:CB	3:4:452:LYS:HB2	2.50	0.42
4:A:1690:A:H2'	4:A:1691:A:C8	2.54	0.42
4:A:2527:G:H2'	4:A:2528:G:C8	2.55	0.42
4:A:2753:G:H5"	4:A:2754:G:H5"	2.02	0.42
9:F:23:LEU:HD21	9:F:172:GLU:HG3	2.01	0.42
3:4:187:ALA:C	3:4:189:GLY:N	2.71	0.42
3:4:245:ILE:HG21	3:4:294:PRO:HG2	1.99	0.42
3:4:250:ILE:HG23	3:4:250:ILE:O	2.19	0.42
4:A:1212:U:H2'	4:A:1213:A:H5"	2.01	0.42
4:A:1479:G:H4'	4:A:2025:C:H5	1.85	0.42
18:O:38:GLU:OE1	18:O:42:ARG:NH2	2.47	0.42
3:4:55:TRP:O	3:4:55:TRP:CD1	2.73	0.42
4:A:928:U:H2'	4:A:929:C:C6	2.54	0.42
4:A:1621:C:H2'	4:A:1622:G:H4'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1728:U:H4'	4:A:1729:A:H5'	2.02	0.42
19:P:111:GLY:H	19:P:114:ALA:HB3	1.85	0.42
3:4:143:ARG:NH2	3:4:305:ARG:O	2.51	0.42
4:A:1179:U:H2'	13:J:13:LEU:HA	2.01	0.42
4:A:1619:U:H2'	4:A:1620:U:C2	2.55	0.42
6:C:40:LYS:HB3	6:C:40:LYS:HE3	4.70	0.42
9:F:87:ARG:H	9:F:90:MET:HE1	1.84	0.42
16:M:104:VAL:HG11	16:M:110:VAL:HG13	2.02	0.42
3:4:93:ASP:HA	3:4:94:PRO:HD3	1.91	0.42
3:4:246:PRO:HA	3:4:326:ASP:OD2	2.20	0.42
3:4:283:THR:CG2	3:4:299:ASP:HB3	2.49	0.42
3:4:291:ASP:OD2	3:4:293:ARG:HG3	2.20	0.42
4:A:389:G:H21	4:A:412:A:H61	1.65	0.42
4:A:857:U:H2'	4:A:858:A:C8	2.54	0.42
4:A:960:G:OP2	4:A:960:G:N2	2.47	0.42
6:C:222:ARG:HE	6:C:222:ARG:HB2	1.67	0.42
6:C:258:ARG:NH2	6:C:264:SER:OG	2.53	0.42
12:I:33:VAL:HG21	13:J:117:ASP:HB2	2.02	0.42
3:4:184:SER:O	3:4:185:ARG:HB2	2.20	0.41
3:4:445:THR:HG23	3:4:450:ARG:H	1.84	0.41
6:C:163:ILE:HD12	6:C:175:LEU:HB3	2.01	0.41
11:H:119:LEU:HA	11:H:132:VAL:HG21	2.01	0.41
12:I:101:LYS:HD2	12:I:101:LYS:HA	1.78	0.41
26:W:86:HIS:CD2	26:W:87:PRO:HD2	2.55	0.41
3:4:410:LEU:HD12	3:4:410:LEU:N	2.34	0.41
4:A:1000:C:O2	4:A:1008:G:N1	2.53	0.41
5:B:9:G:H2'	5:B:10:G:C4	2.54	0.41
3:4:56:THR:HG23	3:4:57:GLU:OE2	2.21	0.41
3:4:319:LEU:HD12	3:4:319:LEU:N	2.35	0.41
3:4:424:TYR:CD1	3:4:424:TYR:N	2.88	0.41
4:A:1008:G:H2'	4:A:1009:U:C6	2.55	0.41
5:B:9:G:H5'	5:B:10:G:C8	2.56	0.41
6:C:132:PRO:HA	6:C:190:ARG:HA	2.01	0.41
6:C:147:LEU:HD23	6:C:147:LEU:HA	1.92	0.41
14:K:2:PRO:HB2	14:K:3:THR:H	1.60	0.41
19:P:56:ASN:OD1	19:P:56:ASN:N	2.51	0.41
25:V:40:ARG:HD3	25:V:61:THR:HG22	2.02	0.41
26:W:177:LEU:HD23	26:W:180:ASN:HB3	2.02	0.41
29:Z:11:ARG:O	29:Z:64:ARG:NH2	2.53	0.41
1:2:40:ASN:OD1	1:2:40:ASN:N	2.52	0.41
3:4:100:SER:HG	4:A:2131:G:H4'	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:357:TYR:O	3:4:358:ASP:C	2.59	0.41
4:A:264:G:H4'	4:A:516:G:H22	1.85	0.41
8:E:9:THR:HG22	8:E:128:THR:HG21	2.02	0.41
8:E:152:LYS:HG3	8:E:153:LYS:HG2	2.02	0.41
12:I:26:THR:H	12:I:78:ALA:HB3	1.86	0.41
19:P:87:LEU:HD23	19:P:87:LEU:HA	1.86	0.41
3:4:187:ALA:HB2	4:A:2826:A:N7	2.35	0.41
3:4:327:LEU:HD21	3:4:329:ILE:HD11	2.02	0.41
3:4:372:ASP:N	3:4:374:ALA:H	2.18	0.41
3:4:386:LEU:HD23	3:4:386:LEU:HA	1.76	0.41
4:A:1089:C:O2'	4:A:1101:A:N3	2.46	0.41
3:4:386:LEU:HA	3:4:387:PRO:HD3	1.89	0.41
3:4:429:LEU:HD13	3:4:429:LEU:HA	1.70	0.41
5:B:9:G:H2'	5:B:10:G:N9	2.36	0.41
6:C:79:VAL:HG22	6:C:115:ASP:H	1.86	0.41
7:D:125:GLY:O	7:D:129:ARG:HB3	2.20	0.41
3:4:284:THR:HG22	3:4:298:THR:HG23	2.02	0.41
3:4:308:PRO:HG2	3:4:311:LEU:HD21	2.01	0.41
5:B:27:A:N3	5:B:115:A:O2'	2.53	0.41
8:E:42:LEU:HD23	8:E:42:LEU:HA	1.94	0.41
9:F:110:LEU:HD23	9:F:114:ALA:HB3	2.03	0.41
10:G:27:LYS:NZ	10:G:28:GLY:O	2.47	0.41
12:I:3:LYS:HE3	12:I:59:ARG:HH11	1.85	0.41
3:4:186:GLN:CB	3:4:207:LYS:NZ	2.83	0.41
3:4:198:VAL:O	4:A:2286:A:N6	2.54	0.41
3:4:257:GLY:HA2	36:4:501:GCP:O5'	2.21	0.41
3:4:369:ASN:C	3:4:371:ILE:N	2.73	0.41
4:A:1758:G:O2'	4:A:1759:A:O4'	2.36	0.41
10:G:33:LEU:HB3	10:G:76:LEU:HG	2.02	0.41
1:2:47:ILE:O	1:2:51:HIS:HB3	2.21	0.41
3:4:47:GLU:CA	3:4:79:SER:HB3	2.51	0.41
3:4:171:TYR:CD1	3:4:171:TYR:C	2.95	0.41
3:4:202:GLY:CA	4:A:2676:C:O4'	2.67	0.41
3:4:237:ARG:HE	3:4:240:ARG:NH2	2.19	0.41
3:4:275:ALA:C	3:4:276:LEU:HD12	2.40	0.41
4:A:2902:A:H2'	4:A:2903:A:C8	2.56	0.41
3:4:43:GLN:HA	3:4:43:GLN:HE21	1.85	0.41
3:4:148:LEU:HA	3:4:311:LEU:CD1	2.49	0.41
3:4:199:GLY:CA	3:4:201:ARG:CD	2.98	0.41
3:4:334:GLY:C	3:4:336:ASP:H	2.24	0.41
3:4:337:VAL:HG23	3:4:338:ASN:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:406:ARG:HA	3:4:409:GLU:CD	2.42	0.41
4:A:368:U:O2	4:A:434:G:N2	2.44	0.41
3:4:141:ILE:HG22	3:4:145:ALA:HB3	2.04	0.40
3:4:440:ASP:HB3	3:4:453:ALA:HA	2.03	0.40
4:A:159:A:N3	4:A:2431:C:O2'	2.42	0.40
4:A:2314:U:H4'	28:Y:56:ILE:HD11	2.03	0.40
8:E:101:ARG:HH11	8:E:101:ARG:HD3	1.76	0.40
14:K:92:LEU:HA	14:K:92:LEU:HD23	1.89	0.40
20:Q:3:THR:HG23	20:Q:4:LEU:HG	2.02	0.40
3:4:250:ILE:CG2	3:4:299:ASP:HA	2.51	0.40
3:4:261:LEU:HD13	3:4:261:LEU:HA	1.93	0.40
3:4:371:ILE:CG2	3:4:391:PHE:CD2	3.03	0.40
4:A:2601:A:HO2'	4:A:2602:A:H8	1.68	0.40
4:A:2905:C:OP2	7:D:119:LYS:NZ	2.52	0.40
28:Y:5:CYS:SG	28:Y:8:CYS:N	2.75	0.40
3:4:42:ARG:NH1	3:4:44:LEU:CB	2.79	0.40
3:4:52:VAL:HG12	3:4:106:LEU:HD11	2.03	0.40
3:4:178:GLY:C	3:4:180:GLY:N	2.73	0.40
3:4:215:ILE:HG23	3:4:216:ARG:N	2.35	0.40
3:4:288:GLU:HA	3:4:295:PHE:HD2	1.87	0.40
3:4:290:GLU:CD	3:4:291:ASP:N	2.75	0.40
16:M:137:ILE:HG21	16:M:144:ALA:HB2	2.03	0.40
3:4:462:THR:O	3:4:463:LEU:C	2.60	0.40
26:W:109:GLU:HG2	26:W:130:THR:HB	2.04	0.40
3:4:371:ILE:CG2	3:4:372:ASP:H	2.28	0.40
4:A:978:A:H2'	4:A:979:G:H8	1.86	0.40
4:A:1007:G:N1	4:A:1008:G:N3	2.70	0.40
4:A:2599:G:N2	4:A:2601:A:O2'	2.55	0.40
9:F:43:VAL:HG13	9:F:161:ILE:HG22	2.02	0.40
14:K:7:LYS:HD3	14:K:7:LYS:HA	1.77	0.40
17:N:71:ASP:N	17:N:71:ASP:OD1	2.55	0.40
19:P:50:GLN:HB2	19:P:63:ALA:N	2.36	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	2	57/61 (93%)	56 (98%)	1 (2%)	0	100	100
2	3	21/24 (88%)	20 (95%)	1 (5%)	0	100	100
3	4	424/470 (90%)	343 (81%)	79 (19%)	2 (0%)	25	55
6	C	273/278 (98%)	258 (94%)	15 (6%)	0	100	100
7	D	212/217 (98%)	196 (92%)	16 (8%)	0	100	100
8	E	207/215 (96%)	192 (93%)	15 (7%)	0	100	100
9	F	180/187 (96%)	146 (81%)	34 (19%)	0	100	100
10	G	174/179 (97%)	151 (87%)	23 (13%)	0	100	100
11	H	149/151 (99%)	110 (74%)	39 (26%)	0	100	100
12	I	124/175 (71%)	108 (87%)	16 (13%)	0	100	100
13	J	131/142 (92%)	100 (76%)	31 (24%)	0	100	100
14	K	144/147 (98%)	137 (95%)	7 (5%)	0	100	100
15	L	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
16	M	143/147 (97%)	130 (91%)	13 (9%)	0	100	100
17	N	134/138 (97%)	124 (92%)	10 (8%)	0	100	100
18	O	116/199 (58%)	107 (92%)	9 (8%)	0	100	100
19	P	124/127 (98%)	88 (71%)	36 (29%)	0	100	100
20	Q	111/113 (98%)	95 (86%)	16 (14%)	0	100	100
21	R	122/129 (95%)	118 (97%)	4 (3%)	0	100	100
22	S	98/103 (95%)	92 (94%)	6 (6%)	0	100	100
23	T	112/153 (73%)	110 (98%)	2 (2%)	0	100	100
24	U	95/100 (95%)	90 (95%)	5 (5%)	0	100	100
25	V	93/105 (89%)	82 (88%)	11 (12%)	0	100	100
26	W	190/215 (88%)	170 (90%)	20 (10%)	0	100	100
27	X	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
28	Y	61/64 (95%)	55 (90%)	6 (10%)	0	100	100
29	Z	62/77 (80%)	62 (100%)	0	0	100	100
30	b	52/57 (91%)	52 (100%)	0	0	100	100
31	c	47/55 (86%)	45 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	d	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
33	e	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
34	f	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
35	g	46/75 (61%)	41 (89%)	5 (11%)	0	100	100
All	All	4039/4461 (90%)	3594 (89%)	443 (11%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	4	294	PRO
3	4	431	ALA

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	2	52/54 (96%)	52 (100%)	0	100	100
2	3	18/19 (95%)	18 (100%)	0	100	100
3	4	337/372 (91%)	310 (92%)	27 (8%)	10	31
6	C	215/218 (99%)	214 (100%)	1 (0%)	86	92
7	D	160/163 (98%)	160 (100%)	0	100	100
8	E	169/173 (98%)	169 (100%)	0	100	100
9	F	151/156 (97%)	149 (99%)	2 (1%)	65	80
10	G	148/150 (99%)	145 (98%)	3 (2%)	50	71
11	H	90/116 (78%)	90 (100%)	0	100	100
12	I	89/120 (74%)	89 (100%)	0	100	100
13	J	102/108 (94%)	100 (98%)	2 (2%)	50	71
14	K	119/120 (99%)	119 (100%)	0	100	100
15	L	100/100 (100%)	99 (99%)	1 (1%)	73	85
16	M	112/114 (98%)	111 (99%)	1 (1%)	75	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	N	114/116 (98%)	112 (98%)	2 (2%)	54 74
18	O	97/158 (61%)	97 (100%)	0	100 100
19	P	93/94 (99%)	88 (95%)	5 (5%)	18 44
20	Q	100/100 (100%)	100 (100%)	0	100 100
21	R	97/99 (98%)	97 (100%)	0	100 100
22	S	81/83 (98%)	81 (100%)	0	100 100
23	T	90/117 (77%)	89 (99%)	1 (1%)	70 83
24	U	83/85 (98%)	83 (100%)	0	100 100
25	V	81/86 (94%)	80 (99%)	1 (1%)	67 81
26	W	155/168 (92%)	155 (100%)	0	100 100
27	X	58/63 (92%)	57 (98%)	1 (2%)	56 75
28	Y	50/51 (98%)	49 (98%)	1 (2%)	50 71
29	Z	58/66 (88%)	57 (98%)	1 (2%)	56 75
30	b	43/46 (94%)	43 (100%)	0	100 100
31	c	47/52 (90%)	47 (100%)	0	100 100
32	d	35/36 (97%)	35 (100%)	0	100 100
33	e	53/54 (98%)	53 (100%)	0	100 100
34	f	35/35 (100%)	35 (100%)	0	100 100
35	g	43/63 (68%)	43 (100%)	0	100 100
All	All	3275/3555 (92%)	3226 (98%)	49 (2%)	60 78

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	4	46	LEU
3	4	56	THR
3	4	57	GLU
3	4	64	GLU
3	4	85	LEU
3	4	98	ILE
3	4	106	LEU
3	4	140	VAL
3	4	147	ILE
3	4	148	LEU
3	4	172	MET

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Mol	Chain	Res	Type
3	4	186	GLN
3	4	201	ARG
3	4	218	ARG
3	4	226	ILE
3	4	274	ASN
3	4	283	THR
3	4	295	PHE
3	4	311	LEU
3	4	384	ARG
3	4	391	PHE
3	4	430	VAL
3	4	438	HIS
3	4	439	VAL
3	4	446	ASP
3	4	450	ARG
3	4	464	ARG
6	C	134	ARG
9	F	52	ARG
9	F	74	VAL
10	G	36	ASP
10	G	45	ARG
10	G	66	HIS
13	J	108	ARG
13	J	135	ARG
15	L	73	ASP
16	M	49	MET
17	N	60	ARG
17	N	120	ARG
19	P	45	ARG
19	P	47	ILE
19	P	50	GLN
19	P	51	LEU
19	P	108	THR
23	T	99	ARG
25	V	44	HIS
27	X	14	ARG
28	Y	5	CYS
29	Z	58	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
3	4	43	GLN
3	4	87	GLN
3	4	128	GLN
3	4	154	HIS
3	4	434	HIS
3	4	444	HIS
6	C	91	ASN
6	C	261	ASN
7	D	34	ASN
8	E	100	GLN
9	F	58	ASN
9	F	62	ASN
10	G	103	ASN
11	H	102	ASN
11	H	118	GLN
12	I	54	ASN
13	J	14	GLN
13	J	21	ASN
13	J	36	ASN
13	J	45	ASN
14	K	132	HIS
14	K	144	GLN
15	L	91	ASN
16	M	76	GLN
19	P	16	ASN
21	R	39	GLN
22	S	76	HIS
22	S	90	HIS
23	T	67	ASN
23	T	109	HIS
24	U	34	HIS
24	U	41	GLN
26	W	14	ASN
26	W	46	HIS
26	W	76	GLN
27	X	50	ASN
35	g	40	GLN
35	g	42	HIS

5.3.3 RNA

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	A	3118/3120 (99%)	760 (24%)	22 (0%)
5	B	117/118 (99%)	37 (31%)	2 (1%)
All	All	3235/3238 (99%)	797 (24%)	24 (0%)

All (797) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	A	7	U
4	A	9	U
4	A	11	A
4	A	12	G
4	A	20	G
4	A	31	U
4	A	32	G
4	A	33	G
4	A	42	G
4	A	46	A
4	A	48	G
4	A	55	G
4	A	58	G
4	A	60	A
4	A	68	A
4	A	71	A
4	A	72	G
4	A	80	G
4	A	81	A
4	A	88	A
4	A	91	C
4	A	94	G
4	A	95	C
4	A	98	U
4	A	99	G
4	A	107	G
4	A	115	A
4	A	116	A
4	A	117	U
4	A	122	A
4	A	125	C
4	A	137	G
4	A	162	A
4	A	164	A

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Mol	Chain	Res	Type
4	A	180	A
4	A	195	A
4	A	198	A
4	A	200	C
4	A	203	A
4	A	212	A
4	A	214	G
4	A	215	A
4	A	220	A
4	A	221	A
4	A	227	A
4	A	229	U
4	A	230	G
4	A	241	A
4	A	248	G
4	A	266	U
4	A	267	G
4	A	273	A
4	A	274	C
4	A	276	G
4	A	280	G
4	A	281	C
4	A	286	G
4	A	288	U
4	A	289	A
4	A	290	C
4	A	292	G
4	A	296	A
4	A	299	G
4	A	300	G
4	A	302	U
4	A	303	G
4	A	305	G
4	A	306	U
4	A	307	G
4	A	309	G
4	A	314	G
4	A	315	U
4	A	316	U
4	A	317	G
4	A	318	U
4	A	319	G

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Mol	Chain	Res	Type
4	A	325	U
4	A	326	A
4	A	327	U
4	A	329	U
4	A	330	U
4	A	331	U
4	A	334	G
4	A	337	U
4	A	338	C
4	A	340	A
4	A	341	C
4	A	342	C
4	A	344	G
4	A	351	G
4	A	357	U
4	A	358	G
4	A	361	A
4	A	363	A
4	A	364	A
4	A	366	G
4	A	370	U
4	A	371	G
4	A	382	A
4	A	384	G
4	A	391	G
4	A	393	U
4	A	399	G
4	A	405	G
4	A	412	A
4	A	413	G
4	A	415	G
4	A	416	C
4	A	427	A
4	A	437	G
4	A	438	U
4	A	441	G
4	A	445	U
4	A	446	G
4	A	451	U
4	A	453	U
4	A	460	G
4	A	474	G

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Mol	Chain	Res	Type
4	A	489	A
4	A	492	C
4	A	493	U
4	A	494	G
4	A	511	A
4	A	512	G
4	A	543	U
4	A	544	U
4	A	555	G
4	A	563	U
4	A	566	A
4	A	567	A
4	A	569	G
4	A	570	U
4	A	571	A
4	A	572	C
4	A	573	C
4	A	578	G
4	A	581	G
4	A	591	G
4	A	592	A
4	A	593	G
4	A	594	U
4	A	595	A
4	A	596	C
4	A	605	G
4	A	612	U
4	A	617	U
4	A	618	C
4	A	619	C
4	A	620	G
4	A	633	A
4	A	635	G
4	A	636	U
4	A	637	G
4	A	639	C
4	A	640	G
4	A	642	G
4	A	644	G
4	A	655	G
4	A	665	G
4	A	667	A

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Mol	Chain	Res	Type
4	A	678	A
4	A	679	G
4	A	684	G
4	A	696	A
4	A	706	G
4	A	707	G
4	A	708	G
4	A	709	U
4	A	721	A
4	A	725	A
4	A	728	G
4	A	731	A
4	A	736	G
4	A	737	A
4	A	739	U
4	A	740	A
4	A	742	G
4	A	747	A
4	A	748	U
4	A	757	G
4	A	758	A
4	A	759	G
4	A	760	U
4	A	763	G
4	A	765	G
4	A	766	G
4	A	768	G
4	A	769	U
4	A	801	U
4	A	826	G
4	A	830	A
4	A	831	A
4	A	842	A
4	A	843	G
4	A	845	C
4	A	862	U
4	A	868	C
4	A	872	G
4	A	877	U
4	A	879	A
4	A	880	G
4	A	890	G

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Mol	Chain	Res	Type
4	A	891	G
4	A	897	A
4	A	899	G
4	A	904	A
4	A	908	A
4	A	919	A
4	A	920	G
4	A	927	C
4	A	942	U
4	A	944	A
4	A	974	G
4	A	975	U
4	A	981	U
4	A	982	A
4	A	990	G
4	A	994	A
4	A	995	U
4	A	996	G
4	A	1001	C
4	A	1002	C
4	A	1004	C
4	A	1005	A
4	A	1006	G
4	A	1008	G
4	A	1010	U
4	A	1011	A
4	A	1012	C
4	A	1014	G
4	A	1016	C
4	A	1025	A
4	A	1027	C
4	A	1046	C
4	A	1047	A
4	A	1048	A
4	A	1049	G
4	A	1063	G
4	A	1074	A
4	A	1076	A
4	A	1078	G
4	A	1085	G
4	A	1091	A
4	A	1092	G

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Mol	Chain	Res	Type
4	A	1097	A
4	A	1101	A
4	A	1114	G
4	A	1127	A
4	A	1130	C
4	A	1131	G
4	A	1143	G
4	A	1144	A
4	A	1148	G
4	A	1151	U
4	A	1156	A
4	A	1162	G
4	A	1163	A
4	A	1164	A
4	A	1165	G
4	A	1167	C
4	A	1171	C
4	A	1172	A
4	A	1173	G
4	A	1174	G
4	A	1175	A
4	A	1176	G
4	A	1178	U
4	A	1179	U
4	A	1180	G
4	A	1181	G
4	A	1182	C
4	A	1184	U
4	A	1185	A
4	A	1186	G
4	A	1187	A
4	A	1188	A
4	A	1190	C
4	A	1191	A
4	A	1195	A
4	A	1196	C
4	A	1197	C
4	A	1198	C
4	A	1199	U
4	A	1200	U
4	A	1201	G
4	A	1202	A

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Mol	Chain	Res	Type
4	A	1203	A
4	A	1204	A
4	A	1205	G
4	A	1206	A
4	A	1207	G
4	A	1212	U
4	A	1213	A
4	A	1214	A
4	A	1216	A
4	A	1217	G
4	A	1219	U
4	A	1222	C
4	A	1225	G
4	A	1226	U
4	A	1227	C
4	A	1228	A
4	A	1229	A
4	A	1230	G
4	A	1231	U
4	A	1236	G
4	A	1237	U
4	A	1238	G
4	A	1239	C
4	A	1240	G
4	A	1246	A
4	A	1248	U
4	A	1251	A
4	A	1253	C
4	A	1254	G
4	A	1260	C
4	A	1261	A
4	A	1270	G
4	A	1275	A
4	A	1292	U
4	A	1293	G
4	A	1332	G
4	A	1343	G
4	A	1344	A
4	A	1353	G
4	A	1362	A
4	A	1365	G
4	A	1371	G

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Mol	Chain	Res	Type
4	A	1377	A
4	A	1380	A
4	A	1386	G
4	A	1387	A
4	A	1389	U
4	A	1399	A
4	A	1401	A
4	A	1402	A
4	A	1404	C
4	A	1415	A
4	A	1416	A
4	A	1436	C
4	A	1444	U
4	A	1456	G
4	A	1465	C
4	A	1467	U
4	A	1480	A
4	A	1493	A
4	A	1494	U
4	A	1499	A
4	A	1508	A
4	A	1510	A
4	A	1518	A
4	A	1522	G
4	A	1530	G
4	A	1531	C
4	A	1532	G
4	A	1533	U
4	A	1535	C
4	A	1536	A
4	A	1538	G
4	A	1542	A
4	A	1546	A
4	A	1548	C
4	A	1549	G
4	A	1550	G
4	A	1551	U
4	A	1553	C
4	A	1556	A
4	A	1564	A
4	A	1566	A
4	A	1567	C

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Mol	Chain	Res	Type
4	A	1573	U
4	A	1574	G
4	A	1575	A
4	A	1577	C
4	A	1578	G
4	A	1580	A
4	A	1582	C
4	A	1583	U
4	A	1584	U
4	A	1585	U
4	A	1586	C
4	A	1587	G
4	A	1588	G
4	A	1589	G
4	A	1592	G
4	A	1593	U
4	A	1597	G
4	A	1598	U
4	A	1599	U
4	A	1600	G
4	A	1601	G
4	A	1603	G
4	A	1608	U
4	A	1609	G
4	A	1610	C
4	A	1616	A
4	A	1617	C
4	A	1618	C
4	A	1619	U
4	A	1621	C
4	A	1622	G
4	A	1623	U
4	A	1624	U
4	A	1625	G
4	A	1628	A
4	A	1629	G
4	A	1630	U
4	A	1632	G
4	A	1636	A
4	A	1638	C
4	A	1640	A
4	A	1648	A

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Mol	Chain	Res	Type
4	A	1649	C
4	A	1670	G
4	A	1671	U
4	A	1673	A
4	A	1674	G
4	A	1676	G
4	A	1678	U
4	A	1679	A
4	A	1681	U
4	A	1688	G
4	A	1703	G
4	A	1708	A
4	A	1709	U
4	A	1710	A
4	A	1713	U
4	A	1716	A
4	A	1717	U
4	A	1718	C
4	A	1723	U
4	A	1728	U
4	A	1730	U
4	A	1731	A
4	A	1737	A
4	A	1744	A
4	A	1746	G
4	A	1754	G
4	A	1756	G
4	A	1757	U
4	A	1759	A
4	A	1767	U
4	A	1768	C
4	A	1769	G
4	A	1777	U
4	A	1778	A
4	A	1786	G
4	A	1787	A
4	A	1789	A
4	A	1798	U
4	A	1803	A
4	A	1813	C
4	A	1825	C
4	A	1826	A

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Mol	Chain	Res	Type
4	A	1835	C
4	A	1844	A
4	A	1847	U
4	A	1848	A
4	A	1851	G
4	A	1852	A
4	A	1864	U
4	A	1866	C
4	A	1871	G
4	A	1872	A
4	A	1892	G
4	A	1893	C
4	A	1904	C
4	A	1911	U
4	A	1912	C
4	A	1916	A
4	A	1931	A
4	A	1940	A
4	A	1941	A
4	A	1942	G
4	A	1943	C
4	A	1945	U
4	A	1946	U
4	A	1947	U
4	A	1948	A
4	A	1949	C
4	A	1955	A
4	A	1961	G
4	A	1972	A
4	A	1973	C
4	A	1975	A
4	A	1981	U
4	A	1990	A
4	A	1999	U
4	A	2017	C
4	A	2018	G
4	A	2026	A
4	A	2033	U
4	A	2046	A
4	A	2075	G
4	A	2083	A
4	A	2085	C

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Mol	Chain	Res	Type
4	A	2086	U
4	A	2089	C
4	A	2092	U
4	A	2093	G
4	A	2094	G
4	A	2095	G
4	A	2107	G
4	A	2113	A
4	A	2128	G
4	A	2130	G
4	A	2131	G
4	A	2132	U
4	A	2133	G
4	A	2134	G
4	A	2135	U
4	A	2136	A
4	A	2137	A
4	A	2138	C
4	A	2139	U
4	A	2140	A
4	A	2141	U
4	A	2142	A
4	A	2145	C
4	A	2146	A
4	A	2147	U
4	A	2148	C
4	A	2151	A
4	A	2152	A
4	A	2153	G
4	A	2154	G
4	A	2160	A
4	A	2161	A
4	A	2162	A
4	A	2163	U
4	A	2179	U
4	A	2187	U
4	A	2190	A
4	A	2191	C
4	A	2194	A
4	A	2195	U
4	A	2196	G
4	A	2215	U

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Mol	Chain	Res	Type
4	A	2216	G
4	A	2217	U
4	A	2221	A
4	A	2227	A
4	A	2246	U
4	A	2247	A
4	A	2251	G
4	A	2254	A
4	A	2255	A
4	A	2256	G
4	A	2257	A
4	A	2263	G
4	A	2267	C
4	A	2276	G
4	A	2279	C
4	A	2280	G
4	A	2284	A
4	A	2285	G
4	A	2286	A
4	A	2310	G
4	A	2316	G
4	A	2320	C
4	A	2321	U
4	A	2323	G
4	A	2326	A
4	A	2327	C
4	A	2329	G
4	A	2330	U
4	A	2332	U
4	A	2333	G
4	A	2334	U
4	A	2335	G
4	A	2336	U
4	A	2339	G
4	A	2340	A
4	A	2341	U
4	A	2342	A
4	A	2343	G
4	A	2345	U
4	A	2346	G
4	A	2348	G
4	A	2350	G

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Mol	Chain	Res	Type
4	A	2351	A
4	A	2353	U
4	A	2354	G
4	A	2355	U
4	A	2356	G
4	A	2357	A
4	A	2358	A
4	A	2362	C
4	A	2363	A
4	A	2365	A
4	A	2366	C
4	A	2367	G
4	A	2368	C
4	A	2369	C
4	A	2371	G
4	A	2374	U
4	A	2376	G
4	A	2379	G
4	A	2380	G
4	A	2381	A
4	A	2382	G
4	A	2384	C
4	A	2385	G
4	A	2386	U
4	A	2387	U
4	A	2388	G
4	A	2389	U
4	A	2390	U
4	A	2391	G
4	A	2392	A
4	A	2393	A
4	A	2394	A
4	A	2395	U
4	A	2396	A
4	A	2398	C
4	A	2399	A
4	A	2400	C
4	A	2401	U
4	A	2402	C
4	A	2403	U
4	A	2405	A
4	A	2407	C

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Mol	Chain	Res	Type
4	A	2410	A
4	A	2413	G
4	A	2421	A
4	A	2422	A
4	A	2434	A
4	A	2446	G
4	A	2449	A
4	A	2462	G
4	A	2463	G
4	A	2467	U
4	A	2470	A
4	A	2474	G
4	A	2475	G
4	A	2476	G
4	A	2483	G
4	A	2490	A
4	A	2492	A
4	A	2503	G
4	A	2506	G
4	A	2507	C
4	A	2511	A
4	A	2516	U
4	A	2528	G
4	A	2529	A
4	A	2531	G
4	A	2532	G
4	A	2533	C
4	A	2534	A
4	A	2535	A
4	A	2536	U
4	A	2538	A
4	A	2544	U
4	A	2545	G
4	A	2549	G
4	A	2559	A
4	A	2567	U
4	A	2569	G
4	A	2571	C
4	A	2572	U
4	A	2574	C
4	A	2582	A
4	A	2585	U

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Mol	Chain	Res	Type
4	A	2600	A
4	A	2601	A
4	A	2602	A
4	A	2607	G
4	A	2609	A
4	A	2620	G
4	A	2630	A
4	A	2631	G
4	A	2646	C
4	A	2647	U
4	A	2649	A
4	A	2653	G
4	A	2654	A
4	A	2655	U
4	A	2656	A
4	A	2657	A
4	A	2659	A
4	A	2665	C
4	A	2672	A
4	A	2676	C
4	A	2683	A
4	A	2694	G
4	A	2698	C
4	A	2700	A
4	A	2702	A
4	A	2715	U
4	A	2718	G
4	A	2726	G
4	A	2728	U
4	A	2729	G
4	A	2742	A
4	A	2744	C
4	A	2749	G
4	A	2753	G
4	A	2759	G
4	A	2780	C
4	A	2786	U
4	A	2790	A
4	A	2791	G
4	A	2796	A
4	A	2797	C
4	A	2822	A

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Mol	Chain	Res	Type
4	A	2823	G
4	A	2826	A
4	A	2827	G
4	A	2832	G
4	A	2833	U
4	A	2834	C
4	A	2837	U
4	A	2839	U
4	A	2853	C
4	A	2854	A
4	A	2865	G
4	A	2870	C
4	A	2884	A
4	A	2893	G
4	A	2913	U
4	A	2915	C
4	A	2936	C
4	A	2938	G
4	A	2950	C
4	A	2956	G
4	A	2957	A
4	A	2963	U
4	A	2969	C
4	A	2972	A
4	A	2976	C
4	A	2985	G
4	A	2990	A
4	A	3002	A
4	A	3005	A
4	A	3009	U
4	A	3015	C
4	A	3021	A
4	A	3022	G
4	A	3023	G
4	A	3029	U
4	A	3039	C
4	A	3041	C
4	A	3042	A
4	A	3044	A
4	A	3050	G
4	A	3056	A
4	A	3080	A

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Mol	Chain	Res	Type
4	A	3082	U
4	A	3088	C
4	A	3093	A
4	A	3101	C
4	A	3105	C
4	A	3106	C
4	A	3107	G
4	A	3112	A
4	A	3114	A
4	A	3115	A
4	A	3119	A
4	A	3120	C
5	B	3	U
5	B	4	A
5	B	5	C
5	B	8	C
5	B	9	G
5	B	10	G
5	B	11	U
5	B	13	C
5	B	14	A
5	B	17	G
5	B	23	G
5	B	25	G
5	B	31	C
5	B	33	C
5	B	36	U
5	B	41	U
5	B	42	C
5	B	43	C
5	B	53	A
5	B	56	C
5	B	57	U
5	B	59	A
5	B	66	C
5	B	67	A
5	B	74	A
5	B	86	A
5	B	89	C
5	B	97	A
5	B	100	G
5	B	103	G

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Mol	Chain	Res	Type
5	B	106	C
5	B	107	A
5	B	109	C
5	B	113	G
5	B	114	A
5	B	117	A
5	B	118	C

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	A	97	U
4	A	272	A
4	A	336	C
4	A	357	U
4	A	643	G
4	A	842	A
4	A	974	G
4	A	981	U
4	A	1199	U
4	A	1206	A
4	A	1230	G
4	A	1292	U
4	A	1947	U
4	A	2094	G
4	A	2135	U
4	A	2141	U
4	A	2320	C
4	A	2328	G
4	A	2345	U
4	A	2397	C
4	A	2656	A
4	A	2779	U
5	B	10	G
5	B	113	G

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
36	GCP	4	501	-	27,34,34	1.36	3 (11%)	35,54,54	1.93	7 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	GCP	4	501	-	-	5/15/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	4	501	GCP	C5-C6	3.99	1.48	1.41
36	4	501	GCP	PG-O2G	2.85	1.61	1.55
36	4	501	GCP	PG-O3G	2.61	1.60	1.55

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	4	501	GCP	C2-N3-C4	4.84	120.70	115.48
36	4	501	GCP	PB-O3A-PA	-4.58	117.42	132.37
36	4	501	GCP	C2-N1-C6	4.23	121.85	115.96
36	4	501	GCP	C5-C6-N1	-3.91	118.19	123.42
36	4	501	GCP	N3-C2-N1	-3.17	123.18	127.21
36	4	501	GCP	C4-C5-N7	-2.86	106.32	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	4	501	GCP	C4-C5-C6	-2.84	116.88	121.23

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	4	501	GCP	PB-C3B-PG-O1G
36	4	501	GCP	PB-C3B-PG-O2G
36	4	501	GCP	PB-C3B-PG-O3G
36	4	501	GCP	C5'-O5'-PA-O1A
36	4	501	GCP	C4'-C5'-O5'-PA

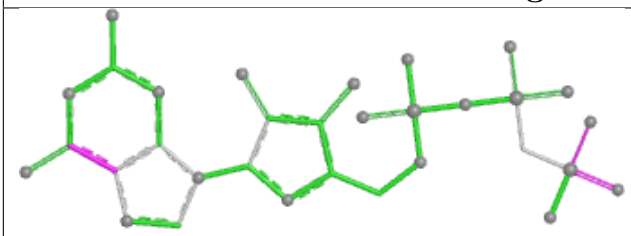
There are no ring outliers.

1 monomer is involved in 15 short contacts:

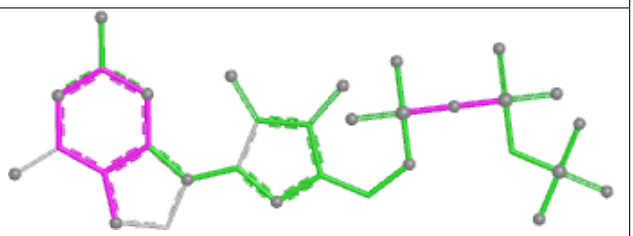
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	4	501	GCP	15	0

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

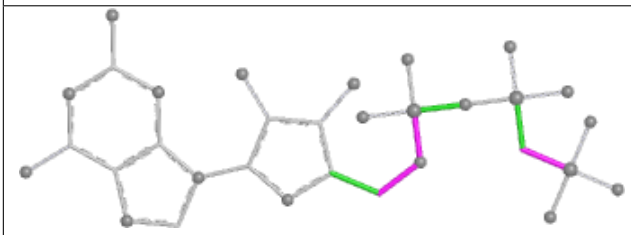
Ligand GCP 4 501



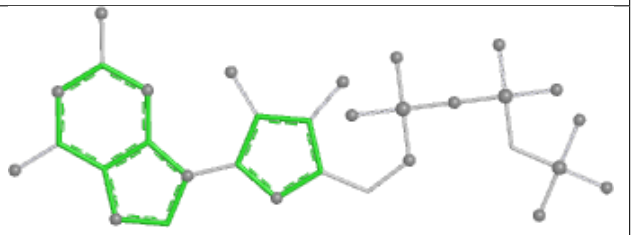
Bond lengths



Bond angles



Torsions



Rings

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.

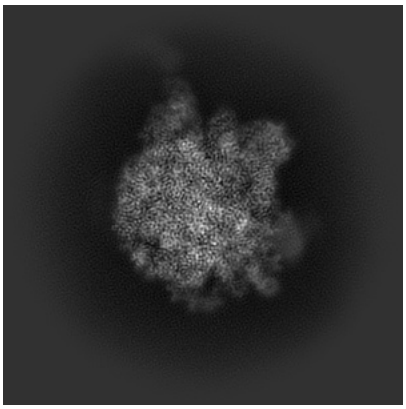
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43294. These allow visual inspection of the internal detail of the map and identification of artifacts.

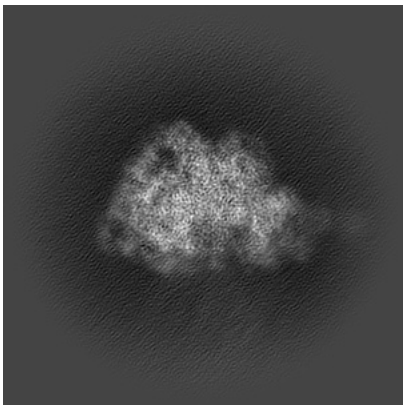
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

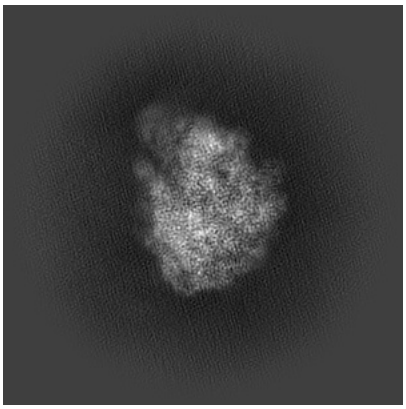
6.1.1 Primary map



X

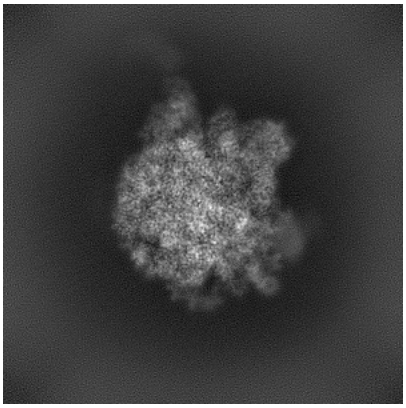


Y

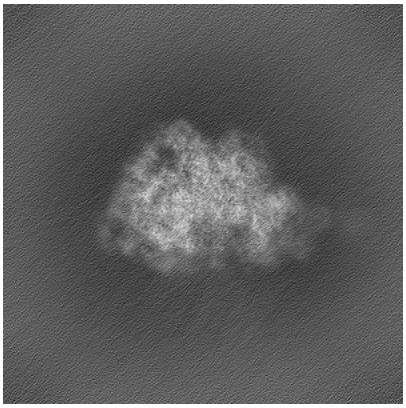


Z

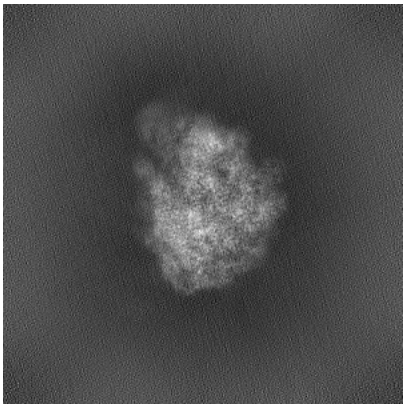
6.1.2 Raw map



X



Y

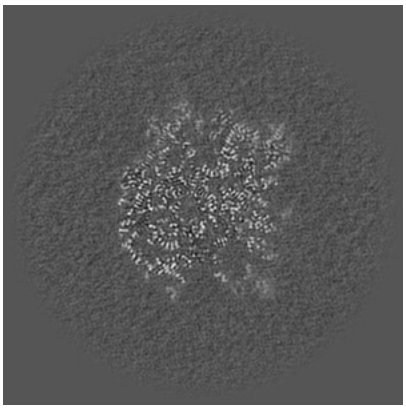


Z

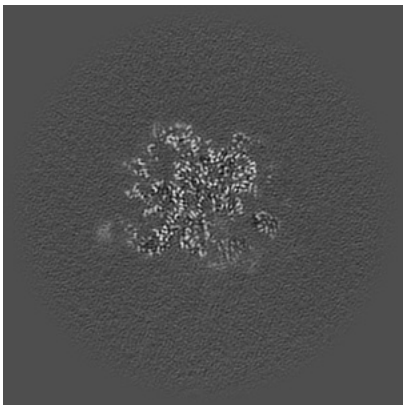
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

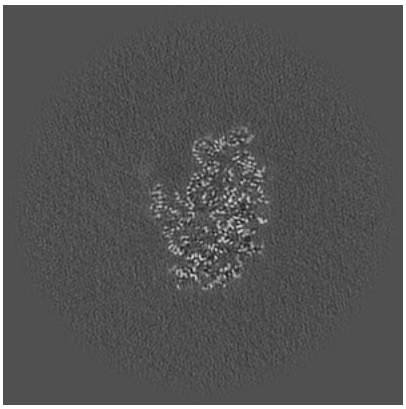
6.2.1 Primary map



X Index: 200

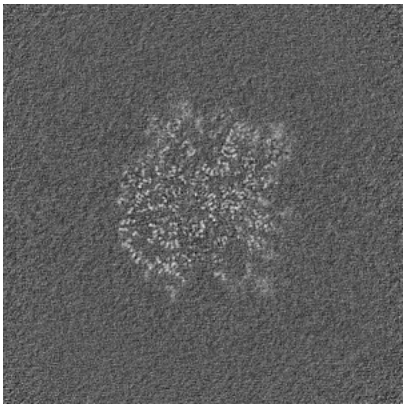


Y Index: 200

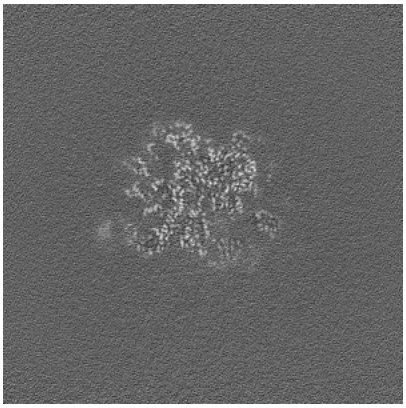


Z Index: 200

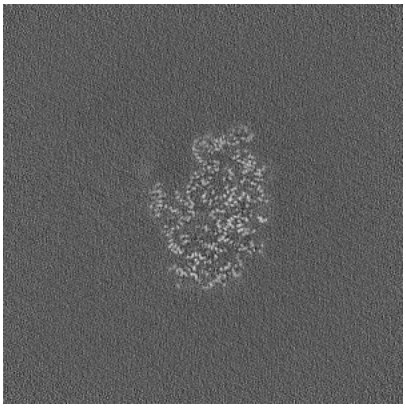
6.2.2 Raw map



X Index: 200



Y Index: 200

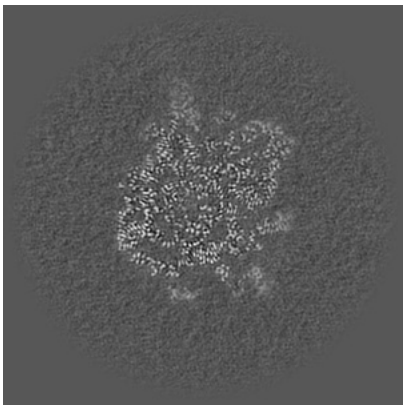


Z Index: 200

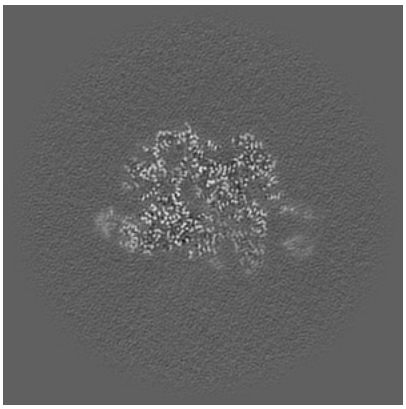
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

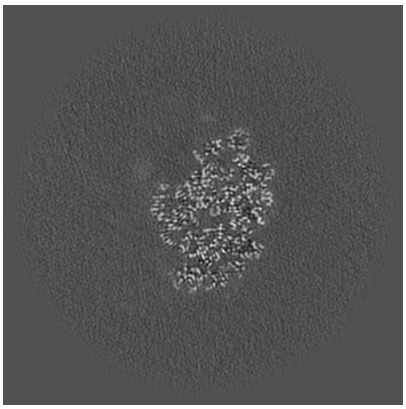
6.3.1 Primary map



X Index: 194

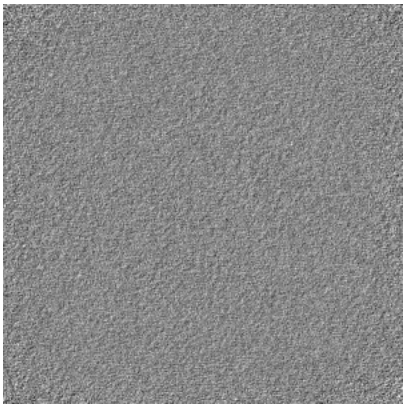


Y Index: 190

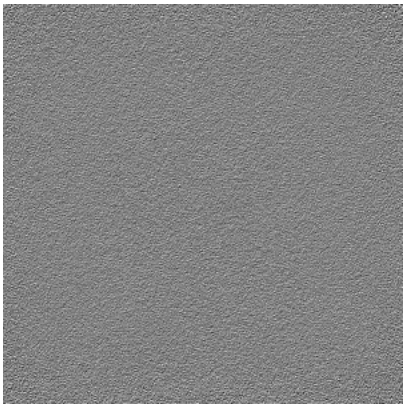


Z Index: 196

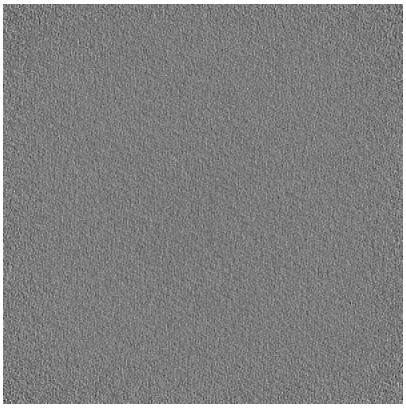
6.3.2 Raw map



X Index: 0



Y Index: 0

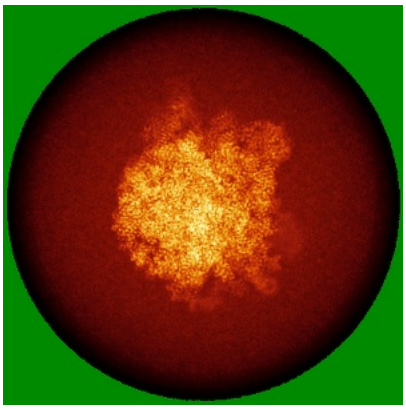


Z Index: 0

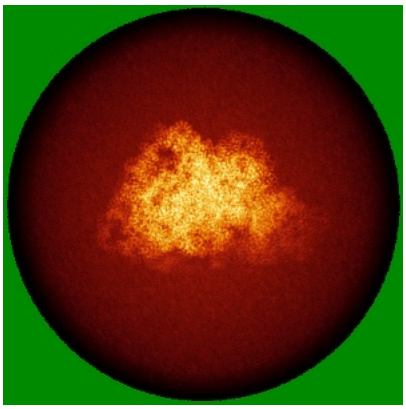
The images above show the largest variance slices of the map in three orthogonal directions.

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

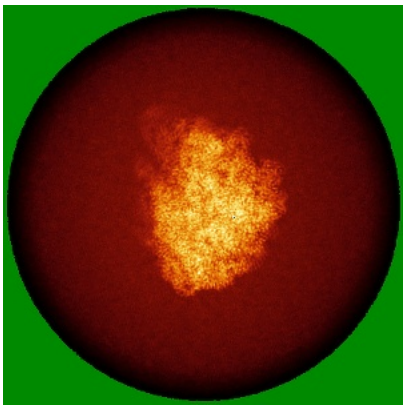
6.4.1 Primary map



X

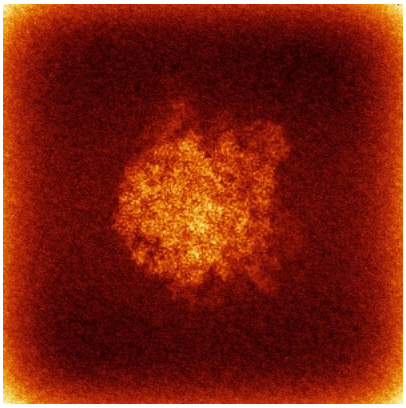


Y

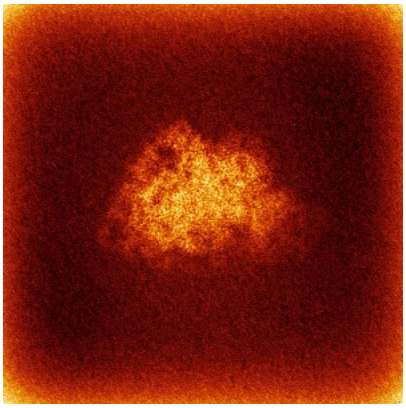


Z

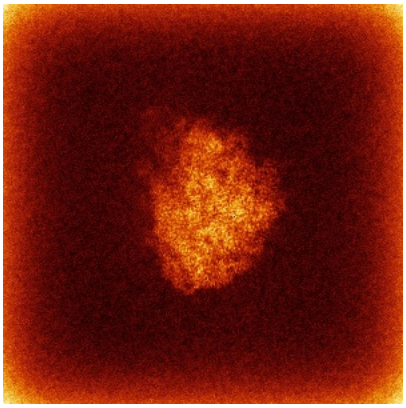
6.4.2 Raw map



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.

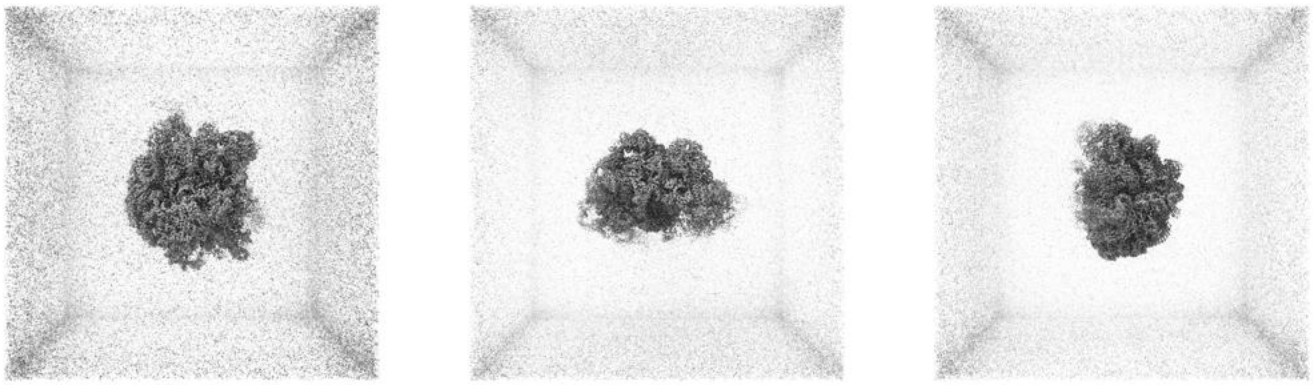
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.19. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

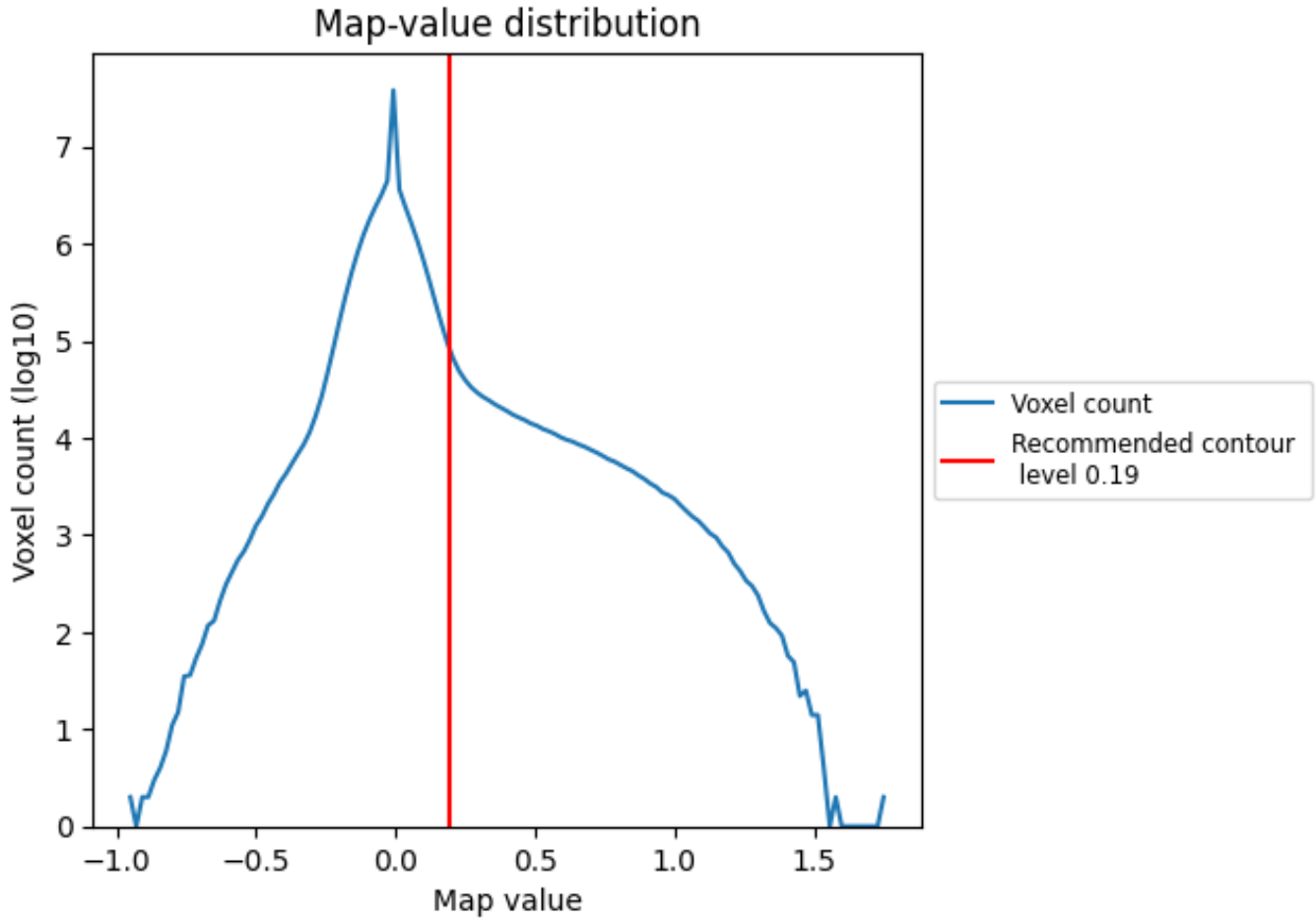
6.6 Mask visualisation (i)

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

7 Map analysis

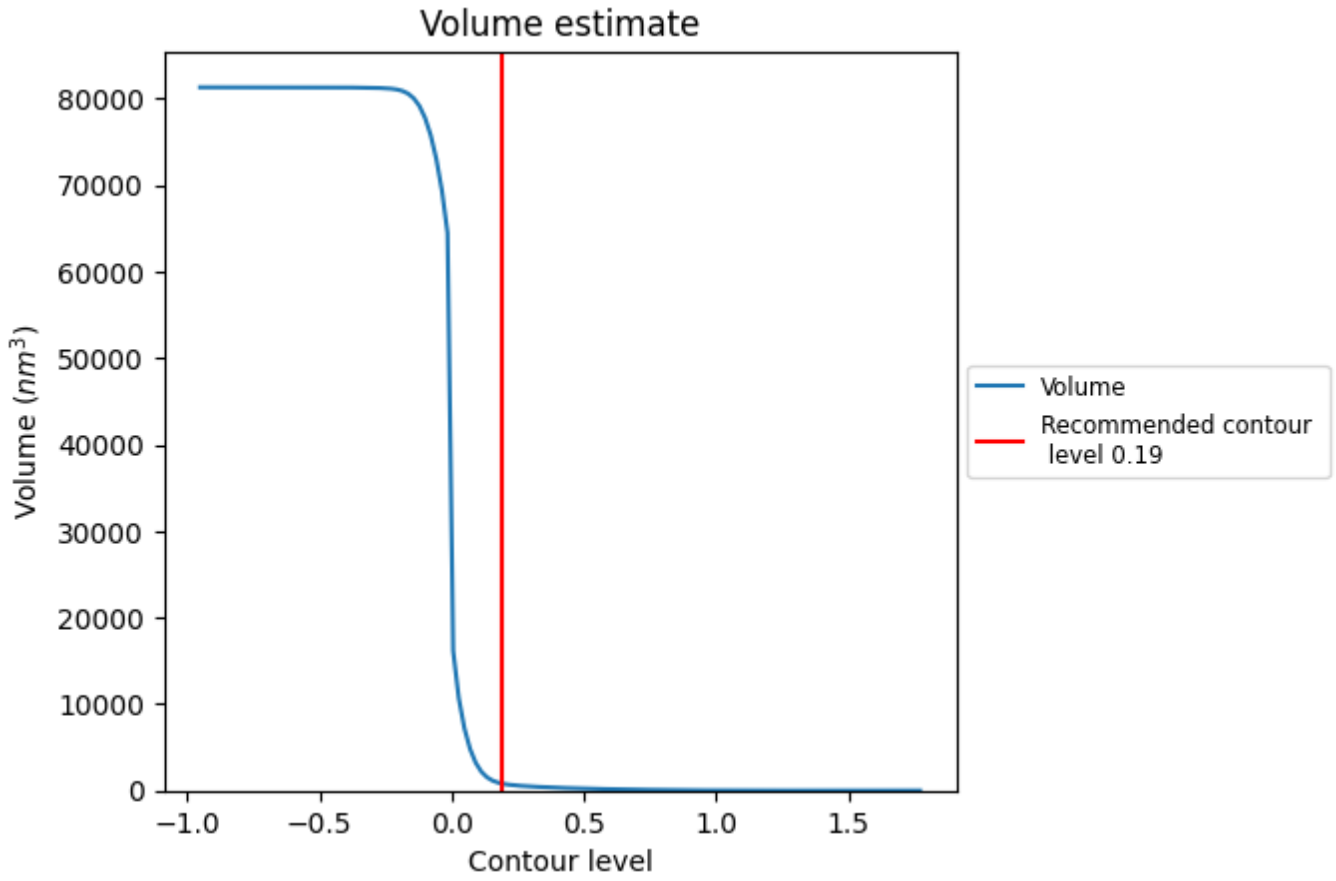
This section contains the results of statistical analysis of the map.

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.

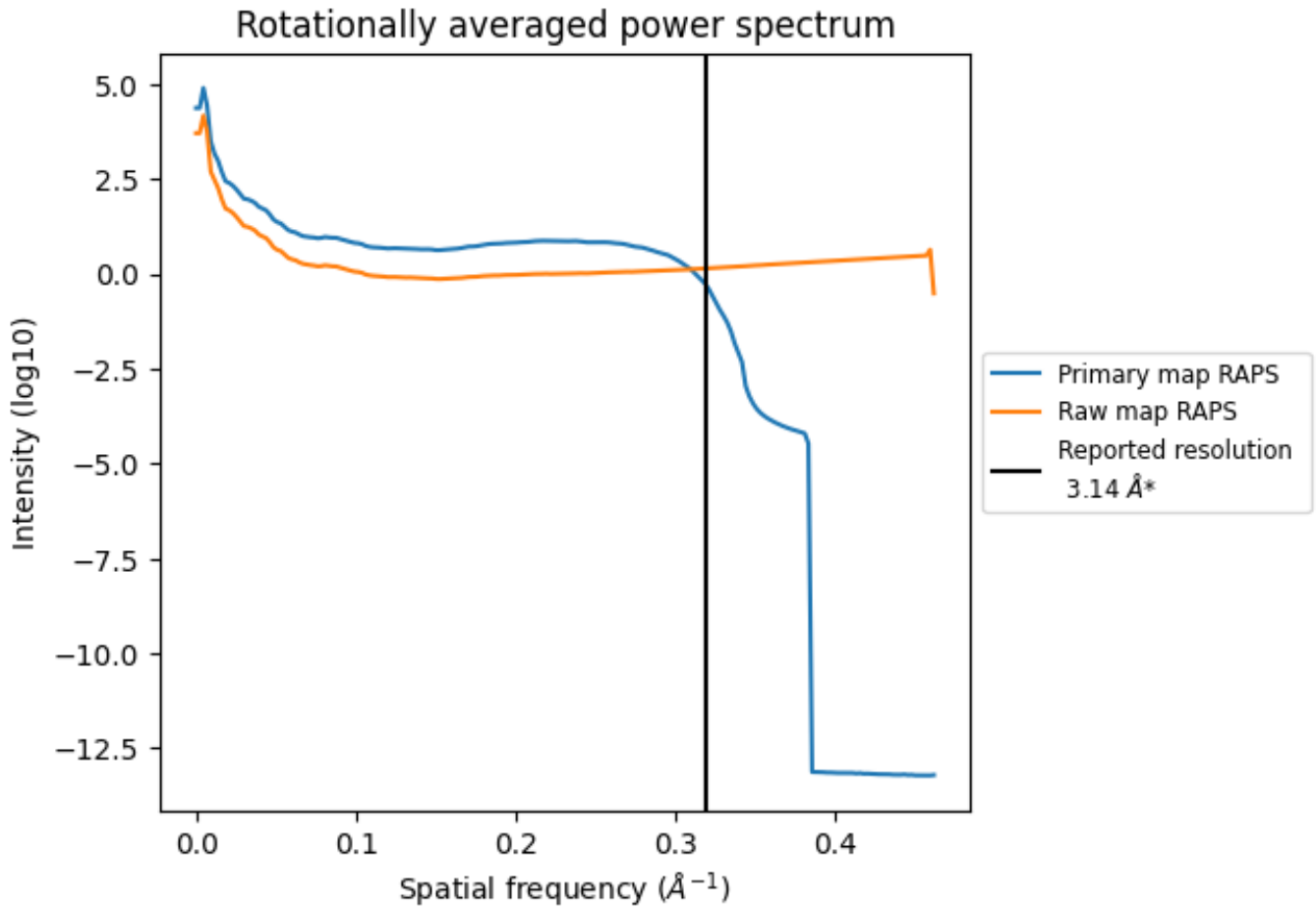
7.2 Volume estimate



The volume at the recommended contour level is 817 nm^3; this corresponds to an approximate mass of 738 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)

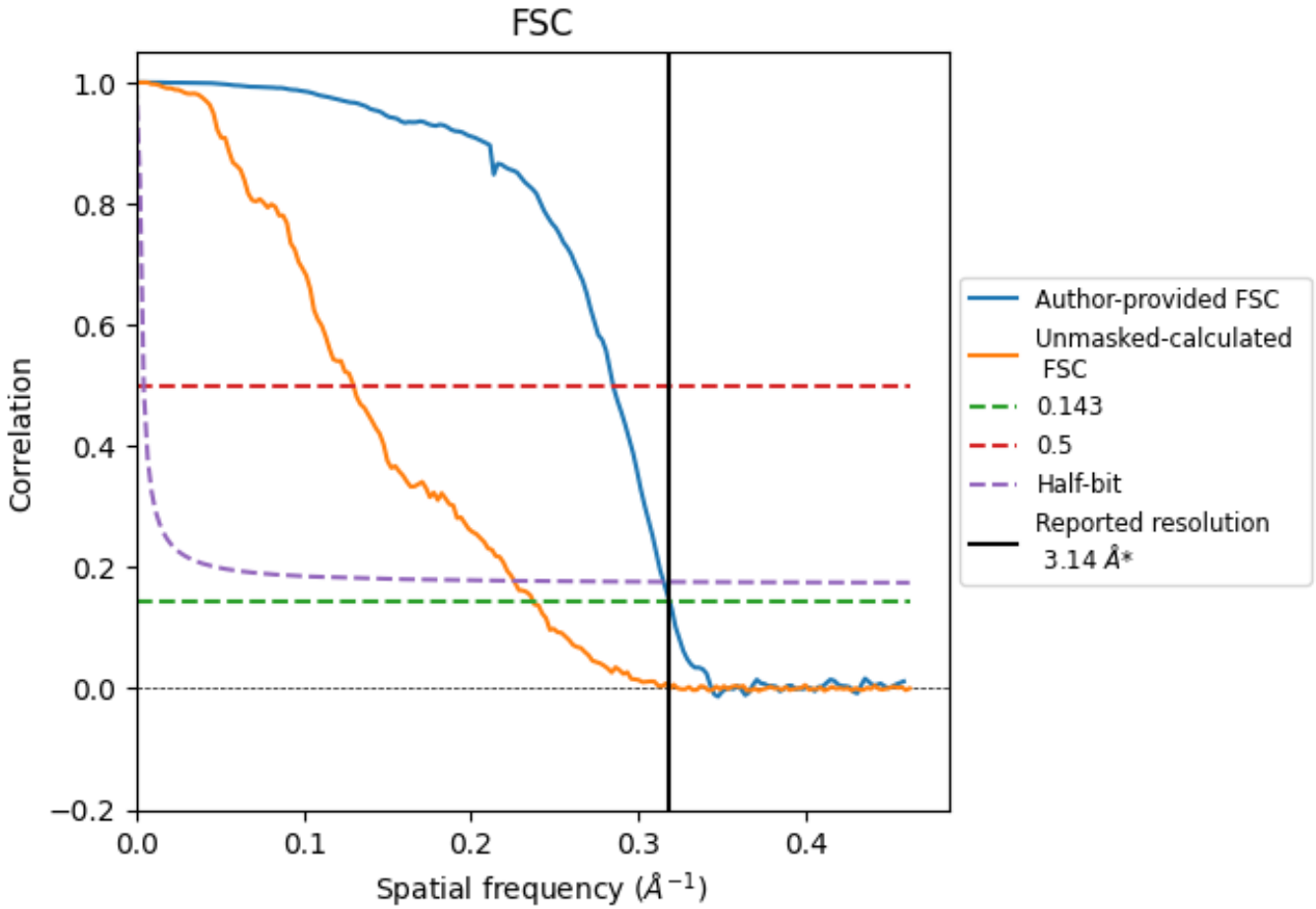


*Reported resolution corresponds to spatial frequency of 0.318 $Å^{-1}$

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 0.318 Å^{-1}

8.2 Resolution estimates (i)

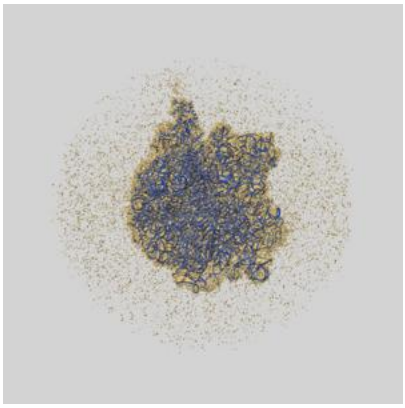
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.14	-	-
Author-provided FSC curve	3.14	3.51	3.18
Unmasked-calculated*	4.22	7.72	4.43

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.22 differs from the reported value 3.14 by more than 10 %

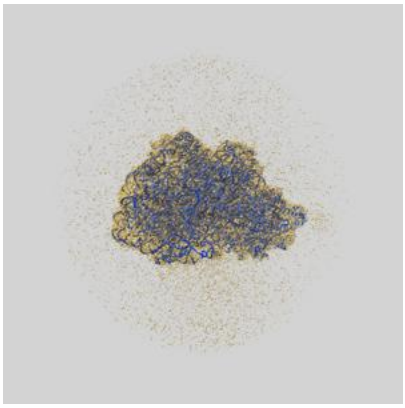
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43294 and PDB model 8VK0. Per-residue inclusion information can be found in section 3 on page 11.

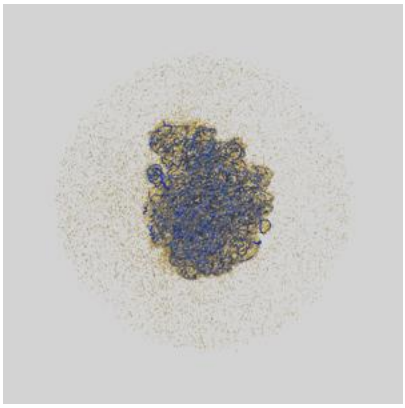
9.1 Map-model overlay



X



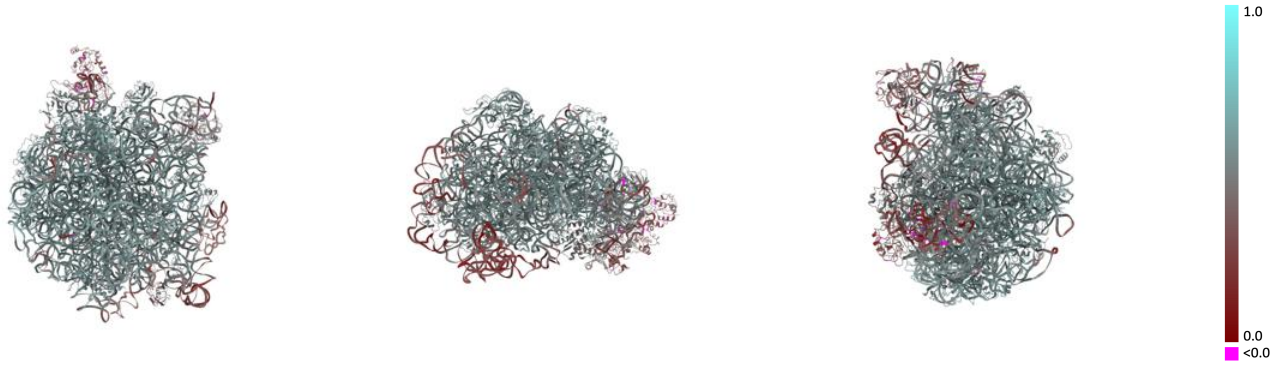
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.19 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.

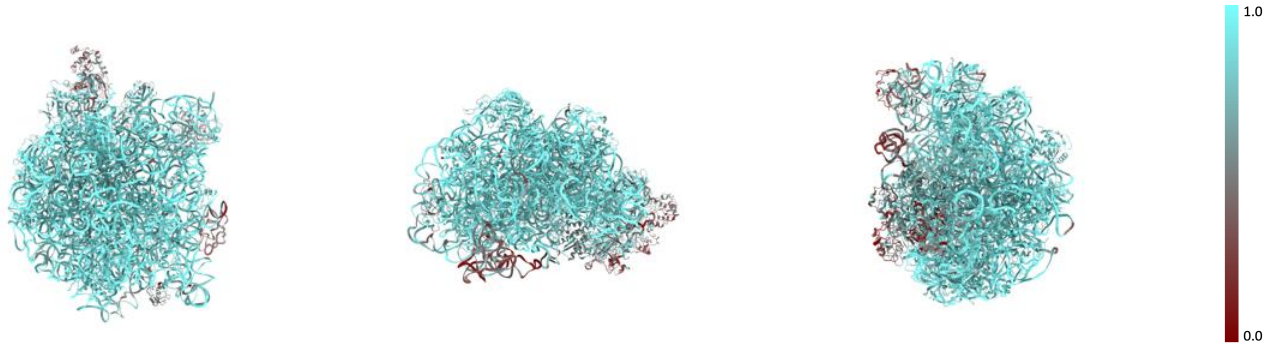
9.2 Q-score mapped to coordinate model (i)



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.

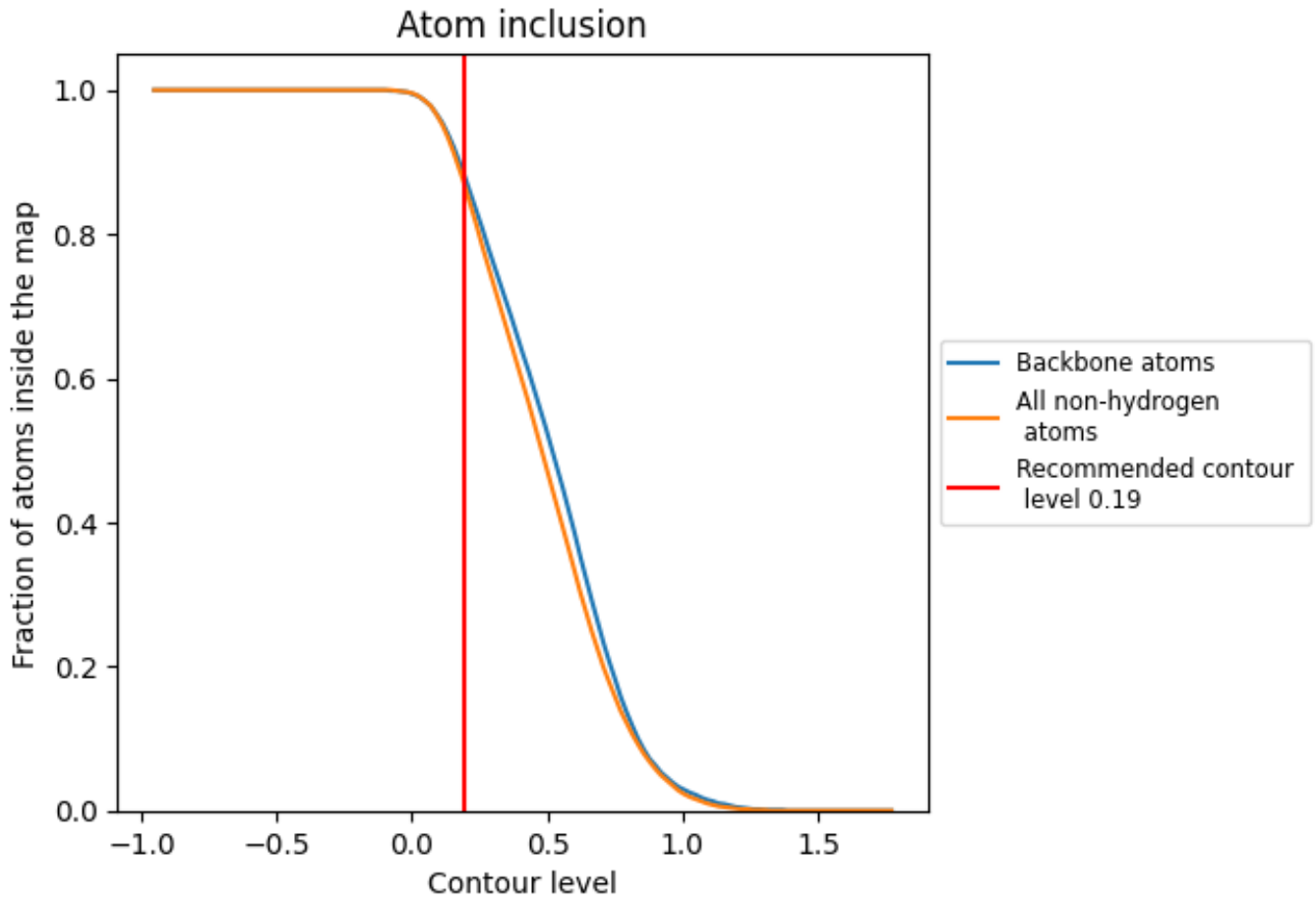
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.19).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 87% 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 (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8740	0.5190
2	0.9410	0.5870
3	0.8660	0.5910
4	0.6210	0.4740
A	0.9060	0.5190
B	0.9180	0.4820
C	0.9240	0.5820
D	0.9270	0.5810
E	0.9000	0.5690
F	0.6140	0.3960
G	0.7870	0.4960
H	0.5930	0.4280
I	0.3830	0.2960
J	0.3570	0.2730
K	0.9350	0.5860
L	0.8990	0.5700
M	0.9170	0.5720
N	0.8540	0.5740
O	0.9300	0.5840
P	0.7640	0.4290
Q	0.8660	0.5520
R	0.9370	0.5890
S	0.9310	0.5870
T	0.9240	0.5810
U	0.9120	0.5700
V	0.8560	0.5250
W	0.7330	0.5330
X	0.9190	0.5790
Y	0.9230	0.5720
Z	0.8900	0.5520
b	0.9030	0.5800
c	0.9090	0.5780
d	0.9230	0.5910
e	0.9190	0.5970
f	0.8570	0.5790
g	0.3360	0.3560