Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 04:05 pm GMT

PDB ID	:	5NCO
EMDB ID	:	EMD-3617
Title	:	Quaternary complex between SRP, SR, and SecYEG bound to the translating ribosome
Authors	:	Jomaa, A.; Hwang Fu, Y.; Boerhinger, D.; Leibundgut, M.; Shan, S.O.; Ban, N.
Deposited on	:	2017-03-06
Resolution	:	4.80 Å(reported)

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

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

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

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

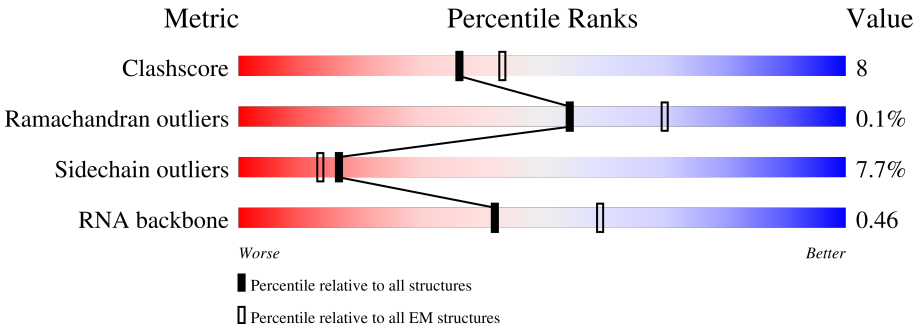
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 4.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	1	104	12% 69% 26% 5%
2	2	3	33% 33% 33%
3	A	2903	55% 36% 8%
4	B	120	72% 24%
5	C	271	8% 71% 25%
6	D	209	6% 78% 20%
7	E	201	8% 77% 21%

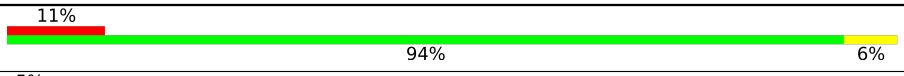
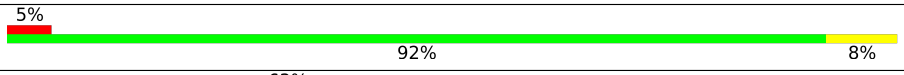
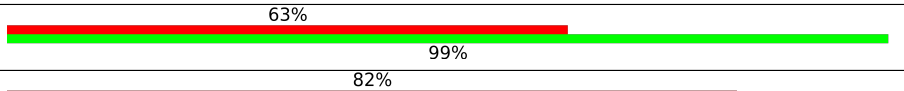
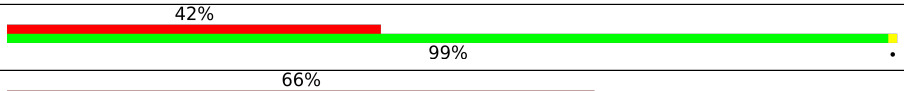
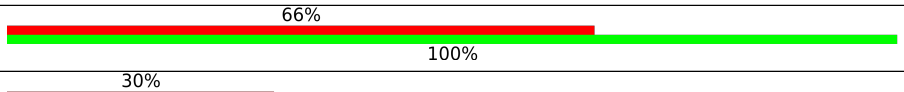
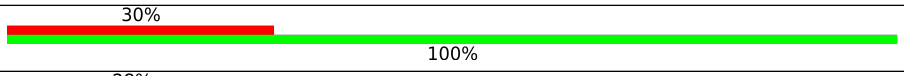
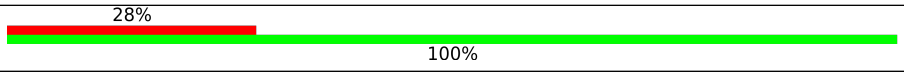
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	F	177	16% 60% 36% 5%
9	G	176	7% 69% 30%
10	H	149	50% 65% 32%
11	I	125	52% 66% 34%
12	J	134	65% 57% 40%
13	K	142	73% 23%
14	L	123	15% 68% 30%
15	M	144	8% 75% 23%
16	N	136	6% 71% 26%
17	O	125	13% 71% 26%
18	P	117	7% 67% 30%
19	Q	114	7% 75% 25%
20	R	117	74% 21%
21	S	103	5% 70% 28%
22	T	110	12% 78% 20%
23	U	95	9% 71% 28%
24	V	102	72% 27%
25	W	94	6% 74% 24%
26	X	76	68% 29%
27	Y	77	8% 64% 36%
28	Z	62	10% 68% 27% 5%
29	a	58	97%
30	b	56	5% 79% 21%
31	c	51	10% 90% 10%
32	d	46	7% 87% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	e	64	
34	f	38	
35	g	416	
36	h	56	
37	i	450	
38	j	71	
39	k	23	
40	l	271	

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 101694 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 RNA chain called 4.5S SRP RNA (Ffs).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	104	2224	991	401	728	104	0	0

- Molecule 2 is a RNA chain called P-site tRNA-CCA end.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	3	62	28	11	20	3	0	0

- Molecule 3 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	A	2883	61902	27613	11397	20009	2883	0	0

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	B	120	2569	1144	468	837	120	0	0

- Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	271	2083	1288	423	365	7	0	0

- Molecule 6 is a protein called 50S ribosomal protein L3.

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

- Molecule 7 is a protein called 50S ribosomal protein L4.

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

- Molecule 8 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 9 is a protein called 50S ribosomal protein L6.

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

- Molecule 10 is a protein called 50S ribosomal protein L9.

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

- Molecule 11 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	125	Total	C	N	O	S	0	0
			946	598	169	175	4		

- Molecule 12 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

- Molecule 13 is a protein called 50S ribosomal protein L13.

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

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 15 is a protein called 50S ribosomal protein L15.

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

- Molecule 16 is a protein called 50S ribosomal protein L16.

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

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	125	Total	C	N	O	S	0	0
			993	613	202	173	5		

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 19 is a protein called 50S ribosomal protein L19.

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

- Molecule 20 is a protein called 50S ribosomal protein L20.

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

- Molecule 21 is a protein called 50S ribosomal protein L21.

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

- Molecule 22 is a protein called 50S ribosomal protein L22.

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

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	95	Total	C	N	O	S	0	0
			756	479	141	135	1		

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	V	102	Total	C	N	O	0	0
			780	492	146	142		

- Molecule 25 is a protein called 50S ribosomal protein L25.

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

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	76	Total	C	N	O	S	0	0
			580	359	117	103	1		

- Molecule 27 is a protein called 50S ribosomal protein L28.

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

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 29 is a protein called 50S ribosomal protein L30.

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

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

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

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	c	51	Total	C	N	O	0	0
			414	266	76	72		

- 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	228	90	57	2		

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

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

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

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

- Molecule 35 is a protein called Protein translocase subunit SecY.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	g	416	Total 1664	C 832	N 416	O 416	0	0

- Molecule 36 is a protein called Protein translocase subunit SecE.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	h	56	Total 224	C 112	N 56	O 56	0	0

- Molecule 37 is a protein called Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	450	Total 3384	C 2129	N 609	O 628	S 18	0	0

- Molecule 38 is a protein called Protein-export membrane protein SecG.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	j	71	Total 284	C 142	N 71	O 71	0	0

- Molecule 39 is a protein called Signal sequence (1A9L).

Mol	Chain	Residues	Atoms				AltConf	Trace
39	k	23	Total 159	C 107	N 25	O 27	0	0

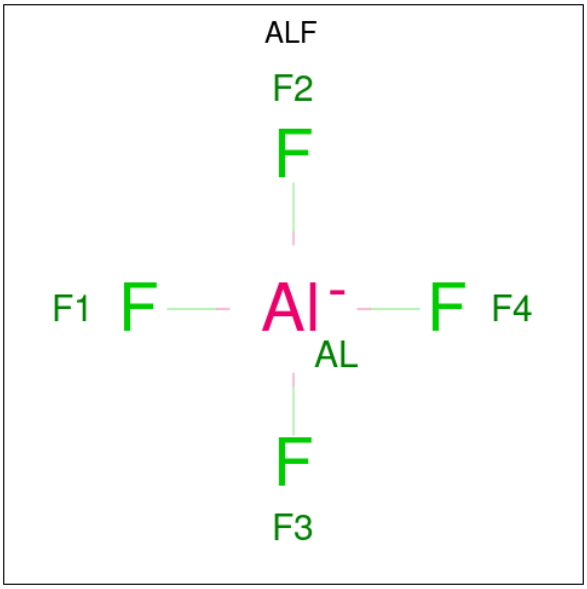
- Molecule 40 is a protein called Signal recognition particle receptor FtsY.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	271	Total 2067	C 1306	N 356	O 399	S 6	0	0

- Molecule 41 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
41	f	1	Total 1	Zn 1	0

- Molecule 42 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).

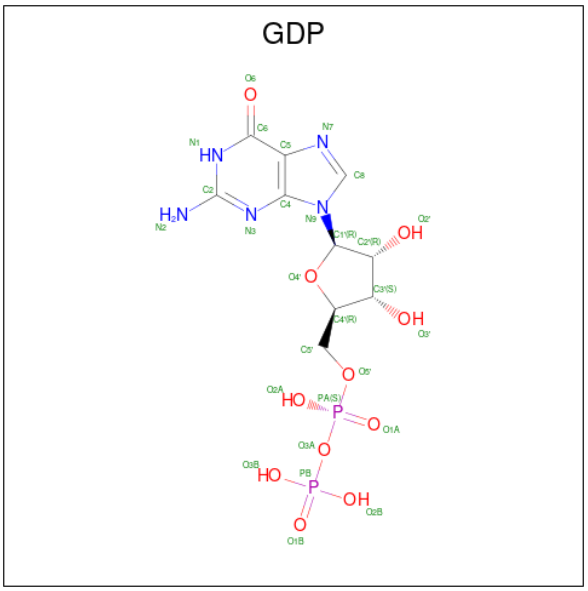


Mol	Chain	Residues	Atoms			AltConf
42	i	1	Total	Al	F	0
			5	1	4	
42	l	1	Total	Al	F	0
			5	1	4	

- Molecule 43 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
43	i	1	Total	Mg	0
			1	1	
43	l	1	Total	Mg	0
			1	1	

- Molecule 44 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



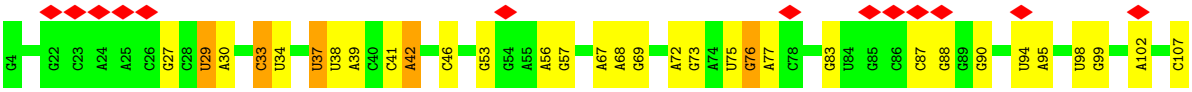
Mol	Chain	Residues	Atoms					AltConf
44	i	1	Total	C	N	O	P	0
			28	10	5	11	2	
44	l	1	Total	C	N	O	P	0
			28	10	5	11	2	

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.

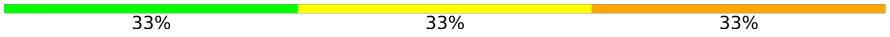
- Molecule 1: 4.5S SRP RNA (Ffs)

Chain 1:



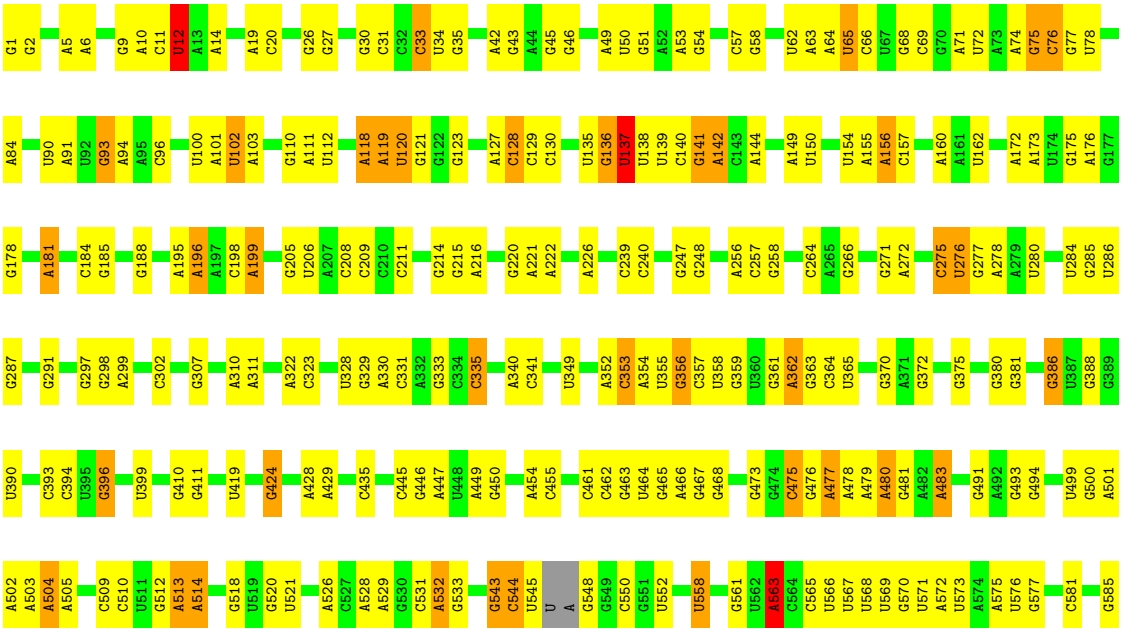
- Molecule 2: P-site tRNA-CCA end

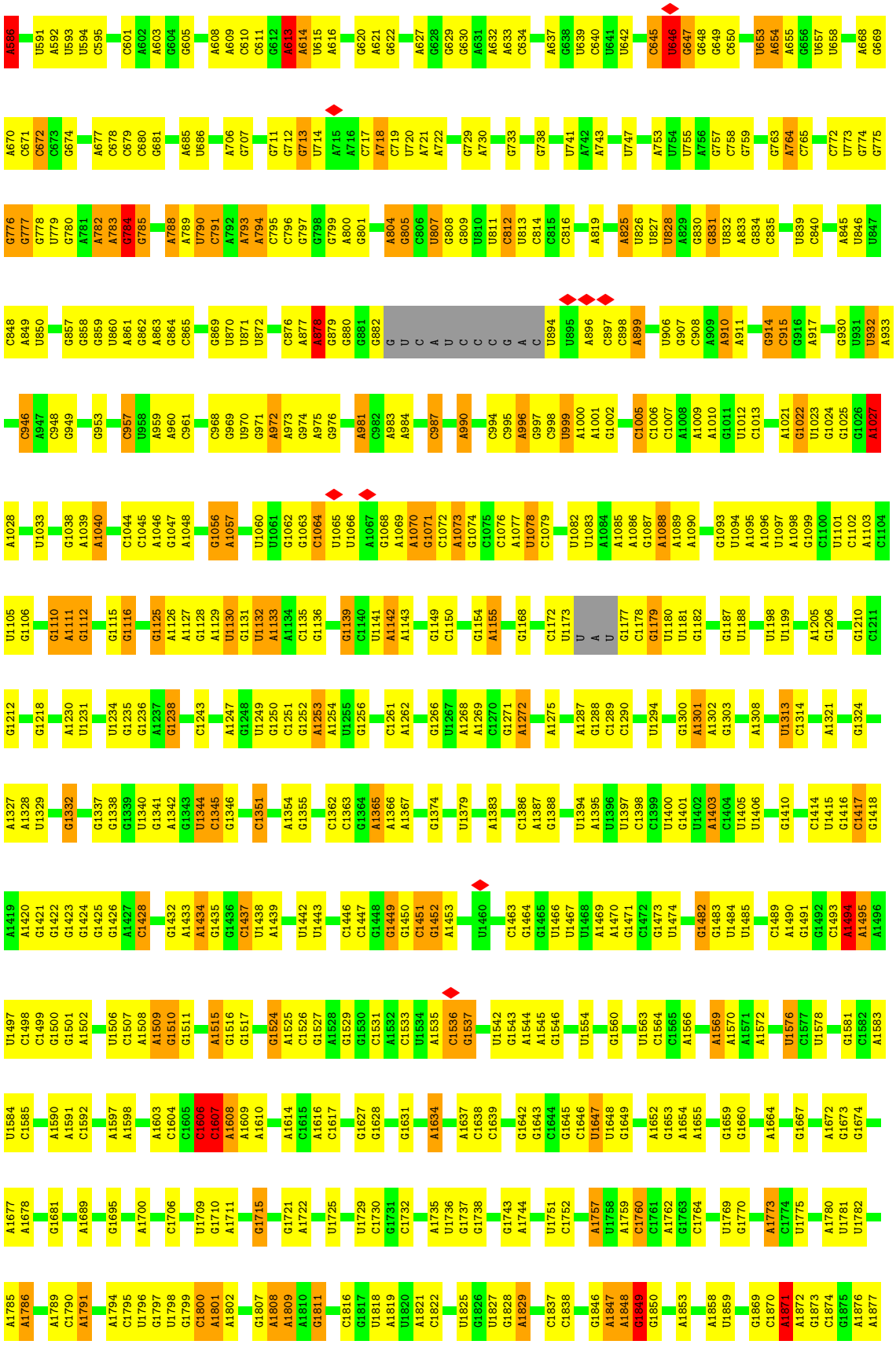
Chain 2:

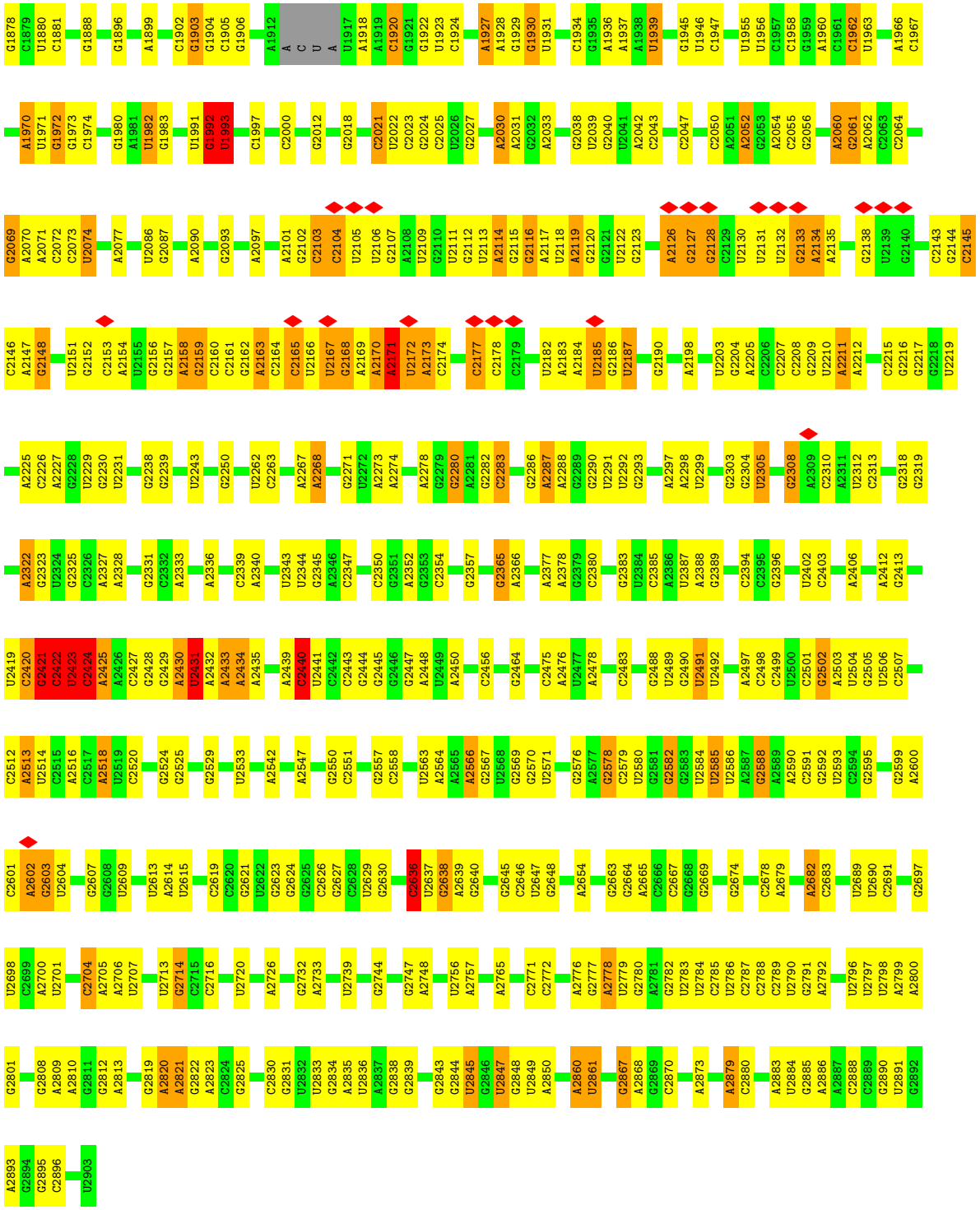


- Molecule 3: 23S rRNA

Chain A:



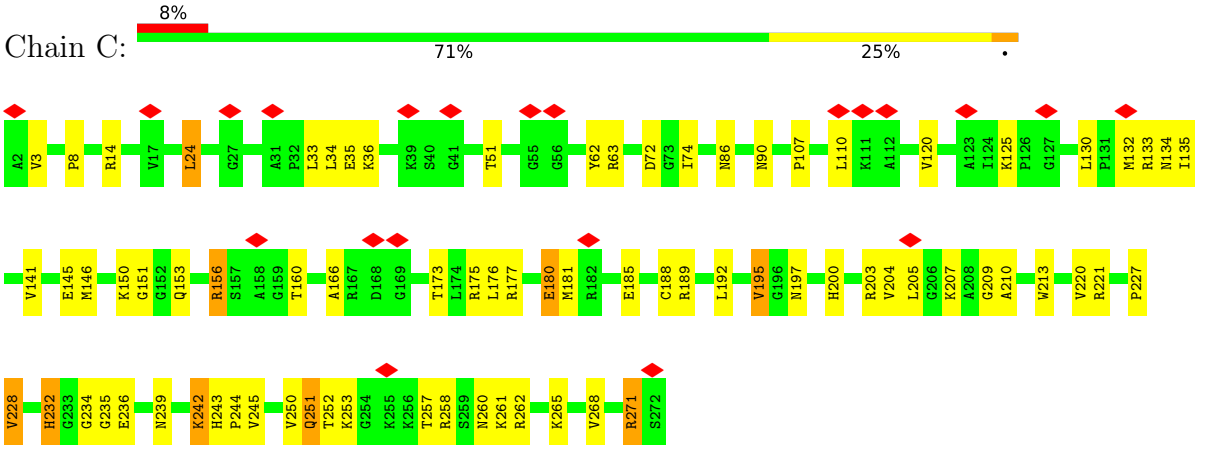

A586 U591 A592 U593 U594 C595 C601 A602 A603 G604 G605 A608 A609 C610 C611 G612 A613 A614 U615 A616 G620 A621 G622 A627 G628 G629 G630 A631 A632 A633 C634 A637 G638 U639 C640 U641 U642 C645 U646 G647 G648 G649 C650 U653 A654 A655 G656 U657 U658 A668 G669
A670 C671 G672 C673 G674 A677 C678 C679 C680 G681 A685 U686 A706 G707 G711 G712 G713 U714 A715 A716 C717 A718 C719 U720 A721 A722 G729 A730 G733 G738 U741 A742 A743 U747 A753 U754 U755 A756 G757 C758 C759 G763 A764 C765 C772 U773 G774 G775
G776 G777 G778 U779 G780 A781 A782 A783 G784 G785 A788 A789 U790 C791 A792 A793 A794 C795 C796 G797 G798 G799 A800 G801 A804 G805 C806 U807 G808 G809 U810 U811 C812 U813 C814 C815 C816 A819 A825 U826 U827 U828 A829 G830 G831 U832 A833 G834 C835 U839 C840 A845 U846 U847
C848 A849 U850 G857 G858 G859 U860 A861 G862 A863 G864 C865 G869 U870 U871 U872 C876 A877 A878 G879 G880 G881 G882 G U C A U C C C G A C U894 U895 A896 C897 C898 A899 U906 G907 C908 A909 A910 A911 G914 C915 G916 A917 G930 U931 U932 A933
C946 A947 C948 G949 G953 C957 U958 A959 A960 C961 C968 G969 U970 G971 A972 A973 G974 A975 G976 A981 C982 A983 A984 C987 A990 C994 C995 A996 G997 C998 U999 A1000 A1001 G1002 C1005 C1006 C1007 A1008 A1009 A1010 G1011 U1012 C1013 A1021 G1022 U1023 G1024 G1025 G1026 A1027
A1028 U1033 G1038 A1039 A1040 C1044 C1045 A1046 G1047 A1048 G1056 A1057 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 U1082 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1090 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104
U1105 G1106 G1110 A1111 C1112 G1115 G1116 G1125 A1126 A1127 G1128 A1129 U1130 G1131 U1132 A1133 A1134 C1135 G1136 G1139 C1140 U1141 A1142 A1143 C1149 C1150 G1154 A1155 G1168 C1172 U1173 U A A U G1177 C1178 G1179 U1180 U1181 G1182 G1187 U1188 U1198 U1199 A1205 G1206 G1210 C1211
G1212 G1218 A1230 U1231 U1234 G1235 G1236 A1237 G1238 C1243 A1247 G1248 U1249 G1250 C1251 G1252 A1253 A1254 U1255 G1256 C1261 A1262 G1266 U1267 A1268 A1269 C1270 G1271 A1272 A1275 A1287 G1288 C1289 C1290 U1294 G1300 A1301 A1302 G1303 A1308 U1313 C1314 A1321 G1324
A1327 A1328 U1329 G1332 G1337 G1338 G1339 U1340 G1341 A1342 G1343 U1344 C1345 G1346 C1351 A1354 G1355 C1362 C1363 G1364 A1365 A1366 A1367 G1374 U1379 A1383 C1386 A1387 G1388 U1394 A1395 U1396 U1397 C1398 C1399 U1400 G1401 U1402 A1403 C1404 U1405 U1406 G1410 C1414 U1415 G1416 C1417 G1418
A1419 A1420 G1421 G1422 G1423 G1424 G1425 G1426 A1427 C1428 G1432 A1433 A1434 G1435 G1436 C1437 U1438 A1439 U1442 U1443 C1446 C1447 G1448 G1449 G1450 C1451 G1452 A1453 U1460 C1463 G1464 G1465 U1466 U1467 U1468 A1469 A1470 G1471 C1472 G1473 U1474 G1482 G1483 U1484 U1485 C1489 A1490 G1491 C1492 C1493 A1494 A1495 A1496
U1497 C1498 C1499 G1500 G1501 A1502 U1506 C1507 A1508 A1509 G1510 G1511 A1515 G1516 G1517 G1524 A1525 C1526 G1527 A1528 G1529 G1530 C1531 A1532 C1533 U1534 A1535 C1536 G1537 U1542 G1543 A1544 A1545 G1546 U1554 G1560 U1563 C1564 C1565 A1566 A1569 A1570 A1571 A1572 U1576 C1577 U1578 G1581 C1582 A1583
U1584 C1585 A1590 A1591 C1592 A1597 A1598 A1603 C1604 C1605 C1606 C1607 A1608 A1609 A1610 A1614 C1615 A1616 C1617 G1627 G1628 G1631 A1634 A1637 C1638 C1639 G1642 G1643 C1644 G1645 C1646 U1647 U1648 G1649 A1652 G1653 A1654 A1655 G1659 G1660 A1664 G1667 A1672 G1673 G1674
A1677 A1678 G1681 A1689 G1695 A1700 C1706 U1709 G1710 A1711 G1715 G1721 A1722 U1725 U1729 C1730 C1731 C1732 A1735 U1736 G1737 G1738 G1743 A1744 U1751 C1752 A1757 U1758 A1759 C1760 C1761 A1762 G1763 C1764 U1769 G1770 A1773 C1774 U1775 A1780 U1781 U1782
A1785 A1786 A1789 C1790 A1791 A1794 C1795 U1796 G1797 U1798 G1799 C1800 A1801 A1802 G1807 A1808 A1809 A1810 G1811 C1816 G1817 U1818 A1819 U1820 A1821 C1822 U1825 G1826 U1827 G1828 A1829 C1837 C1838 G1846 A1847 A1848 G1849 G1850 A1853 A1858 U1859 G1869 C1870 A1871 A1872 G1873 C1874 G1875 A1876 A1877



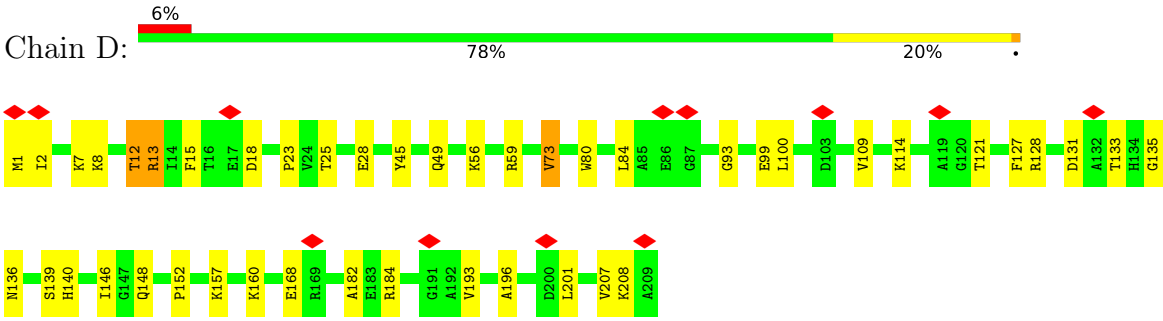
• Molecule 4: 5S rRNA

Chain B:

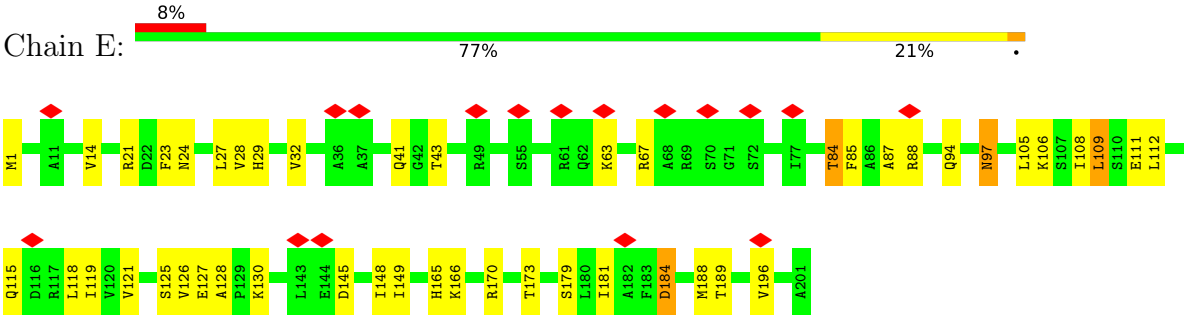
• Molecule 5: 50S ribosomal protein L2



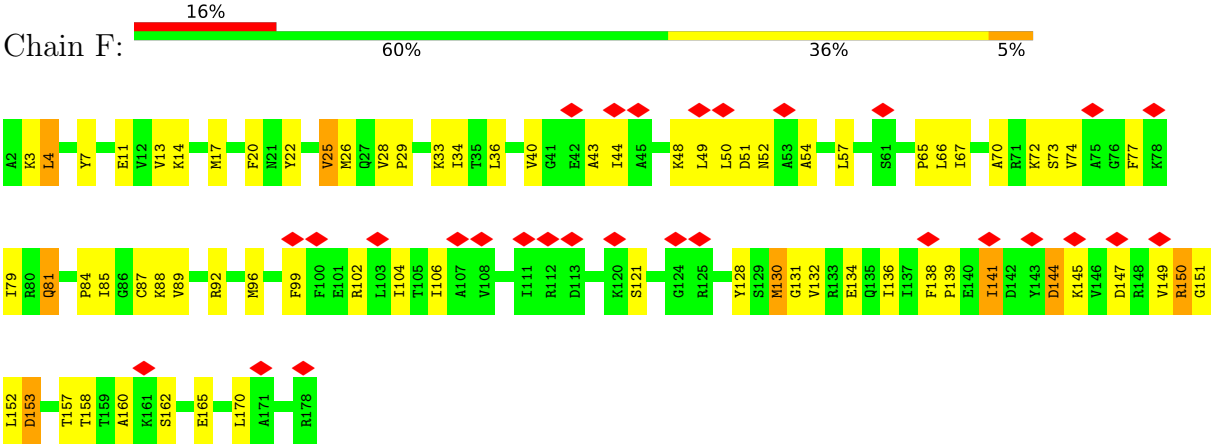
• Molecule 6: 50S ribosomal protein L3



• Molecule 7: 50S ribosomal protein L4

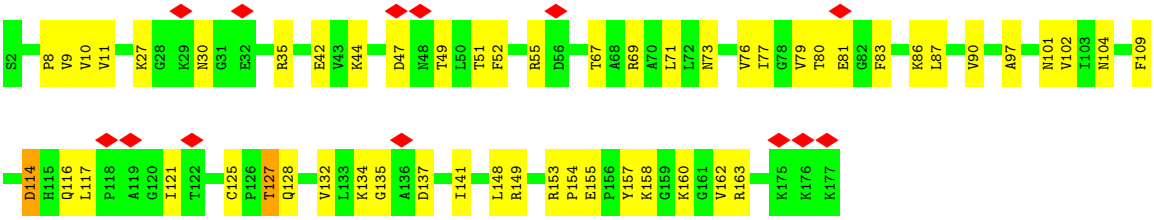


• Molecule 8: 50S ribosomal protein L5



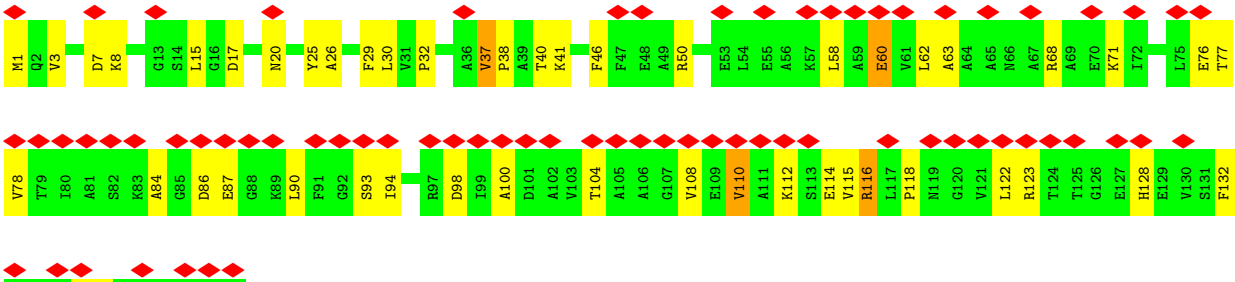
• Molecule 9: 50S ribosomal protein L6

Chain G:



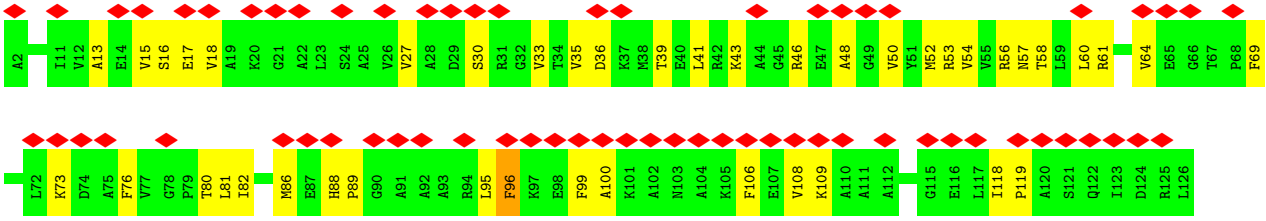
• Molecule 10: 50S ribosomal protein L9

Chain H:



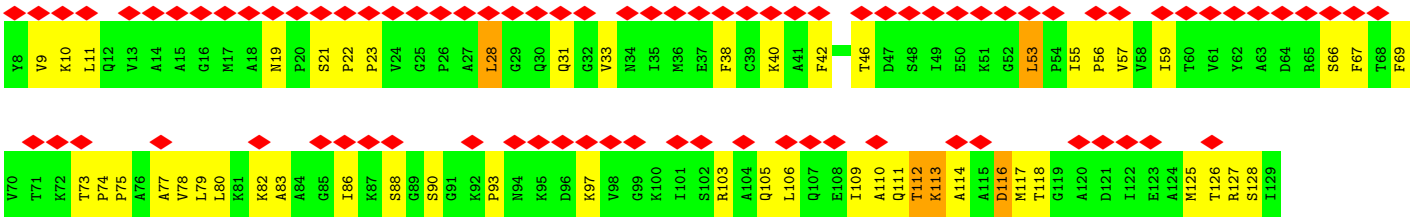
• Molecule 11: 50S ribosomal protein L10

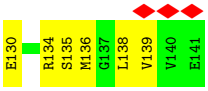
Chain I:



• Molecule 12: 50S ribosomal protein L11

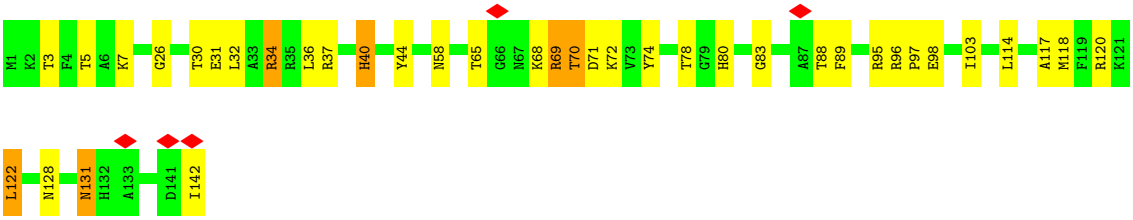
Chain J:





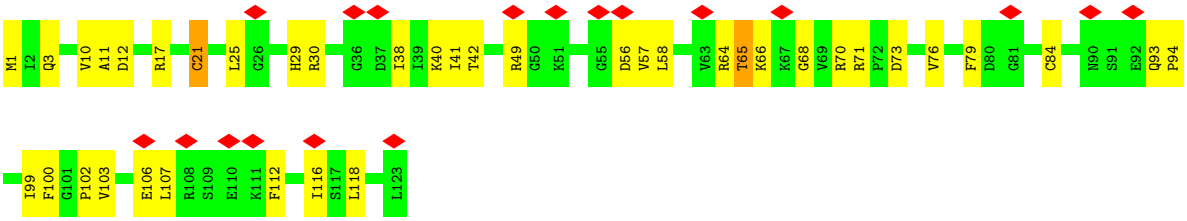
• Molecule 13: 50S ribosomal protein L13

Chain K:



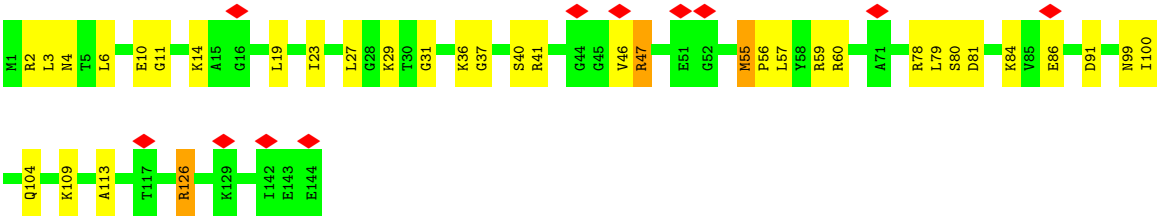
• Molecule 14: 50S ribosomal protein L14

Chain L:



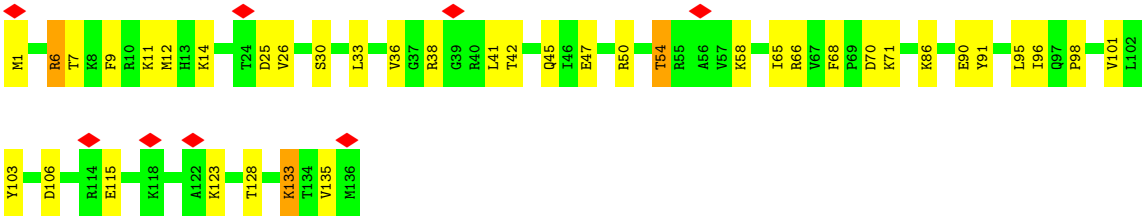
• Molecule 15: 50S ribosomal protein L15

Chain M:



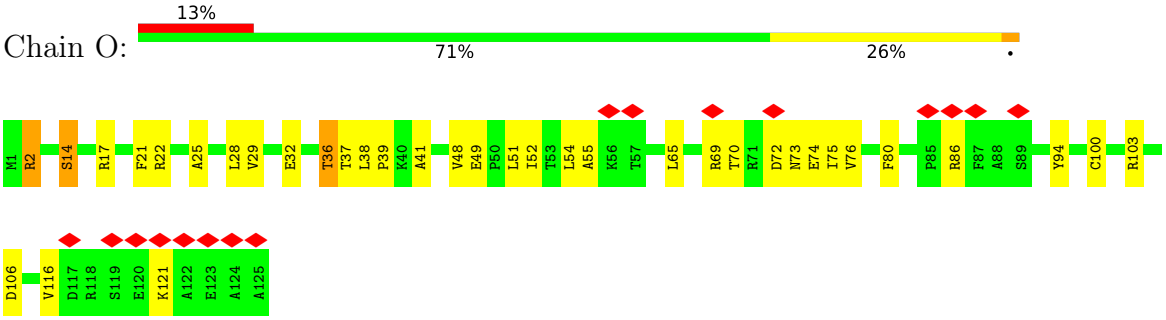
• Molecule 16: 50S ribosomal protein L16

Chain N:



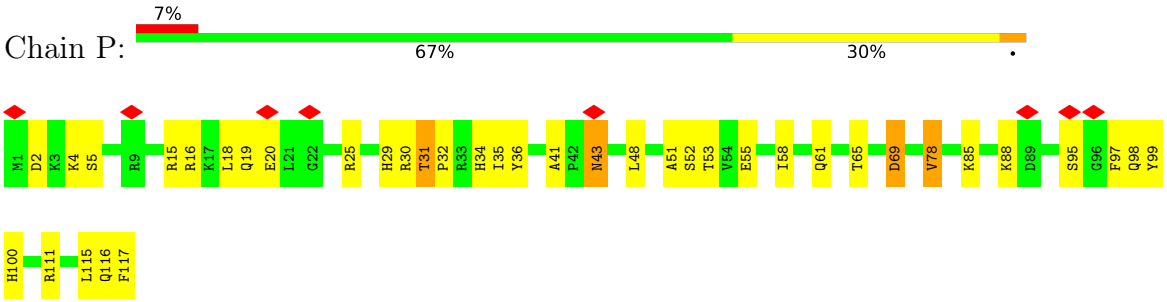
• Molecule 17: 50S ribosomal protein L17

Chain O:



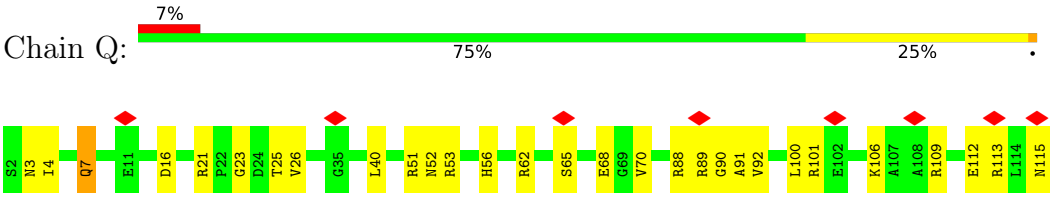
• Molecule 18: 50S ribosomal protein L18

Chain P:



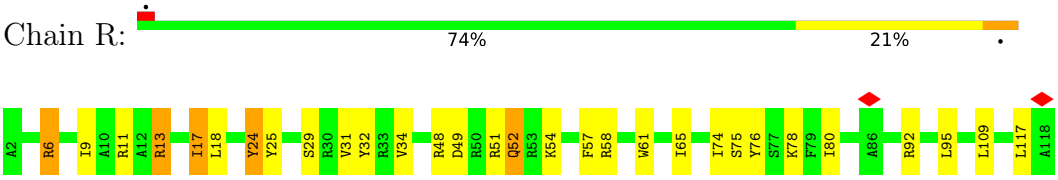
• Molecule 19: 50S ribosomal protein L19

Chain Q:



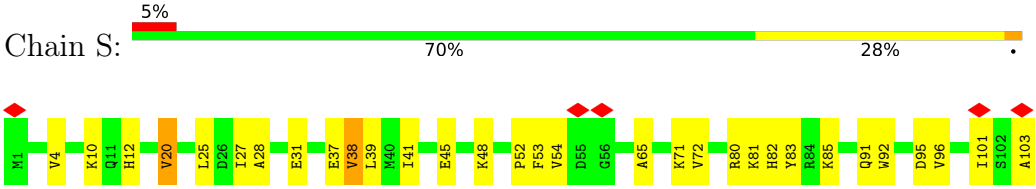
• Molecule 20: 50S ribosomal protein L20

Chain R:



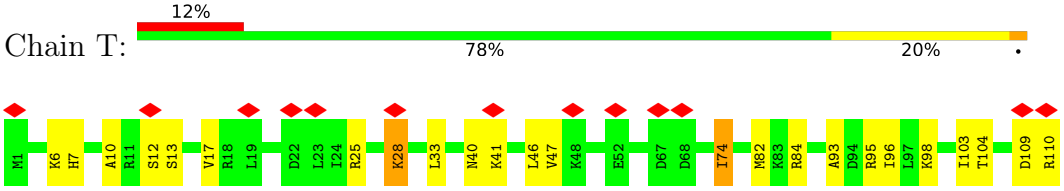
• Molecule 21: 50S ribosomal protein L21

Chain S:



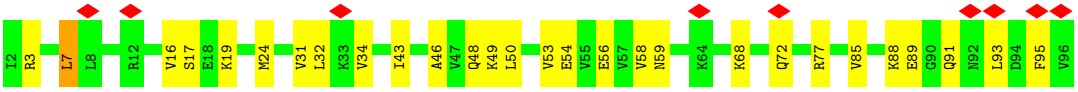
• Molecule 22: 50S ribosomal protein L22

Chain T:



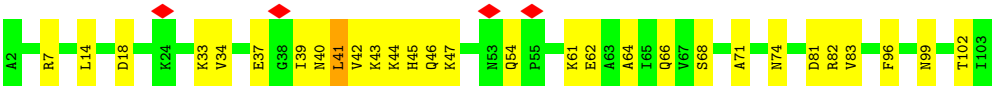
• Molecule 23: 50S ribosomal protein L23

Chain U:



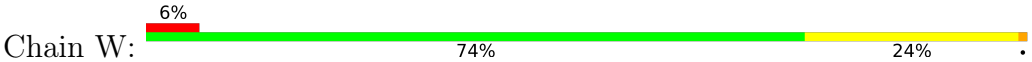
• Molecule 24: 50S ribosomal protein L24

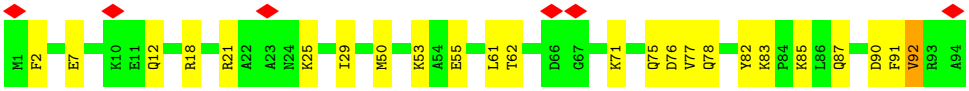
Chain V:



• Molecule 25: 50S ribosomal protein L25

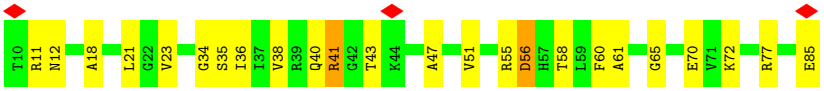
Chain W:





• Molecule 26: 50S ribosomal protein L27

Chain X:

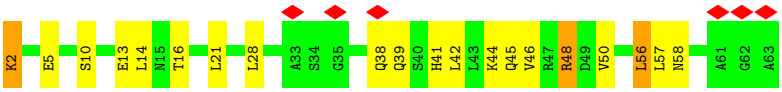


• Molecule 27: 50S ribosomal protein L28

Chain Y:

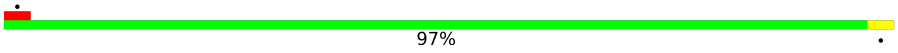
• Molecule 28: 50S ribosomal protein L29

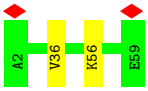
Chain Z:



• Molecule 29: 50S ribosomal protein L30

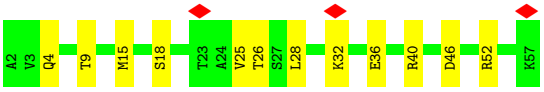
Chain a:





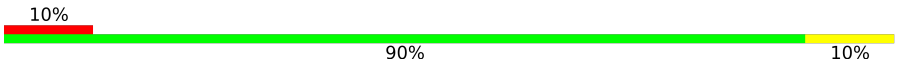
• Molecule 30: 50S ribosomal protein L32

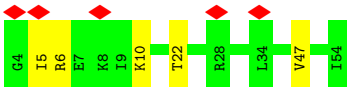
Chain b:



• Molecule 31: 50S ribosomal protein L33

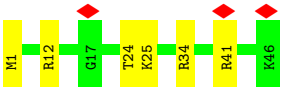
Chain c:





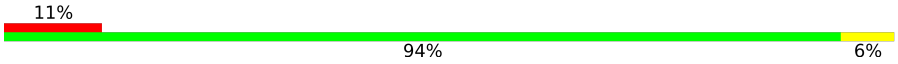
• Molecule 32: 50S ribosomal protein L34

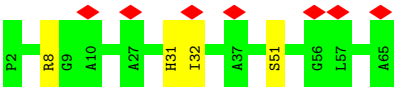
Chain d:



• Molecule 33: 50S ribosomal protein L35

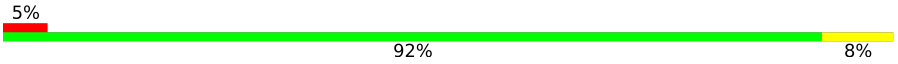
Chain e:

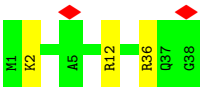




• Molecule 34: 50S ribosomal protein L36

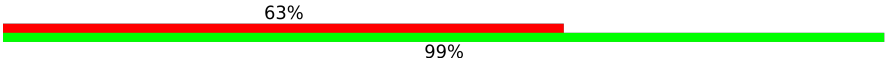
Chain f:

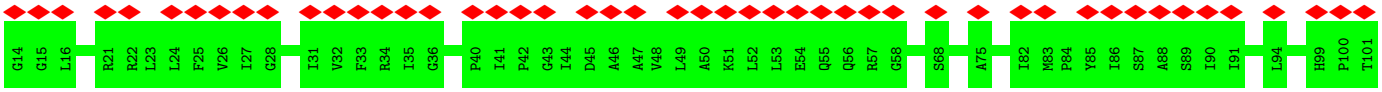


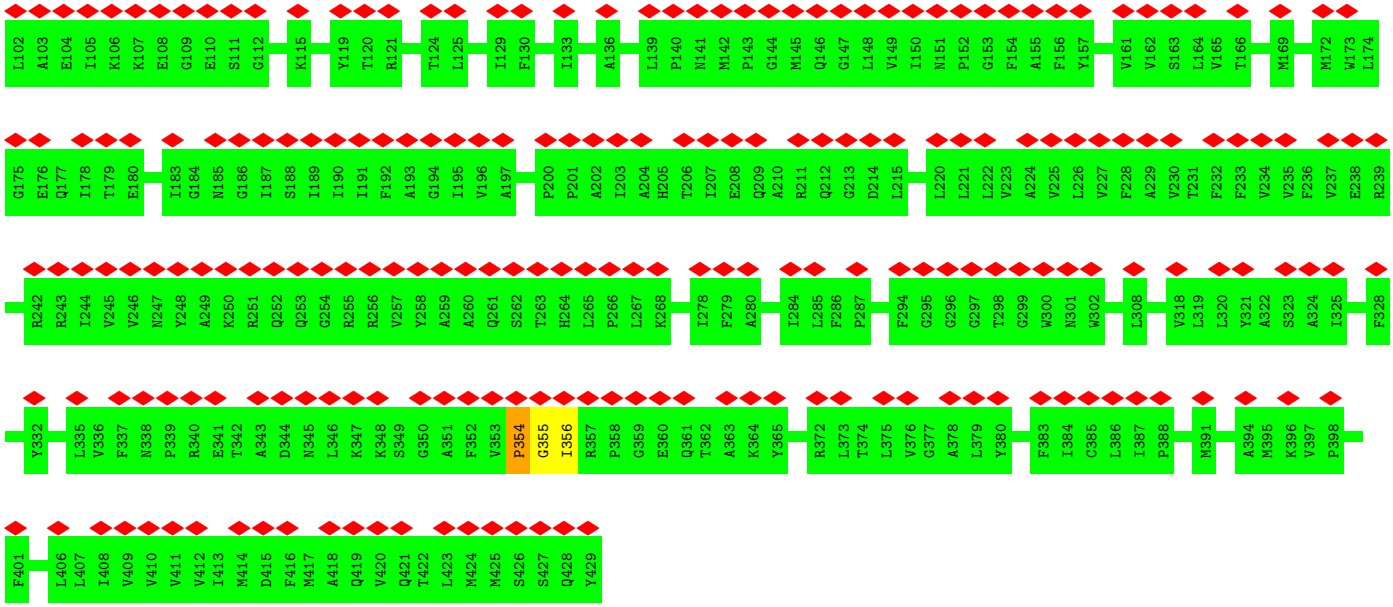


• Molecule 35: Protein translocase subunit SecY

Chain g:

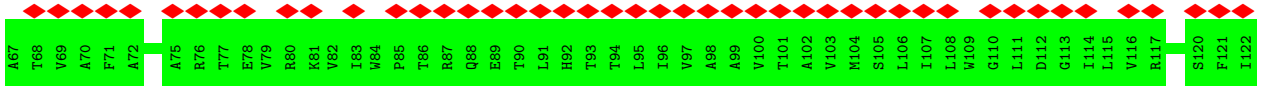






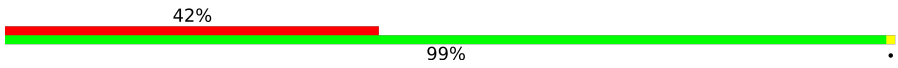
• Molecule 36: Protein translocase subunit SecE

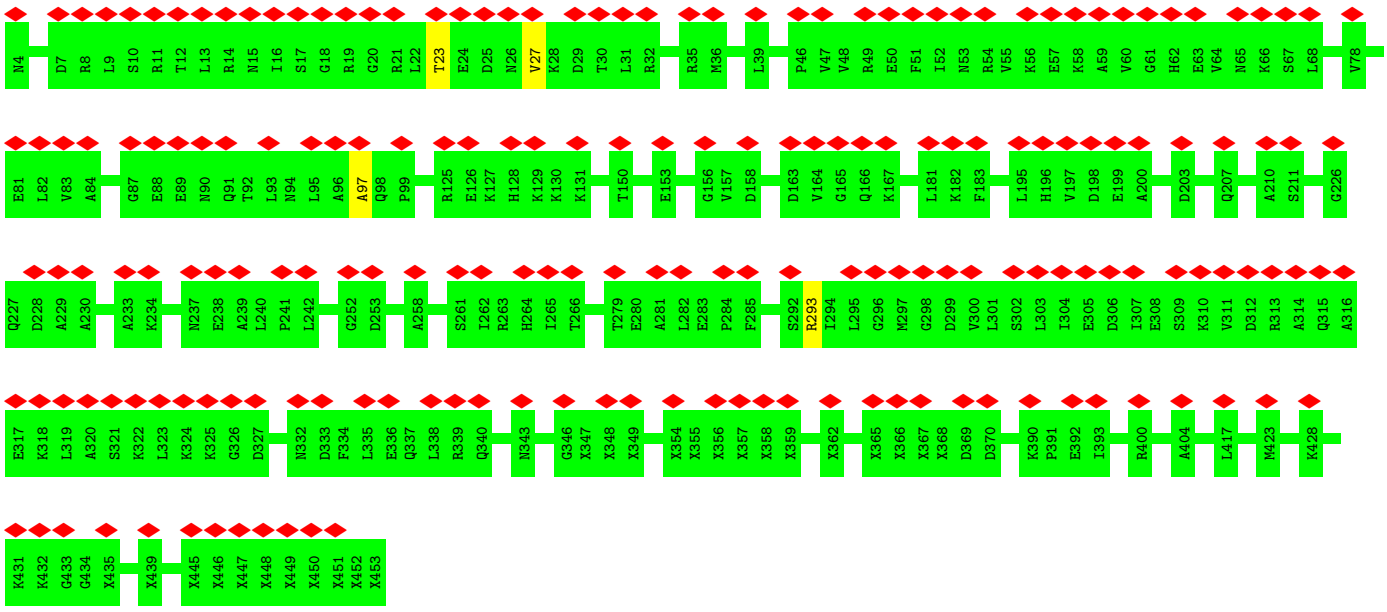
Chain h:



• Molecule 37: Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein

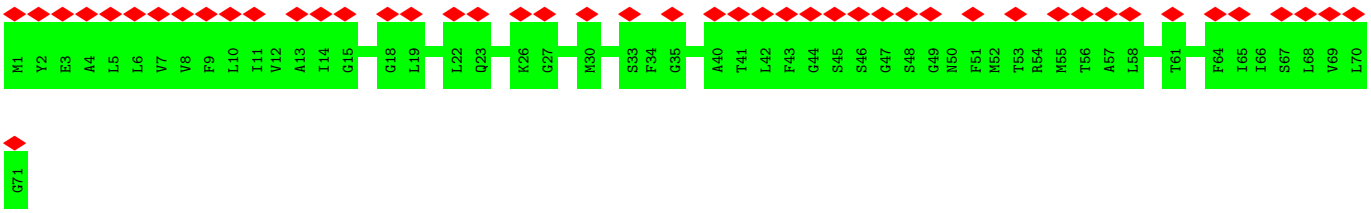
Chain i:





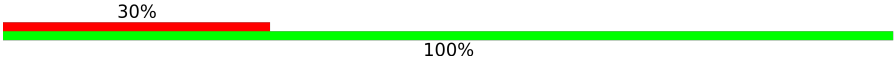
• Molecule 38: Protein-export membrane protein SecG

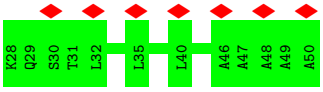
Chain j:



• Molecule 39: Signal sequence (1A9L)

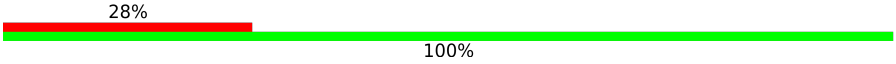
Chain k:

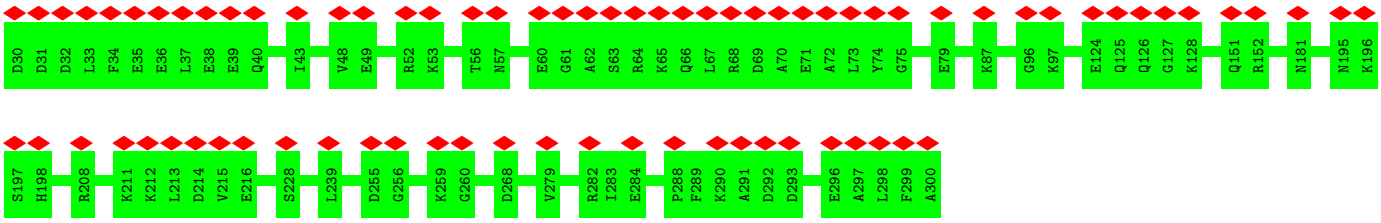




• Molecule 40: Signal recognition particle receptor FtsY

Chain l:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	13926	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; After 3D reconstruction 3D maps were sharpened	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	100719	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.210	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

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

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	1	0.15	0/2486	0.70	0/3874
2	2	0.57	0/68	1.27	1/103 (1.0%)
3	A	0.69	13/69329 (0.0%)	1.17	188/108152 (0.2%)
4	B	0.51	0/2872	1.04	1/4478 (0.0%)
5	C	0.47	0/2122	0.65	0/2852
6	D	0.47	0/1586	0.63	0/2134
7	E	0.44	0/1571	0.61	1/2113 (0.0%)
8	F	0.39	0/1435	0.56	0/1926
9	G	0.39	0/1343	0.58	0/1816
10	H	0.43	0/1121	0.57	0/1515
11	I	0.48	0/958	0.62	1/1290 (0.1%)
12	J	0.58	0/993	0.69	1/1341 (0.1%)
13	K	0.46	0/1152	0.57	0/1551
14	L	0.45	0/955	0.63	0/1279
15	M	0.47	0/1062	0.64	0/1413
16	N	0.48	0/1093	0.60	0/1460
17	O	0.47	0/1006	0.67	0/1345
18	P	0.41	0/910	0.56	0/1219
19	Q	0.48	0/929	0.60	0/1242
20	R	0.56	0/960	0.59	0/1278
21	S	0.46	0/829	0.62	0/1107
22	T	0.52	0/864	0.71	0/1156
23	U	0.46	0/763	0.65	0/1021
24	V	0.38	0/788	0.54	0/1051
25	W	0.40	0/766	0.57	0/1025
26	X	0.50	0/587	0.60	0/776
27	Y	0.48	0/635	0.61	0/848
28	Z	0.42	0/502	0.54	0/667
29	a	0.38	0/453	0.56	0/605
30	b	0.43	0/450	0.62	0/599
31	c	0.44	0/421	0.61	0/561
32	d	0.51	0/380	0.66	0/498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	e	0.47	0/513	0.63	0/676
34	f	0.49	0/303	0.58	0/397
35	g	0.27	0/1663	0.51	5/2077 (0.2%)
36	h	0.16	0/223	0.29	0/277
37	i	0.21	0/3170	0.39	0/4255
38	j	0.16	0/283	0.27	0/352
39	k	0.21	0/159	0.40	0/218
40	l	0.20	0/2091	0.36	0/2822
All	All	0.60	13/109794 (0.0%)	1.02	198/163369 (0.1%)

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
5	C	0	1
9	G	0	1
12	J	0	1
35	g	0	1
37	i	0	1
All	All	0	5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2542	A	N9-C4	-6.93	1.33	1.37
3	A	1254	A	N9-C4	-6.48	1.33	1.37
3	A	1321	A	N9-C4	6.30	1.41	1.37
3	A	776	G	N9-C4	6.01	1.42	1.38
3	A	1490	A	N9-C4	5.92	1.41	1.37
3	A	2114	A	N9-C4	5.90	1.41	1.37
3	A	563	A	N9-C4	-5.71	1.34	1.37
3	A	1254	A	N3-C4	-5.48	1.31	1.34
3	A	1010	A	N9-C4	-5.33	1.34	1.37
3	A	960	A	N9-C4	-5.27	1.34	1.37
3	A	586	A	N3-C4	-5.24	1.31	1.34
3	A	1678	A	N9-C4	-5.21	1.34	1.37
3	A	514	A	N9-C4	-5.11	1.34	1.37

All (198) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2423	U	C6-N1-C2	-12.21	113.67	121.00
3	A	2422	C	O4'-C1'-N1	9.37	115.69	108.20
3	A	1838	C	C6-N1-C2	9.15	123.96	120.30
35	g	354	PRO	C-N-CA	-8.94	103.53	122.30
3	A	2423	U	C5-C6-N1	8.77	127.08	122.70
3	A	1584	U	C2-N1-C1'	8.55	127.95	117.70
3	A	776	G	C8-N9-C4	-7.97	103.21	106.40
3	A	2431	U	N3-C2-O2	-7.91	116.67	122.20
3	A	275	C	C6-N1-C2	-7.67	117.23	120.30
3	A	1760	C	C6-N1-C2	7.58	123.33	120.30
3	A	2422	C	N3-C2-O2	-7.30	116.79	121.90
3	A	1584	U	N1-C2-O2	7.26	127.88	122.80
3	A	2177	C	C6-N1-C2	-7.10	117.46	120.30
3	A	1992	G	C4-C5-N7	7.02	113.61	110.80
3	A	2614	A	C6-N1-C2	-6.92	114.45	118.60
3	A	2431	U	C5-C4-O4	6.90	130.04	125.90
3	A	214	G	N3-C4-C5	-6.89	125.16	128.60
3	A	137	U	C5-C4-O4	-6.85	121.79	125.90
3	A	2422	C	C6-N1-C2	-6.83	117.57	120.30
3	A	2636	C	C2-N1-C1'	6.80	126.28	118.80
3	A	2424	C	O4'-C1'-N1	6.78	113.62	108.20
3	A	2207	C	C6-N1-C2	-6.76	117.60	120.30
35	g	355	GLY	CA-C-O	-6.75	108.44	120.60
3	A	1607	C	C6-N1-C2	-6.71	117.62	120.30
3	A	1027	A	C8-N9-C4	6.62	108.45	105.80
3	A	102	U	C2-N1-C1'	6.62	125.64	117.70
3	A	776	G	C4-N9-C1'	6.54	135.01	126.50
3	A	1064	C	C6-N1-C2	-6.49	117.70	120.30
3	A	2542	A	C2-N3-C4	-6.48	107.36	110.60
3	A	1531	C	C5-C6-N1	6.47	124.24	121.00
3	A	784	G	P-O3'-C3'	6.47	127.47	119.70
3	A	906	U	C5-C4-O4	6.47	129.78	125.90
3	A	1849	G	C8-N9-C4	-6.46	103.81	106.40
3	A	2000	C	C6-N1-C2	6.46	122.88	120.30
3	A	1313	U	N3-C2-O2	-6.45	117.68	122.20
3	A	1128	G	C8-N9-C4	6.43	108.97	106.40
3	A	1849	G	N7-C8-N9	6.38	116.29	113.10
3	A	2456	C	C6-N1-C2	-6.32	117.77	120.30
3	A	1652	A	C8-N9-C4	6.28	108.31	105.80
3	A	12	U	N3-C2-O2	-6.28	117.81	122.20
3	A	733	G	C4-C5-N7	6.28	113.31	110.80
3	A	2104	C	C6-N1-C2	-6.27	117.79	120.30
3	A	483	A	C8-N9-C4	6.24	108.30	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1606	C	N3-C2-O2	-6.24	117.53	121.90
3	A	1848	A	C8-N9-C4	-6.23	103.31	105.80
3	A	1695	G	N9-C4-C5	-6.21	102.92	105.40
3	A	832	U	C5-C6-N1	-6.18	119.61	122.70
3	A	611	C	C6-N1-C2	-6.17	117.83	120.30
3	A	805	G	C8-N9-C4	6.15	108.86	106.40
3	A	774	G	C8-N9-C4	6.13	108.85	106.40
3	A	1470	A	C8-N9-C4	-6.11	103.36	105.80
3	A	804	A	C8-N9-C4	6.11	108.24	105.80
3	A	758	C	C6-N1-C2	-6.10	117.86	120.30
3	A	1362	C	C6-N1-C2	-6.10	117.86	120.30
3	A	776	G	N3-C4-C5	-6.07	125.56	128.60
3	A	2691	C	C6-N1-C2	6.07	122.73	120.30
3	A	2499	C	N1-C2-O2	6.07	122.54	118.90
3	A	1261	C	C6-N1-C2	6.06	122.72	120.30
3	A	2704	C	C6-N1-C2	-6.04	117.89	120.30
3	A	1272	A	C8-N9-C4	6.03	108.21	105.80
3	A	2052	A	N1-C6-N6	6.02	122.21	118.60
3	A	102	U	N1-C2-O2	6.00	127.00	122.80
3	A	2542	A	N3-C4-C5	6.00	131.00	126.80
3	A	2171	A	O4'-C1'-N9	6.00	113.00	108.20
3	A	2109	U	C6-N1-C2	-5.98	117.41	121.00
3	A	130	C	N3-C4-C5	5.97	124.29	121.90
3	A	1992	G	N9-C4-C5	-5.97	103.01	105.40
3	A	1584	U	C5-C6-N1	5.96	125.68	122.70
3	A	2433	A	N1-C2-N3	5.96	132.28	129.30
3	A	832	U	C2-N3-C4	-5.93	123.44	127.00
3	A	2440	C	C6-N1-C2	5.89	122.66	120.30
3	A	2423	U	N3-C4-C5	-5.88	111.07	114.60
3	A	776	G	O4'-C1'-N9	5.87	112.90	108.20
3	A	2820	A	C8-N9-C4	5.87	108.15	105.80
3	A	1531	C	C6-N1-C2	-5.86	117.96	120.30
3	A	205	G	O4'-C1'-N9	5.84	112.87	108.20
12	J	53	LEU	CA-CB-CG	5.82	128.69	115.30
3	A	790	U	N1-C2-O2	5.82	126.88	122.80
3	A	2077	A	C6-N1-C2	-5.81	115.11	118.60
3	A	1072	C	C6-N1-C2	-5.80	117.98	120.30
3	A	141	G	N7-C8-N9	5.79	116.00	113.10
3	A	1584	U	N3-C2-O2	-5.78	118.15	122.20
3	A	793	A	C2-N3-C4	5.77	113.49	110.60
3	A	2580	U	C6-N1-C2	-5.74	117.56	121.00
3	A	2153	C	C5-C6-N1	5.71	123.86	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	741	U	C5-C6-N1	-5.71	119.84	122.70
3	A	1871	A	C8-N9-C4	-5.70	103.52	105.80
3	A	1643	G	C8-N9-C4	-5.70	104.12	106.40
3	A	1045	C	C6-N1-C2	5.69	122.58	120.30
7	E	109	LEU	CA-CB-CG	-5.68	102.23	115.30
3	A	2588	G	N3-C4-C5	5.68	131.44	128.60
3	A	1659	G	N3-C4-C5	5.67	131.44	128.60
3	A	2582	G	N3-C4-C5	-5.67	125.76	128.60
3	A	816	C	C6-N1-C2	-5.67	118.03	120.30
3	A	1993	U	C5-C6-N1	-5.67	119.87	122.70
3	A	76	C	C5-C6-N1	5.66	123.83	121.00
3	A	2243	U	C5-C6-N1	-5.66	119.87	122.70
3	A	2845	U	C2-N3-C4	-5.65	123.61	127.00
3	A	793	A	C5-C6-N6	-5.63	119.20	123.70
11	I	95	LEU	CA-CB-CG	5.62	128.24	115.30
3	A	987	C	N3-C4-C5	5.62	124.15	121.90
35	g	355	GLY	N-CA-C	-5.61	99.08	113.10
3	A	130	C	C6-N1-C2	5.60	122.54	120.30
3	A	783	A	C8-N9-C4	-5.58	103.57	105.80
3	A	410	G	N3-C4-C5	-5.57	125.82	128.60
3	A	2636	C	C6-N1-C1'	-5.56	114.13	120.80
3	A	1303	G	C8-N9-C4	5.56	108.62	106.40
3	A	2145	C	C6-N1-C2	-5.55	118.08	120.30
3	A	1526	C	C6-N1-C2	-5.54	118.08	120.30
3	A	972	A	N1-C6-N6	-5.54	115.28	118.60
3	A	1078	U	C5-C6-N1	5.51	125.45	122.70
3	A	2498	C	C6-N1-C2	-5.51	118.10	120.30
3	A	825	A	C6-N1-C2	-5.51	115.30	118.60
3	A	1125	G	C8-N9-C4	-5.50	104.20	106.40
3	A	2022	U	C6-N1-C2	5.50	124.30	121.00
3	A	2614	A	C5-C6-N1	5.49	120.45	117.70
3	A	1314	C	C6-N1-C2	-5.49	118.11	120.30
3	A	1604	C	C5-C6-N1	-5.48	118.26	121.00
3	A	1351	C	C6-N1-C2	5.48	122.49	120.30
3	A	1584	U	C6-N1-C1'	-5.48	113.53	121.20
3	A	776	G	N7-C8-N9	5.45	115.82	113.10
3	A	206	U	C2-N1-C1'	5.44	124.23	117.70
3	A	135	U	C5-C6-N1	5.44	125.42	122.70
3	A	2153	C	C6-N1-C2	-5.42	118.13	120.30
3	A	280	U	P-O3'-C3'	5.41	126.19	119.70
3	A	2595	G	C4-N9-C1'	-5.41	119.47	126.50
3	A	613	A	P-O3'-C3'	5.40	126.18	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	g	356	ILE	N-CA-C	5.39	125.54	111.00
3	A	2423	U	N1-C2-N3	5.38	118.13	114.90
3	A	755	U	C5-C6-N1	-5.38	120.01	122.70
3	A	1642	G	N3-C4-C5	5.37	131.29	128.60
3	A	12	U	N1-C2-O2	5.37	126.56	122.80
3	A	793	A	C5-C6-N1	5.37	120.38	117.70
3	A	1172	C	C6-N1-C2	-5.36	118.16	120.30
3	A	2090	A	C8-N9-C4	5.35	107.94	105.80
3	A	1848	A	N7-C8-N9	5.34	116.47	113.80
3	A	2380	C	C6-N1-C2	-5.34	118.17	120.30
3	A	790	U	C2-N1-C1'	5.33	124.10	117.70
3	A	1606	C	N1-C2-O2	5.33	122.10	118.90
3	A	1494	A	P-O3'-C3'	5.33	126.09	119.70
3	A	672	C	N3-C2-O2	-5.32	118.17	121.90
3	A	642	U	O4'-C1'-N1	5.31	112.45	108.20
3	A	2645	G	C4-N9-C1'	5.31	133.41	126.50
4	B	42	C	C6-N1-C2	-5.31	118.18	120.30
3	A	569	U	C5-C6-N1	-5.30	120.05	122.70
3	A	946	C	N3-C2-O2	-5.30	118.19	121.90
3	A	906	U	O4'-C1'-N1	5.30	112.44	108.20
3	A	2645	G	N3-C4-C5	-5.29	125.96	128.60
3	A	1664	A	C8-N9-C4	-5.29	103.69	105.80
35	g	356	ILE	C-N-CA	5.27	134.87	121.70
3	A	1848	A	O4'-C1'-N9	5.26	112.41	108.20
3	A	2000	C	C5-C6-N1	-5.24	118.38	121.00
3	A	264	C	N3-C2-O2	-5.24	118.23	121.90
3	A	375	G	N3-C4-N9	5.22	129.13	126.00
3	A	128	C	C6-N1-C2	5.22	122.39	120.30
3	A	809	G	N3-C4-C5	-5.22	125.99	128.60
3	A	906	U	C2-N1-C1'	-5.21	111.45	117.70
3	A	1072	C	C5-C6-N1	5.21	123.60	121.00
3	A	375	G	N3-C4-C5	-5.20	126.00	128.60
3	A	1769	U	C5-C6-N1	-5.20	120.10	122.70
3	A	1970	A	N1-C2-N3	5.20	131.90	129.30
3	A	2516	A	C8-N9-C4	5.20	107.88	105.80
3	A	2074	U	N3-C2-O2	-5.19	118.57	122.20
2	2	74	C	C5-C6-N1	5.19	123.59	121.00
3	A	2022	U	C5-C6-N1	-5.18	120.11	122.70
3	A	2074	U	C2-N1-C1'	5.18	123.91	117.70
3	A	972	A	N9-C4-C5	5.15	107.86	105.80
3	A	828	U	C5-C6-N1	-5.15	120.12	122.70
3	A	981	A	C8-N9-C4	5.13	107.85	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1617	C	C5-C6-N1	-5.13	118.43	121.00
3	A	2847	U	C5-C6-N1	-5.12	120.14	122.70
3	A	66	C	N3-C2-O2	-5.11	118.32	121.90
3	A	1617	C	C2-N3-C4	-5.11	117.34	119.90
3	A	2421	G	C4-C5-N7	5.11	112.84	110.80
3	A	807	U	C5-C6-N1	-5.09	120.15	122.70
3	A	2115	G	N3-C4-C5	-5.09	126.05	128.60
3	A	646	U	C6-N1-C2	-5.07	117.96	121.00
3	A	1958	C	C6-N1-C2	-5.07	118.27	120.30
3	A	2614	A	C8-N9-C4	-5.07	103.77	105.80
3	A	906	U	C6-N1-C1'	5.06	128.28	121.20
3	A	809	G	C8-N9-C4	-5.05	104.38	106.40
3	A	30	G	C8-N9-C4	5.05	108.42	106.40
3	A	878	A	C8-N9-C4	-5.05	103.78	105.80
3	A	2365	G	C8-N9-C4	5.05	108.42	106.40
3	A	76	C	C6-N1-C2	-5.04	118.28	120.30
3	A	1903	G	C8-N9-C4	5.04	108.42	106.40
3	A	1470	A	N9-C4-C5	5.04	107.82	105.80
3	A	2114	A	C8-N9-C4	-5.04	103.79	105.80
3	A	2421	G	C6-C5-N7	-5.04	127.38	130.40
3	A	211	C	C6-N1-C2	5.03	122.31	120.30
3	A	1314	C	C2-N1-C1'	5.03	124.33	118.80
3	A	733	G	C5-N7-C8	-5.02	101.79	104.30
3	A	2064	C	C6-N1-C2	-5.02	118.29	120.30
3	A	102	U	C6-N1-C1'	-5.02	114.17	121.20
3	A	2542	A	C8-N9-C4	5.02	107.81	105.80
3	A	271	G	C8-N9-C4	5.01	108.41	106.40
3	A	804	A	C2-N3-C4	-5.00	108.10	110.60
3	A	1102	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	C	232	HIS	Peptide
9	G	47	ASP	Peptide
12	J	19	ASN	Peptide
35	g	354	PRO	Peptide
37	i	293	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2224	0	1124	11	0
2	2	62	0	34	1	0
3	A	61902	0	31134	679	0
4	B	2569	0	1301	19	0
5	C	2083	0	2154	51	0
6	D	1565	0	1616	33	0
7	E	1552	0	1619	27	0
8	F	1411	0	1444	44	0
9	G	1323	0	1371	33	0
10	H	1110	0	1148	24	0
11	I	946	0	976	30	0
12	J	979	0	1028	39	0
13	K	1129	0	1162	23	0
14	L	946	0	1023	21	0
15	M	1053	0	1129	26	0
16	N	1074	0	1157	24	0
17	O	993	0	1034	24	0
18	P	900	0	935	22	0
19	Q	917	0	962	19	0
20	R	947	0	1019	24	0
21	S	816	0	839	20	0
22	T	857	0	922	14	0
23	U	756	0	817	20	0
24	V	780	0	831	16	0
25	W	753	0	780	14	0
26	X	580	0	594	16	0
27	Y	625	0	652	16	0
28	Z	501	0	531	13	0
29	a	449	0	488	0	0
30	b	444	0	458	0	0
31	c	414	0	442	0	0
32	d	377	0	418	0	0
33	e	504	0	572	0	0
34	f	302	0	340	0	0
35	g	1664	0	476	0	0
36	h	224	0	58	0	0
37	i	3384	0	3512	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	j	284	0	95	0	0
39	k	159	0	189	0	0
40	l	2067	0	2114	0	0
41	f	1	0	0	0	0
42	i	5	0	0	0	0
42	l	5	0	0	0	0
43	i	1	0	0	0	0
43	l	1	0	0	0	0
44	i	28	0	12	0	0
44	l	28	0	12	0	0
All	All	101694	0	68522	1166	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 8.

All (1166) 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:A:1818:U:OP2	5:C:156:ARG:NH1	2.00	0.95
23:U:24:MET:SD	23:U:93:LEU:CD1	2.60	0.90
3:A:1168:G:H1	3:A:1181:U:H3	1.20	0.90
10:H:3:VAL:HG12	10:H:38:PRO:HA	1.57	0.86
3:A:276:U:O2	3:A:278:A:N6	2.07	0.86
1:1:42:A:H61	1:1:67:A:H62	1.23	0.86
3:A:1827:U:OP2	5:C:221:ARG:NH1	2.08	0.86
3:A:287:G:O6	3:A:352:A:N6	2.10	0.85
3:A:2135:A:HO2'	3:A:2159:G:HO2'	1.24	0.85
3:A:2135:A:N6	3:A:2156:G:O2'	2.10	0.84
3:A:2107:G:H1	3:A:2182:U:H3	1.22	0.83
5:C:107:PRO:HD2	5:C:110:LEU:HD22	1.59	0.83
3:A:807:U:OP2	15:M:41:ARG:NH1	2.14	0.81
15:M:109:LYS:HG2	15:M:126:ARG:HB2	1.64	0.80
3:A:994:C:O2	21:S:10:LYS:NZ	2.16	0.79
3:A:2128:G:N3	3:A:2173:A:O2'	2.14	0.78
11:I:18:VAL:HG13	11:I:86:MET:SD	2.23	0.78
18:P:15:ARG:NH2	18:P:95:SER:OG	2.18	0.77
11:I:41:LEU:HD21	11:I:96:PHE:HE1	1.50	0.76
3:A:614:A:O2'	3:A:616:A:N7	2.18	0.76
5:C:245:VAL:HG12	5:C:251:GLN:HA	1.67	0.76
3:A:2599:G:N7	5:C:236:GLU:HB2	2.02	0.75
5:C:181:MET:HB2	5:C:268:VAL:HB	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2848:G:O2'	3:A:2867:G:N2	2.19	0.73
23:U:24:MET:SD	23:U:93:LEU:HD12	2.27	0.73
3:A:720:U:H2'	3:A:721:A:C8	2.24	0.72
3:A:331:C:H41	3:A:1210:G:H22	1.37	0.72
3:A:2119:A:N6	3:A:2167:U:O2	2.22	0.72
13:K:70:THR:OG1	13:K:71:ASP:OD1	2.08	0.72
7:E:1:MET:HG3	7:E:14:VAL:HG23	1.71	0.71
13:K:131:ASN:OD1	13:K:131:ASN:N	2.22	0.71
3:A:2423:U:H2'	3:A:2424:C:O4'	1.89	0.71
3:A:331:C:H41	3:A:1210:G:N2	1.88	0.71
3:A:2310:C:H2'	8:F:77:PHE:HE2	1.54	0.71
3:A:1069:A:H4'	3:A:1070:A:H5"	1.71	0.70
14:L:70:ARG:HD3	14:L:76:VAL:HG22	1.72	0.70
3:A:2163:A:OP1	3:A:2170:A:O2'	2.08	0.70
3:A:258:G:H1'	15:M:104:GLN:HE22	1.56	0.70
3:A:545:U:O2	3:A:548:G:N1	2.19	0.69
3:A:971:G:H2'	3:A:972:A:O4'	1.92	0.69
3:A:1801:A:OP2	5:C:150:LYS:NZ	2.18	0.69
11:I:43:LYS:HG2	11:I:46:ARG:HH22	1.56	0.69
3:A:513:A:O2'	20:R:11:ARG:NH1	2.26	0.69
3:A:1536:C:H4'	3:A:1537:G:H5"	1.75	0.69
3:A:2830:C:H5"	6:D:56:LYS:HE3	1.75	0.68
9:G:35:ARG:HD3	9:G:71:LEU:HD13	1.73	0.68
14:L:79:PHE:HD1	19:Q:70:VAL:HG22	1.58	0.68
3:A:362:A:H3'	3:A:363:G:H8	1.59	0.68
12:J:79:LEU:HB3	12:J:109:ILE:HG12	1.76	0.68
3:A:878:A:H3'	3:A:879:G:H8	1.60	0.67
14:L:21:CYS:HA	14:L:41:ILE:HG22	1.76	0.67
3:A:1340:U:OP1	23:U:19:LYS:NZ	2.26	0.67
18:P:31:THR:HG22	18:P:34:HIS:H	1.59	0.67
3:A:358:U:H2'	3:A:359:G:H8	1.60	0.67
3:A:1105:U:H2'	3:A:1106:G:C8	2.29	0.67
3:A:2103:C:O2	3:A:2186:G:N1	2.27	0.67
3:A:196:A:OP2	15:M:47:ARG:NH1	2.28	0.67
27:Y:32:ASN:O	27:Y:52:SER:HA	1.95	0.67
3:A:2122:U:OP1	3:A:2168:G:N2	2.26	0.67
3:A:2713:U:H3'	3:A:2714:G:H5"	1.77	0.67
3:A:286:U:H2'	3:A:287:G:H8	1.60	0.66
13:K:31:GLU:HG3	13:K:142:ILE:HG13	1.77	0.66
3:A:2216:G:H2'	3:A:2217:G:H8	1.60	0.66
3:A:2135:A:O2'	3:A:2159:G:O2'	2.06	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2590:A:H2'	3:A:2591:C:H6	1.61	0.66
3:A:286:U:H2'	3:A:287:G:C8	2.31	0.66
3:A:2209:G:H1	3:A:2215:C:H42	1.44	0.66
3:A:2303:G:O2'	8:F:121:SER:O	2.13	0.66
10:H:84:ALA:HA	10:H:90:LEU:HA	1.78	0.66
3:A:2305:U:C2	8:F:151:GLY:HA3	2.31	0.65
4:B:43:C:O2	8:F:92:ARG:NH2	2.28	0.65
3:A:1597:A:H5"	3:A:1598:A:H5'	1.78	0.65
7:E:87:ALA:O	7:E:88:ARG:NH2	2.30	0.65
8:F:158:THR:HG22	8:F:160:ALA:H	1.61	0.65
3:A:572:A:OP2	21:S:80:ARG:NH2	2.27	0.65
3:A:1344:U:O2'	3:A:1345:C:OP1	2.14	0.65
28:Z:10:SER:N	28:Z:13:GLU:OE1	2.26	0.65
9:G:9:VAL:HG22	9:G:69:ARG:HE	1.61	0.65
3:A:860:U:H1'	3:A:2268:A:H5'	1.78	0.65
3:A:2788:C:O2'	3:A:2809:A:N3	2.28	0.65
3:A:1342:A:O2'	3:A:1344:U:OP2	2.16	0.64
3:A:1869:G:N2	3:A:1871:A:O2'	2.30	0.64
3:A:1007:C:OP1	13:K:37:ARG:NH2	2.29	0.64
3:A:370:G:O2'	3:A:424:G:OP1	2.11	0.64
3:A:1794:A:H2'	3:A:1795:C:H6	1.61	0.64
3:A:968:C:H2'	3:A:969:G:H8	1.62	0.64
3:A:284:U:H3	3:A:356:G:H1	1.44	0.64
3:A:322:A:H5'	3:A:340:A:H1'	1.78	0.64
3:A:1094:U:N3	3:A:1097:U:OP2	2.30	0.64
3:A:1105:U:H2'	3:A:1106:G:H8	1.63	0.64
3:A:1510:G:H2'	3:A:1511:G:C8	2.32	0.64
3:A:2674:G:H4'	14:L:30:ARG:HG3	1.78	0.64
26:X:65:GLY:HA2	26:X:85:GLU:HG2	1.78	0.64
3:A:1980:G:O2'	3:A:1982:U:OP2	2.16	0.63
3:A:2102:G:N2	3:A:2187:U:O2	2.31	0.63
25:W:21:ARG:NH2	25:W:87:GLN:O	2.29	0.63
8:F:144:ASP:N	8:F:144:ASP:OD1	2.30	0.63
16:N:14:LYS:O	16:N:71:LYS:NZ	2.32	0.63
20:R:74:ILE:HD11	20:R:78:LYS:HB3	1.80	0.63
3:A:2424:C:H5"	3:A:2425:A:H5'	1.79	0.63
3:A:1614:A:N1	22:T:93:ALA:HB2	2.13	0.63
3:A:2151:U:H2'	3:A:2152:G:C8	2.34	0.63
22:T:82:MET:HB3	22:T:84:ARG:HH22	1.62	0.63
13:K:117:ALA:HA	13:K:120:ARG:HH21	1.63	0.63
1:1:29:U:O4	1:1:77:A:N6	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:91:ALA:HB2	19:Q:113:ARG:HA	1.80	0.63
3:A:825:A:H2'	3:A:826:U:O4'	1.98	0.63
20:R:58:ARG:HA	20:R:61:TRP:CE3	2.34	0.63
3:A:1187:G:OP1	21:S:85:LYS:NZ	2.31	0.62
8:F:74:VAL:HG22	8:F:79:ILE:HD11	1.79	0.62
16:N:50:ARG:O	16:N:54:THR:OG1	2.13	0.62
3:A:2809:A:H2'	3:A:2810:A:C8	2.34	0.62
21:S:41:ILE:HB	21:S:48:LYS:HD2	1.79	0.62
3:A:1433:A:N1	3:A:1434:A:N6	2.48	0.62
3:A:514:A:N3	3:A:581:C:O2'	2.32	0.62
19:Q:4:ILE:HD12	19:Q:4:ILE:H	1.65	0.62
3:A:784:G:C6	5:C:228:VAL:HG11	2.35	0.62
17:O:49:GLU:HA	17:O:52:ILE:HD12	1.79	0.62
10:H:68:ARG:HA	10:H:71:LYS:HD2	1.81	0.62
3:A:2590:A:H2'	3:A:2591:C:C6	2.35	0.62
11:I:57:ASN:ND2	11:I:76:PHE:O	2.33	0.61
3:A:2822:G:O6	17:O:2:ARG:NH1	2.32	0.61
12:J:53:LEU:HD11	12:J:82:LYS:HD2	1.83	0.61
26:X:56:ASP:OD1	26:X:56:ASP:N	2.28	0.61
3:A:2639:A:H2'	3:A:2640:G:O4'	2.01	0.61
11:I:41:LEU:HD21	11:I:96:PHE:CE1	2.34	0.61
15:M:57:LEU:HD13	15:M:60:ARG:HH11	1.65	0.61
3:A:1079:C:O2'	12:J:134:ARG:NH1	2.33	0.61
3:A:2636:C:HO2'	6:D:45:TYR:HH	1.46	0.61
3:A:503:A:H4'	3:A:504:A:H5'	1.82	0.61
3:A:2060:A:H3'	7:E:63:LYS:HZ1	1.65	0.61
3:A:1001:A:H2'	3:A:1002:G:O4'	2.01	0.61
22:T:6:LYS:HG2	22:T:104:THR:HG23	1.82	0.60
3:A:1076:C:H2'	3:A:1077:A:C8	2.37	0.60
1:1:37:U:O4	1:1:68:A:N6	2.34	0.60
3:A:585:G:N7	20:R:6:ARG:NH1	2.48	0.60
3:A:2310:C:H2'	8:F:77:PHE:CE2	2.35	0.60
5:C:235:GLY:HA3	5:C:239:ASN:HB2	1.83	0.60
9:G:137:ASP:O	9:G:141:ILE:HG22	2.01	0.60
11:I:27:VAL:HG22	11:I:82:ILE:HG22	1.83	0.60
6:D:12:THR:OG1	6:D:13:ARG:N	2.34	0.60
7:E:97:ASN:N	7:E:97:ASN:OD1	2.34	0.60
15:M:81:ASP:HA	15:M:84:LYS:HD2	1.82	0.60
3:A:570:G:H2'	3:A:2030:A:N7	2.16	0.60
3:A:1794:A:H2'	3:A:1795:C:C6	2.37	0.60
17:O:54:LEU:HD21	17:O:65:LEU:HD23	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1251:C:OP2	20:R:6:ARG:NH2	2.35	0.60
3:A:2831:G:OP1	6:D:56:LYS:NZ	2.35	0.60
13:K:36:LEU:HD11	13:K:122:LEU:HB2	1.83	0.60
3:A:355:U:H2'	3:A:356:G:C8	2.37	0.59
11:I:64:VAL:HG22	11:I:69:PHE:HB2	1.84	0.59
8:F:44:ILE:HG21	8:F:79:ILE:HG22	1.83	0.59
3:A:1363:C:O2'	3:A:1809:A:N3	2.33	0.59
6:D:2:ILE:HG13	6:D:100:LEU:HD21	1.83	0.59
3:A:776:G:O2'	3:A:777:G:OP1	2.19	0.59
3:A:1796:U:H2'	3:A:1797:G:H8	1.67	0.59
3:A:2819:G:H2'	3:A:2821:A:N7	2.17	0.59
18:P:99:TYR:OH	18:P:111:ARG:NH1	2.36	0.59
3:A:2584:U:H3'	3:A:2585:U:H5"	1.84	0.59
3:A:878:A:H3'	3:A:879:G:C8	2.38	0.59
9:G:27:LYS:NZ	9:G:27:LYS:HB3	2.17	0.59
3:A:2127:G:O2'	3:A:2128:G:O4'	2.20	0.59
12:J:106:LEU:HB3	12:J:126:THR:HG23	1.85	0.59
3:A:1808:A:H3'	3:A:1809:A:C8	2.38	0.58
3:A:2021:C:OP1	20:R:25:TYR:OH	2.21	0.58
21:S:37:GLU:HB3	21:S:53:PHE:CE1	2.39	0.58
24:V:81:ASP:OD1	24:V:82:ARG:N	2.35	0.58
3:A:2205:A:H61	3:A:2219:U:H3	1.50	0.58
17:O:73:ASN:HA	17:O:76:VAL:HG22	1.86	0.58
25:W:76:ASP:OD1	25:W:77:VAL:N	2.37	0.58
3:A:396:G:OP2	27:Y:10:LYS:NZ	2.36	0.58
3:A:1130:U:O2'	3:A:1131:G:H8	1.87	0.58
3:A:2127:G:O2'	3:A:2128:G:O5'	2.19	0.58
3:A:2412:A:H2'	3:A:2413:G:O4'	2.04	0.58
6:D:13:ARG:HD2	6:D:15:PHE:CZ	2.38	0.58
3:A:833:A:H2'	3:A:834:G:C8	2.39	0.58
18:P:41:ALA:HB2	18:P:48:LEU:HD21	1.86	0.58
3:A:1645:G:H5"	3:A:1646:C:H5'	1.86	0.57
5:C:227:PRO:HG3	5:C:234:GLY:H	1.69	0.57
17:O:94:TYR:O	17:O:116:VAL:HG23	2.05	0.57
3:A:2447:G:N2	3:A:2450:A:OP2	2.37	0.57
3:A:849:A:H2'	3:A:850:U:C6	2.39	0.57
3:A:1715:G:O2'	3:A:1743:G:O6	2.17	0.57
6:D:157:LYS:HD2	13:K:80:HIS:CE1	2.40	0.57
7:E:21:ARG:HD3	7:E:106:LYS:HB3	1.85	0.57
12:J:59:ILE:HD13	12:J:69:PHE:HB3	1.86	0.57
3:A:2291:U:H2'	3:A:2292:U:C6	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:148:GLN:HB2	6:D:152:PRO:HD2	1.85	0.57
3:A:340:A:H2'	3:A:341:C:O4'	2.05	0.57
3:A:839:U:H2'	3:A:840:C:C6	2.40	0.57
3:A:1403:A:HO2'	3:A:1471:G:HO2'	1.38	0.57
3:A:1063:G:H5'	12:J:77:ALA:HB1	1.87	0.56
3:A:1076:C:H2'	3:A:1077:A:H8	1.69	0.56
3:A:1905:C:H2'	3:A:1930:G:C8	2.40	0.56
5:C:166:ALA:HB3	5:C:173:THR:HB	1.86	0.56
7:E:112:LEU:HB3	7:E:118:LEU:HB2	1.87	0.56
3:A:876:C:H2'	3:A:877:A:O4'	2.05	0.56
3:A:2216:G:H2'	3:A:2217:G:C8	2.40	0.56
11:I:60:LEU:O	11:I:64:VAL:HB	2.05	0.56
3:A:26:G:C6	3:A:27:G:N1	2.73	0.56
3:A:480:A:OP2	24:V:44:LYS:NZ	2.23	0.56
3:A:721:A:H2'	3:A:722:A:C8	2.41	0.56
3:A:2602:A:H4'	3:A:2603:G:O5'	2.04	0.56
8:F:33:LYS:HG2	8:F:157:THR:HB	1.87	0.56
3:A:1796:U:H2'	3:A:1797:G:C8	2.40	0.56
6:D:1:MET:HG2	6:D:2:ILE:H	1.70	0.56
10:H:37:VAL:HG22	10:H:38:PRO:HD2	1.86	0.56
12:J:53:LEU:HD22	12:J:78:VAL:HG13	1.87	0.56
3:A:2162:G:H5"	3:A:2171:A:H2'	1.86	0.56
13:K:72:LYS:HE3	13:K:74:TYR:CE1	2.39	0.56
3:A:1790:C:H3'	3:A:1828:G:N2	2.21	0.56
3:A:2298:A:H2'	3:A:2299:U:O4'	2.05	0.56
3:A:2430:A:N3	3:A:2430:A:H2'	2.21	0.56
4:B:42:C:C5	8:F:66:LEU:HD22	2.41	0.56
3:A:299:A:N1	3:A:322:A:O2'	2.27	0.56
3:A:1800:C:H5'	5:C:146:MET:HE1	1.88	0.56
3:A:2491:U:H5"	3:A:2570:G:H5"	1.88	0.56
3:A:388:G:N7	3:A:390:U:H2'	2.21	0.56
3:A:849:A:H2'	3:A:850:U:H6	1.70	0.56
9:G:30:ASN:HB3	9:G:79:VAL:HA	1.88	0.56
17:O:2:ARG:NH1	17:O:2:ARG:HB3	2.21	0.56
18:P:16:ARG:HA	18:P:16:ARG:HH21	1.71	0.56
3:A:812:C:H4'	20:R:13:ARG:NH1	2.21	0.55
3:A:1442:U:H2'	3:A:1443:U:C6	2.41	0.55
25:W:62:THR:HG22	25:W:71:LYS:HG2	1.88	0.55
12:J:73:THR:HB	12:J:112:THR:HG22	1.87	0.55
3:A:2783:U:H2'	3:A:2784:U:C6	2.42	0.55
12:J:127:ARG:HA	12:J:130:GLU:HB2	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:19:A:H2'	3:A:20:C:C6	2.41	0.55
3:A:882:G:H1	3:A:894:U:H3	1.54	0.55
10:H:7:ASP:OD1	10:H:8:LYS:N	2.40	0.55
17:O:48:VAL:O	17:O:51:LEU:HB2	2.05	0.55
3:A:591:U:H2'	3:A:592:A:H8	1.72	0.55
3:A:639:U:H2'	3:A:640:C:C6	2.42	0.55
3:A:2133:G:H2'	3:A:2157:G:H1	1.70	0.55
3:A:645:C:O2'	3:A:646:U:OP1	2.24	0.55
3:A:2171:A:H3'	3:A:2173:A:C8	2.41	0.55
3:A:184:C:H2'	3:A:185:G:C8	2.41	0.55
8:F:132:VAL:HG22	8:F:152:LEU:HB3	1.88	0.55
8:F:134:GLU:HB3	8:F:136:ILE:HG12	1.89	0.55
5:C:160:THR:HG22	5:C:177:ARG:HG2	1.89	0.55
24:V:33:LYS:HB3	24:V:64:ALA:HB1	1.87	0.55
3:A:2070:A:H2'	3:A:2071:A:C8	2.42	0.55
3:A:2584:U:H3'	3:A:2585:U:C5'	2.36	0.55
3:A:2591:C:H2'	3:A:2592:G:C8	2.41	0.55
3:A:996:A:OP2	21:S:10:LYS:HD3	2.07	0.54
6:D:8:LYS:HB2	6:D:201:LEU:HD11	1.88	0.54
3:A:586:A:H5'	7:E:84:THR:HG21	1.90	0.54
6:D:184:ARG:NH1	19:Q:7:GLN:OE1	2.40	0.54
3:A:833:A:H2'	3:A:834:G:H8	1.73	0.54
12:J:56:PRO:HD3	12:J:75:PRO:HD3	1.90	0.54
12:J:79:LEU:HA	12:J:82:LYS:HG2	1.88	0.54
3:A:1837:C:H2'	3:A:1899:A:H61	1.73	0.54
3:A:2262:U:H2'	3:A:2263:C:H6	1.72	0.54
13:K:34:ARG:HH22	13:K:40:HIS:HB3	1.71	0.54
3:A:172:A:H2'	3:A:173:A:C8	2.43	0.54
3:A:609:A:H2'	3:A:610:C:O4'	2.08	0.54
3:A:2579:C:O2'	6:D:136:ASN:ND2	2.41	0.54
3:A:2619:C:H5"	6:D:157:LYS:HG3	1.89	0.54
7:E:88:ARG:HA	7:E:88:ARG:HH21	1.72	0.54
21:S:20:VAL:HG13	21:S:96:VAL:HG23	1.89	0.54
3:A:720:U:H2'	3:A:721:A:H8	1.72	0.54
3:A:2267:A:H5"	3:A:2268:A:H5"	1.89	0.54
3:A:2424:C:H5"	3:A:2425:A:C5'	2.37	0.54
21:S:48:LYS:HE3	21:S:103:ALA:HB1	1.90	0.54
23:U:68:LYS:HG3	23:U:77:ARG:NH2	2.23	0.54
3:A:1923:U:H2'	3:A:1924:C:C6	2.43	0.54
3:A:2834:G:O6	3:A:2879:A:H2'	2.08	0.53
3:A:2443:C:H2'	3:A:2444:G:C8	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:104:ASN:ND2	9:G:114:ASP:OD1	2.41	0.53
11:I:54:VAL:HG22	11:I:81:LEU:HD13	1.90	0.53
3:A:2845:U:H5"	19:Q:52:ASN:O	2.08	0.53
14:L:38:ILE:HD11	14:L:112:PHE:HZ	1.73	0.53
14:L:40:LYS:HE3	14:L:57:VAL:HG12	1.91	0.53
3:A:1056:G:H5"	3:A:1057:A:H5'	1.90	0.53
3:A:1056:G:O2'	3:A:1103:A:N6	2.40	0.53
3:A:2547:A:H4'	14:L:29:HIS:CD2	2.44	0.53
17:O:36:THR:OG1	17:O:37:THR:N	2.42	0.53
3:A:9:G:O2'	3:A:2800:A:N6	2.42	0.53
3:A:608:A:H2'	3:A:609:A:C8	2.44	0.53
5:C:145:GLU:HB2	5:C:188:CYS:HB3	1.89	0.53
17:O:36:THR:HG23	17:O:41:ALA:HB2	1.90	0.53
3:A:2171:A:H3'	3:A:2173:A:H8	1.74	0.53
23:U:24:MET:CG	23:U:93:LEU:HD12	2.39	0.53
10:H:116:ARG:HH21	10:H:133:GLN:HB3	1.74	0.53
11:I:88:HIS:ND1	11:I:89:PRO:O	2.42	0.53
3:A:671:C:H2'	3:A:672:C:H6	1.74	0.52
3:A:788:A:OP1	3:A:791:C:N4	2.41	0.52
3:A:1069:A:C2	3:A:1096:A:H5"	2.44	0.52
3:A:2808:G:O2'	3:A:2890:G:O6	2.21	0.52
4:B:93:C:OP2	25:W:18:ARG:NH1	2.41	0.52
5:C:62:TYR:HA	5:C:86:ASN:HD21	1.73	0.52
3:A:1428:C:C5	3:A:1569:A:H5"	2.45	0.52
3:A:1993:U:H4'	6:D:133:THR:OG1	2.10	0.52
3:A:2086:U:H2'	3:A:2087:G:C8	2.44	0.52
3:A:2210:U:H4'	3:A:2211:A:H5'	1.91	0.52
3:A:679:C:H2'	3:A:680:C:C6	2.44	0.52
3:A:1425:G:H2'	3:A:1426:G:O4'	2.09	0.52
13:K:3:THR:HB	20:R:57:PHE:HE1	1.75	0.52
3:A:68:G:H2'	3:A:69:C:O4'	2.10	0.52
3:A:120:U:H4'	3:A:121:G:H5"	1.89	0.52
3:A:284:U:O2	3:A:356:G:N2	2.37	0.52
3:A:1873:G:H2'	3:A:1874:C:H6	1.74	0.52
3:A:2127:G:H2'	3:A:2128:G:C8	2.45	0.52
8:F:99:PHE:HD1	8:F:102:ARG:HH22	1.57	0.52
18:P:69:ASP:N	18:P:69:ASP:OD1	2.40	0.52
3:A:1289:C:H2'	3:A:1290:C:C6	2.45	0.52
3:A:1421:G:C2	3:A:1422:G:C8	2.98	0.52
3:A:1791:A:N6	3:A:1828:G:O2'	2.42	0.52
7:E:28:VAL:O	7:E:32:VAL:HG13	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:52:PRO:HG2	21:S:53:PHE:CD2	2.45	0.52
23:U:53:VAL:HB	23:U:91:GLN:CD	2.30	0.52
3:A:90:U:H3'	3:A:91:A:H8	1.74	0.52
3:A:2133:G:H21	3:A:2158:A:H62	1.58	0.52
3:A:2637:U:C2'	3:A:2638:G:H5'	2.39	0.52
6:D:114:LYS:HD3	6:D:196:ALA:HB2	1.92	0.52
25:W:55:GLU:H	25:W:55:GLU:CD	2.13	0.52
3:A:653:U:H1'	3:A:654:A:H5"	1.91	0.52
3:A:845:A:H61	3:A:932:U:H3	1.58	0.52
3:A:898:C:H2'	3:A:899:A:O4'	2.10	0.52
28:Z:2:LYS:HG3	28:Z:5:GLU:OE1	2.10	0.52
3:A:1115:G:O2'	3:A:1116:G:H5"	2.10	0.52
3:A:1410:G:H1	3:A:1592:C:H42	1.57	0.52
7:E:41:GLN:HG2	7:E:43:THR:HG23	1.92	0.52
3:A:1451:C:H1'	3:A:1452:G:C2	2.45	0.51
23:U:93:LEU:HD13	23:U:95:PHE:CZ	2.45	0.51
3:A:1681:G:H21	3:A:1762:A:H3'	1.75	0.51
3:A:1798:U:H5"	5:C:258:ARG:HB2	1.92	0.51
19:Q:16:ASP:OD1	19:Q:16:ASP:N	2.33	0.51
23:U:56:GLU:HA	23:U:88:LYS:HE3	1.92	0.51
3:A:364:C:H2'	3:A:365:U:C6	2.45	0.51
3:A:968:C:H2'	3:A:969:G:C8	2.42	0.51
8:F:128:TYR:HE2	8:F:130:MET:HG2	1.76	0.51
3:A:576:U:H2'	3:A:577:G:C8	2.46	0.51
3:A:1790:C:H2'	3:A:1791:A:C5	2.45	0.51
3:A:2502:G:H5"	3:A:2503:A:H5"	1.92	0.51
3:A:2647:U:H2'	3:A:2648:G:H8	1.76	0.51
7:E:24:ASN:ND2	7:E:27:LEU:HB2	2.25	0.51
17:O:55:ALA:HA	17:O:80:PHE:CE2	2.45	0.51
24:V:18:ASP:OD2	24:V:40:ASN:N	2.38	0.51
24:V:74:ASN:HD21	24:V:99:ASN:HD21	1.58	0.51
3:A:499:U:H2'	3:A:500:G:O4'	2.10	0.51
3:A:1414:C:H2'	3:A:1415:U:O4'	2.11	0.51
3:A:1437:C:H2'	3:A:1438:U:C6	2.46	0.51
3:A:2439:A:H4'	3:A:2440:C:H5"	1.91	0.51
3:A:141:G:H2'	3:A:142:A:O4'	2.11	0.51
3:A:948:C:H2'	3:A:949:G:C8	2.45	0.51
20:R:24:TYR:N	20:R:24:TYR:CD1	2.78	0.51
21:S:28:ALA:HB3	21:S:31:GLU:HG3	1.93	0.51
3:A:2271:G:H5"	26:X:18:ALA:HB1	1.93	0.51
3:A:2720:U:OP1	19:Q:53:ARG:NH2	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:113:LYS:HE3	12:J:116:ASP:HB3	1.92	0.51
3:A:256:A:H2'	3:A:257:C:H6	1.74	0.51
7:E:145:ASP:HA	7:E:166:LYS:HB3	1.93	0.51
8:F:40:VAL:HG11	8:F:43:ALA:HB2	1.92	0.51
3:A:1000:A:OP2	3:A:1154:G:N1	2.32	0.51
3:A:621:A:OP2	15:M:99:ASN:ND2	2.40	0.51
3:A:1927:A:H2'	3:A:1928:A:C8	2.46	0.51
15:M:36:LYS:O	15:M:40:SER:HB3	2.11	0.51
3:A:1132:U:H2'	3:A:1133:A:C8	2.46	0.50
3:A:1394:U:H4'	3:A:1603:A:H4'	1.92	0.50
3:A:2333:A:P	26:X:77:ARG:HH22	2.34	0.50
13:K:32:LEU:O	13:K:36:LEU:HB2	2.12	0.50
16:N:1:MET:HA	16:N:47:GLU:HG3	1.93	0.50
3:A:2564:A:OP1	3:A:2648:G:O2'	2.19	0.50
15:M:23:ILE:HG12	21:S:82:HIS:CD2	2.47	0.50
16:N:30:SER:H	16:N:106:ASP:HB3	1.75	0.50
3:A:2024:G:H2'	3:A:2025:C:H6	1.76	0.50
3:A:2809:A:H2'	3:A:2810:A:H8	1.75	0.50
20:R:76:TYR:CZ	20:R:80:ILE:HG13	2.46	0.50
3:A:128:C:H2'	3:A:129:C:C6	2.46	0.50
3:A:357:C:H2'	3:A:358:U:C6	2.46	0.50
3:A:1405:U:H2'	3:A:1406:U:C6	2.46	0.50
3:A:2282:G:C6	3:A:2425:A:C2	3.00	0.50
12:J:73:THR:OG1	12:J:113:LYS:NZ	2.40	0.50
14:L:64:ARG:NH1	14:L:102:PRO:O	2.44	0.50
22:T:40:ASN:O	22:T:41:LYS:HG2	2.10	0.50
23:U:7:LEU:HD13	23:U:46:ALA:HA	1.92	0.50
3:A:1939:U:OP1	3:A:2604:U:O2'	2.28	0.50
3:A:90:U:C2	3:A:91:A:N7	2.80	0.50
3:A:256:A:H2'	3:A:257:C:C6	2.46	0.50
8:F:17:MET:SD	8:F:22:TYR:HB2	2.52	0.50
20:R:65:ILE:HD11	20:R:95:LEU:HB2	1.93	0.50
23:U:54:GLU:H	23:U:91:GLN:NE2	2.08	0.50
3:A:878:A:N6	3:A:899:A:O2'	2.45	0.50
3:A:1327:A:N6	3:A:1647:U:O2	2.45	0.50
3:A:2850:A:N7	3:A:2868:A:O2'	2.39	0.50
9:G:127:THR:HG22	9:G:128:GLN:H	1.77	0.50
3:A:738:G:H1'	3:A:759:G:N2	2.27	0.50
3:A:2576:G:O2'	3:A:2579:C:OP2	2.23	0.50
4:B:2:G:H2'	4:B:3:C:C6	2.47	0.50
12:J:83:ALA:O	12:J:105:GLN:NE2	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:132:MET:HG2	5:C:135:ILE:HD12	1.94	0.50
23:U:24:MET:SD	23:U:93:LEU:HD13	2.50	0.50
3:A:1638:C:H1'	3:A:2698:U:O2'	2.12	0.49
9:G:83:PHE:O	9:G:134:LYS:HA	2.12	0.49
10:H:94:ILE:HB	10:H:122:LEU:HB2	1.94	0.49
28:Z:39:GLN:HB3	28:Z:41:HIS:CE1	2.47	0.49
3:A:1021:A:H3'	3:A:1021:A:N3	2.27	0.49
3:A:2183:A:H2'	3:A:2184:A:C8	2.46	0.49
24:V:46:GLN:OE1	24:V:54:GLN:NE2	2.44	0.49
3:A:184:C:H2'	3:A:185:G:H8	1.76	0.49
3:A:1506:U:H2'	3:A:1507:C:C6	2.48	0.49
3:A:2626:C:H2'	3:A:2627:G:O4'	2.12	0.49
15:M:4:ASN:OD1	15:M:4:ASN:N	2.39	0.49
19:Q:23:GLY:O	19:Q:90:GLY:HA3	2.11	0.49
25:W:75:GLN:HB2	25:W:92:VAL:HG12	1.94	0.49
3:A:671:C:H2'	3:A:672:C:C6	2.48	0.49
3:A:1187:G:HO2'	3:A:1188:U:H6	1.60	0.49
3:A:2747:G:O2'	9:G:67:THR:HG23	2.12	0.49
9:G:8:PRO:HB3	9:G:51:THR:HG22	1.94	0.49
3:A:27:G:N2	3:A:512:G:H1'	2.28	0.49
3:A:613:A:O2'	3:A:614:A:O5'	2.30	0.49
3:A:2073:C:H2'	3:A:2074:U:H6	1.77	0.49
3:A:2151:U:H2'	3:A:2152:G:H8	1.77	0.49
3:A:2171:A:H5'	3:A:2173:A:N7	2.26	0.49
3:A:2308:G:H3'	3:A:2310:C:OP2	2.11	0.49
3:A:1005:C:H2'	3:A:1006:C:C6	2.47	0.49
3:A:1903:G:C2	3:A:1904:G:C8	3.00	0.49
8:F:50:LEU:O	8:F:54:ALA:N	2.38	0.49
14:L:10:VAL:HG12	14:L:12:ASP:H	1.78	0.49
17:O:14:SER:HA	17:O:17:ARG:NH1	2.27	0.49
3:A:563:A:C4	3:A:2018:G:C2	3.01	0.49
4:B:7:G:OP1	18:P:4:LYS:NZ	2.27	0.49
3:A:1088:A:N6	12:J:135:SER:HB3	2.26	0.49
3:A:1243:C:H1'	15:M:4:ASN:O	2.13	0.49
9:G:101:ASN:ND2	9:G:116:GLN:OE1	2.45	0.49
18:P:30:ARG:HG3	18:P:35:ILE:HD12	1.94	0.49
3:A:1606:C:H5'	3:A:1607:C:OP1	2.13	0.49
15:M:19:LEU:HD23	15:M:27:LEU:HD13	1.95	0.49
3:A:160:A:N3	3:A:2208:C:O2'	2.43	0.48
7:E:23:PHE:CD1	7:E:111:GLU:HG3	2.48	0.48
22:T:96:ILE:HD13	22:T:96:ILE:HA	1.74	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:17:ASN:HB2	27:Y:25:THR:OG1	2.13	0.48
1:1:98:U:H2'	1:1:99:G:H8	1.79	0.48
3:A:467:G:H2'	3:A:468:G:O4'	2.13	0.48
3:A:719:C:H2'	3:A:720:U:H6	1.78	0.48
3:A:1093:G:C2'	3:A:1098:A:H61	2.26	0.48
3:A:2290:G:H2'	3:A:2291:U:O4'	2.12	0.48
4:B:116:G:H2'	4:B:117:G:C8	2.49	0.48
5:C:175:ARG:HG3	5:C:181:MET:HE1	1.95	0.48
10:H:110:VAL:HG12	10:H:114:GLU:HB2	1.94	0.48
21:S:65:ALA:HB3	21:S:95:ASP:HB2	1.94	0.48
1:1:53:G:N2	1:1:56:A:OP2	2.45	0.48
7:E:184:ASP:OD1	7:E:184:ASP:N	2.43	0.48
27:Y:17:ASN:OD1	27:Y:27:ARG:HD2	2.13	0.48
3:A:813:U:H2'	3:A:814:C:C6	2.49	0.48
3:A:1654:A:H2'	3:A:1655:A:H8	1.78	0.48
3:A:1773:A:N7	3:A:1829:A:H1'	2.28	0.48
3:A:1790:C:H3'	3:A:1828:G:H22	1.77	0.48
3:A:2280:G:O2'	3:A:2388:A:N1	2.37	0.48
11:I:33:VAL:HG21	11:I:106:PHE:CE2	2.48	0.48
25:W:25:LYS:HB3	25:W:25:LYS:HE2	1.71	0.48
26:X:34:GLY:N	26:X:61:ALA:O	2.37	0.48
3:A:1386:C:H2'	3:A:1387:A:C8	2.49	0.48
3:A:1819:A:H5"	5:C:160:THR:HG21	1.94	0.48
3:A:2158:A:H4'	3:A:2159:G:O5'	2.14	0.48
5:C:145:GLU:HG2	5:C:151:GLY:C	2.34	0.48
8:F:7:TYR:CD1	8:F:11:GLU:HG3	2.48	0.48
10:H:115:VAL:HG22	10:H:132:PHE:CE2	2.48	0.48
23:U:68:LYS:HG3	23:U:77:ARG:HH21	1.79	0.48
3:A:136:G:H2'	3:A:137:U:O4'	2.13	0.48
3:A:428:A:H2'	3:A:429:A:C8	2.49	0.48
3:A:784:G:H5'	3:A:785:G:OP1	2.13	0.48
3:A:2116:G:C5	3:A:2165:C:N4	2.82	0.48
3:A:2834:G:H2'	3:A:2879:A:N6	2.29	0.48
9:G:86:LYS:HG2	9:G:132:VAL:HG22	1.96	0.48
10:H:93:SER:HB3	10:H:123:ARG:HG2	1.95	0.48
26:X:41:ARG:HD3	26:X:41:ARG:HA	1.53	0.48
3:A:782:A:N7	5:C:220:VAL:HG21	2.29	0.48
3:A:1268:A:H2'	3:A:1269:A:O4'	2.13	0.48
3:A:483:A:O4'	24:V:45:HIS:HB3	2.14	0.48
3:A:795:C:H2'	3:A:796:C:C6	2.49	0.48
3:A:914:G:H5'	3:A:915:C:OP2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1179:G:H2'	3:A:1180:U:C6	2.48	0.48
3:A:2428:G:H21	15:M:60:ARG:NH2	2.12	0.48
9:G:35:ARG:CD	9:G:71:LEU:HD13	2.43	0.48
12:J:113:LYS:O	12:J:117:MET:N	2.46	0.48
13:K:72:LYS:HE3	13:K:74:TYR:CZ	2.49	0.48
26:X:40:GLN:NE2	26:X:43:THR:HA	2.29	0.48
3:A:957:C:C5	3:A:959:A:C5	3.01	0.48
3:A:1527:G:N1	3:A:1544:A:OP2	2.32	0.48
16:N:41:LEU:HG	16:N:96:ILE:HG13	1.94	0.48
1:1:76:G:H2'	1:1:77:A:C8	2.48	0.48
3:A:1446:C:H2'	3:A:1447:C:C6	2.49	0.48
3:A:2060:A:H3'	7:E:63:LYS:NZ	2.29	0.48
3:A:2209:G:H1	3:A:2215:C:N4	2.12	0.48
6:D:25:THR:HG21	6:D:193:VAL:HG22	1.95	0.48
9:G:80:THR:OG1	9:G:81:GLU:N	2.46	0.48
14:L:66:LYS:HB3	14:L:66:LYS:HE2	1.64	0.48
16:N:11:LYS:HD3	16:N:86:LYS:HD3	1.96	0.48
27:Y:6:GLN:NE2	27:Y:76:GLU:OE2	2.39	0.48
28:Z:14:LEU:HB3	28:Z:57:LEU:HD21	1.96	0.48
3:A:140:C:H4'	3:A:141:G:OP1	2.13	0.47
3:A:156:A:H2'	3:A:157:C:O4'	2.13	0.47
3:A:208:C:H2'	3:A:209:C:H6	1.78	0.47
3:A:477:A:H2'	3:A:478:A:C8	2.49	0.47
3:A:1007:C:H5"	13:K:37:ARG:NH2	2.29	0.47
3:A:1846:G:H5"	3:A:1847:A:OP2	2.14	0.47
3:A:2305:U:H5"	8:F:131:GLY:HA3	1.96	0.47
12:J:42:PHE:O	12:J:46:THR:OG1	2.32	0.47
17:O:38:LEU:HB3	17:O:39:PRO:HD3	1.96	0.47
18:P:31:THR:HG23	18:P:32:PRO:HD2	1.96	0.47
3:A:175:G:N2	3:A:176:A:N3	2.62	0.47
3:A:1132:U:H3'	3:A:1133:A:H5"	1.95	0.47
3:A:2444:G:OP2	7:E:63:LYS:HD2	2.14	0.47
3:A:2570:G:H2'	3:A:2571:U:O4'	2.14	0.47
7:E:125:SER:OG	7:E:126:VAL:N	2.46	0.47
14:L:73:ASP:OD1	14:L:73:ASP:N	2.39	0.47
18:P:51:ALA:HB3	18:P:78:VAL:HG13	1.95	0.47
3:A:910:A:H2'	3:A:911:A:C8	2.49	0.47
3:A:911:A:H2'	16:N:9:PHE:HZ	1.78	0.47
3:A:995:C:OP2	20:R:54:LYS:NZ	2.44	0.47
3:A:1085:A:H61	11:I:35:VAL:HG22	1.78	0.47
3:A:1341:G:O2'	23:U:59:ASN:ND2	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1438:U:H2'	3:A:1439:A:H8	1.79	0.47
3:A:2433:A:H2	27:Y:21:ALA:HB1	1.79	0.47
23:U:58:VAL:HG22	23:U:85:VAL:HG22	1.96	0.47
8:F:25:VAL:O	8:F:28:VAL:HG12	2.14	0.47
10:H:142:VAL:HG12	10:H:143:ILE:H	1.79	0.47
12:J:10:LYS:O	12:J:11:LEU:HD12	2.15	0.47
13:K:78:THR:HG23	13:K:83:GLY:O	2.13	0.47
3:A:1873:G:H2'	3:A:1874:C:C6	2.49	0.47
3:A:2226:C:H2'	3:A:2227:A:O4'	2.13	0.47
6:D:56:LYS:HB2	6:D:59:ARG:HB2	1.95	0.47
6:D:121:THR:HB	6:D:127:PHE:CD2	2.50	0.47
12:J:40:LYS:N	12:J:40:LYS:HD2	2.30	0.47
15:M:55:MET:SD	15:M:56:PRO:HD2	2.55	0.47
18:P:43:ASN:ND2	18:P:43:ASN:H	2.13	0.47
24:V:14:LEU:HD11	24:V:71:ALA:HB2	1.95	0.47
3:A:112:U:H5'	28:Z:58:ASN:HD21	1.80	0.47
3:A:1027:A:C6	3:A:1126:A:C4	3.02	0.47
3:A:2592:G:C6	3:A:2593:U:N3	2.83	0.47
10:H:29:PHE:O	10:H:32:PRO:HD2	2.15	0.47
12:J:75:PRO:HD2	12:J:78:VAL:HB	1.96	0.47
24:V:41:LEU:HD22	24:V:62:GLU:HG2	1.96	0.47
3:A:127:A:H5"	3:A:128:C:O4'	2.14	0.47
3:A:713:G:H2'	3:A:714:U:C6	2.50	0.47
3:A:911:A:H2'	16:N:9:PHE:CZ	2.50	0.47
3:A:975:A:H1'	3:A:990:A:C2	2.50	0.47
3:A:1420:A:N7	3:A:2211:A:N6	2.62	0.47
3:A:2419:U:O2'	3:A:2420:C:H5'	2.15	0.47
3:A:2557:G:H2'	3:A:2558:C:C6	2.50	0.47
5:C:260:ASN:OD1	5:C:262:ARG:N	2.37	0.47
9:G:102:VAL:HG22	9:G:116:GLN:HE22	1.78	0.47
9:G:155:GLU:OE1	9:G:157:TYR:N	2.44	0.47
10:H:40:THR:HG22	10:H:41:LYS:H	1.79	0.47
13:K:98:GLU:OE1	13:K:98:GLU:N	2.41	0.47
17:O:25:ALA:O	17:O:29:VAL:HG23	2.15	0.47
18:P:30:ARG:HB3	18:P:97:PHE:CE1	2.50	0.47
25:W:2:PHE:HB3	25:W:50:MET:CE	2.44	0.47
3:A:323:C:C4	3:A:333:G:C8	3.03	0.47
3:A:1672:A:C6	3:A:1673:G:C6	3.03	0.47
3:A:2047:C:O2'	3:A:2823:A:N1	2.42	0.47
3:A:2431:U:H5	3:A:2433:A:H5"	1.79	0.47
12:J:28:LEU:HD11	12:J:33:VAL:HG11	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:18:LEU:HD11	20:R:32:TYR:HA	1.97	0.47
27:Y:40:VAL:HG12	27:Y:43:GLU:H	1.80	0.47
3:A:1062:G:N2	12:J:93:PRO:HG2	2.29	0.47
3:A:2339:C:H2'	3:A:2340:A:H8	1.80	0.47
11:I:27:VAL:HG13	11:I:80:THR:HG23	1.97	0.47
19:Q:100:LEU:HA	19:Q:100:LEU:HD23	1.67	0.47
20:R:49:ASP:HA	20:R:52:GLN:HB2	1.96	0.47
3:A:2039:U:H2'	3:A:2040:G:C8	2.50	0.47
4:B:116:G:H2'	4:B:117:G:H8	1.80	0.47
7:E:149:ILE:HB	7:E:188:MET:HG2	1.96	0.47
22:T:7:HIS:CE1	22:T:10:ALA:HB2	2.49	0.47
27:Y:62:LYS:HE3	27:Y:66:THR:HG21	1.96	0.47
3:A:861:A:H2'	3:A:862:G:O4'	2.15	0.46
3:A:871:U:H2'	3:A:872:U:C6	2.50	0.46
3:A:1097:U:H2'	3:A:1098:A:O4'	2.15	0.46
3:A:2483:C:N3	16:N:123:LYS:NZ	2.60	0.46
3:A:2788:C:H2'	3:A:2789:C:C6	2.50	0.46
13:K:114:LEU:O	13:K:118:MET:HG3	2.14	0.46
3:A:796:C:H2'	3:A:797:G:C8	2.50	0.46
3:A:825:A:C2	3:A:833:A:C2	3.03	0.46
3:A:857:G:H2'	3:A:858:G:O4'	2.16	0.46
3:A:1510:G:H2'	3:A:1511:G:H8	1.78	0.46
3:A:1689:A:C6	3:A:1700:A:C2	3.03	0.46
3:A:1946:U:H2'	3:A:1947:C:C6	2.51	0.46
3:A:2230:G:H2'	3:A:2231:U:C6	2.51	0.46
11:I:39:THR:HG22	11:I:43:LYS:HE3	1.98	0.46
21:S:38:VAL:O	21:S:54:VAL:HG23	2.15	0.46
3:A:144:A:H1'	23:U:3:ARG:HH22	1.80	0.46
3:A:1038:G:H2'	3:A:1039:A:C8	2.50	0.46
3:A:1060:U:C2	3:A:1062:G:H5'	2.50	0.46
3:A:1508:A:O2'	3:A:1509:A:O4'	2.19	0.46
3:A:2126:A:H61	3:A:2163:A:H5'	1.80	0.46
9:G:42:GLU:CG	9:G:55:ARG:HH21	2.29	0.46
19:Q:88:ARG:NH2	19:Q:112:GLU:HB2	2.31	0.46
3:A:247:G:H4'	3:A:386:G:C5	2.50	0.46
3:A:998:C:H2'	3:A:999:U:O4'	2.14	0.46
3:A:1022:G:O2'	3:A:1024:G:O6	2.27	0.46
5:C:252:THR:OG1	5:C:253:LYS:N	2.48	0.46
9:G:121:ILE:HD13	9:G:135:GLY:HA3	1.98	0.46
18:P:53:THR:HB	18:P:65:THR:HB	1.98	0.46
3:A:861:A:C6	3:A:917:A:C8	3.03	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1387:A:H5'	3:A:1469:A:H1'	1.97	0.46
3:A:1799:G:C5	5:C:176:LEU:HD13	2.50	0.46
3:A:75:G:H4'	28:Z:48:ARG:CZ	2.45	0.46
3:A:358:U:H2'	3:A:359:G:C8	2.44	0.46
3:A:1028:A:N6	3:A:1125:G:H2'	2.30	0.46
3:A:2821:A:H2'	3:A:2822:G:C8	2.51	0.46
4:B:95:U:H2'	4:B:96:G:H8	1.81	0.46
5:C:125:LYS:HE2	5:C:125:LYS:HB2	1.77	0.46
6:D:7:LYS:HB3	6:D:7:LYS:HE2	1.78	0.46
16:N:66:ARG:HB2	16:N:101:VAL:O	2.16	0.46
19:Q:106:LYS:O	19:Q:109:ARG:NH2	2.45	0.46
24:V:81:ASP:OD2	24:V:96:PHE:HB3	2.16	0.46
3:A:880:G:N2	3:A:898:C:C2	2.84	0.46
3:A:1808:A:H3'	3:A:1809:A:H8	1.79	0.46
3:A:2786:U:H2'	3:A:2787:C:H6	1.79	0.46
13:K:95:ARG:HG2	13:K:96:ARG:N	2.30	0.46
14:L:79:PHE:CD1	19:Q:70:VAL:HG22	2.46	0.46
3:A:532:A:N3	3:A:532:A:H2'	2.31	0.46
5:C:232:HIS:NE2	5:C:244:PRO:HA	2.30	0.46
11:I:30:SER:HB3	11:I:81:LEU:HB2	1.98	0.46
3:A:1149:G:H2'	3:A:1150:C:C6	2.50	0.46
3:A:1342:A:C6	3:A:1397:U:C5	3.04	0.46
3:A:1848:A:H3'	3:A:1849:G:H8	1.80	0.46
3:A:1869:G:N2	3:A:1873:G:C5	2.83	0.46
3:A:2069:G:N2	3:A:2443:C:C2	2.83	0.46
3:A:2229:U:H2'	3:A:2230:G:C8	2.51	0.46
5:C:243:HIS:HA	5:C:244:PRO:HD3	1.79	0.46
6:D:184:ARG:HH11	19:Q:7:GLN:CD	2.19	0.46
3:A:1563:U:H2'	3:A:1564:C:C6	2.51	0.45
3:A:1631:G:N2	3:A:1634:A:OP2	2.32	0.45
6:D:207:VAL:HG13	6:D:208:LYS:HG3	1.98	0.45
17:O:28:LEU:O	17:O:32:GLU:N	2.45	0.45
3:A:483:A:H5"	24:V:47:LYS:HG2	1.97	0.45
3:A:772:C:H2'	3:A:773:U:C6	2.52	0.45
3:A:878:A:H5'	3:A:879:G:OP2	2.16	0.45
3:A:1048:A:N1	3:A:1112:G:O2'	2.36	0.45
3:A:1570:A:H5'	5:C:36:LYS:HB2	1.98	0.45
3:A:1706:C:O2'	3:A:1757:A:H5'	2.17	0.45
3:A:1785:A:O2'	3:A:1786:A:H2'	2.16	0.45
12:J:80:LEU:HB3	12:J:138:LEU:CD1	2.46	0.45
22:T:13:SER:O	22:T:17:VAL:HG23	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:25:ARG:NH2	22:T:74:ILE:O	2.49	0.45
3:A:257:C:H2'	3:A:258:G:O4'	2.16	0.45
3:A:1313:U:H2'	3:A:1610:A:C2	2.51	0.45
3:A:1653:G:H3'	17:O:2:ARG:HG3	1.98	0.45
5:C:160:THR:O	5:C:195:VAL:HG23	2.17	0.45
8:F:136:ILE:HG22	8:F:141:ILE:HG21	1.98	0.45
3:A:558:U:OP1	13:K:114:LEU:N	2.46	0.45
3:A:1086:A:H4'	3:A:1103:A:C2	2.52	0.45
3:A:2396:G:N3	3:A:2421:G:N2	2.64	0.45
9:G:155:GLU:OE2	9:G:158:LYS:N	2.48	0.45
11:I:53:ARG:O	11:I:81:LEU:HD12	2.16	0.45
15:M:27:LEU:O	15:M:31:GLY:HA2	2.17	0.45
18:P:88:LYS:HG2	18:P:116:GLN:HB2	1.98	0.45
24:V:37:GLU:O	24:V:39:ILE:HG12	2.17	0.45
3:A:706:A:C2	3:A:707:G:H1'	2.52	0.45
3:A:831:G:H5"	15:M:37:GLY:HA2	1.97	0.45
3:A:908:C:O2'	16:N:70:ASP:OD2	2.30	0.45
3:A:1466:U:H5"	3:A:1467:U:H5'	1.98	0.45
3:A:1709:U:H2'	3:A:1710:G:H8	1.80	0.45
3:A:2165:C:H2'	3:A:2166:U:O4'	2.16	0.45
6:D:99:GLU:OE2	6:D:182:ALA:HB2	2.16	0.45
8:F:20:PHE:CZ	8:F:165:GLU:HA	2.51	0.45
26:X:23:VAL:HG22	26:X:38:VAL:HB	1.99	0.45
3:A:2052:A:OP1	6:D:146:ILE:HG12	2.17	0.45
16:N:65:ILE:HG12	16:N:103:TYR:CD2	2.51	0.45
17:O:17:ARG:HG2	17:O:21:PHE:HE2	1.82	0.45
23:U:34:VAL:HG21	23:U:43:ILE:HD11	1.99	0.45
3:A:111:A:H2'	3:A:112:U:O4'	2.16	0.45
3:A:208:C:H2'	3:A:209:C:C6	2.52	0.45
3:A:499:U:H5"	24:V:43:LYS:HE3	1.99	0.45
3:A:1918:A:O2'	3:A:1920:C:N4	2.50	0.45
3:A:2273:A:H2'	3:A:2274:A:C8	2.52	0.45
3:A:2327:A:H2'	3:A:2328:A:C8	2.51	0.45
3:A:2433:A:H5'	3:A:2434:A:P	2.57	0.45
3:A:2667:C:H1'	9:G:109:PHE:HD1	1.82	0.45
3:A:2683:C:H4'	6:D:13:ARG:HH12	1.81	0.45
8:F:73:SER:OG	8:F:81:GLN:N	2.33	0.45
10:H:62:LEU:HD23	10:H:135:HIS:CD2	2.52	0.45
18:P:85:LYS:HE2	18:P:85:LYS:HB3	1.79	0.45
3:A:593:U:H2'	3:A:594:U:C6	2.52	0.45
3:A:594:U:H2'	3:A:595:C:C6	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1545:A:H2'	3:A:1546:G:O4'	2.17	0.45
11:I:41:LEU:HB2	11:I:99:PHE:CE1	2.52	0.45
12:J:117:MET:HB2	12:J:125:MET:HG2	1.99	0.45
21:S:4:VAL:HA	21:S:12:HIS:O	2.17	0.45
3:A:77:G:H2'	3:A:78:U:O4'	2.16	0.45
3:A:629:G:H5"	3:A:650:C:O2'	2.16	0.45
3:A:976:G:HO2'	3:A:1155:A:HO2'	1.60	0.45
3:A:1848:A:N3	3:A:1849:G:C8	2.84	0.45
3:A:2134:A:H1'	3:A:2159:G:H21	1.82	0.45
6:D:49:GLN:HA	6:D:80:TRP:O	2.16	0.45
12:J:130:GLU:HB3	12:J:134:ARG:NH2	2.32	0.45
14:L:25:LEU:HD23	14:L:25:LEU:HA	1.67	0.45
3:A:198:C:O2'	3:A:199:A:H5'	2.17	0.45
3:A:239:C:H2'	3:A:240:C:O4'	2.16	0.45
3:A:657:U:H2'	3:A:658:U:C6	2.52	0.45
3:A:718:A:H2'	3:A:719:C:O4'	2.16	0.45
3:A:2313:C:H5"	8:F:88:LYS:HD3	1.98	0.45
3:A:2396:G:C2	3:A:2421:G:C2	3.05	0.45
3:A:2524:G:H2'	3:A:2525:G:O4'	2.16	0.45
11:I:52:MET:HE3	11:I:81:LEU:HD11	1.99	0.45
12:J:86:ILE:CD1	12:J:138:LEU:HD21	2.46	0.45
13:K:69:ARG:O	13:K:89:PHE:HB3	2.17	0.45
17:O:2:ARG:HB3	17:O:2:ARG:CZ	2.46	0.45
3:A:141:G:C8	3:A:141:G:H3'	2.51	0.44
3:A:948:C:H1'	3:A:984:A:C8	2.52	0.44
3:A:1287:A:H3'	3:A:1288:G:N2	2.32	0.44
3:A:2667:C:H1'	9:G:109:PHE:CD1	2.52	0.44
15:M:10:GLU:OE2	15:M:11:GLY:N	2.50	0.44
25:W:83:LYS:HB3	25:W:85:LYS:HG3	1.98	0.44
26:X:55:ARG:HE	26:X:55:ARG:HB2	1.45	0.44
3:A:154:U:H2'	3:A:155:A:C8	2.53	0.44
3:A:172:A:H2'	3:A:173:A:H8	1.81	0.44
3:A:620:G:H4'	3:A:621:A:O5'	2.17	0.44
3:A:764:A:H5'	5:C:209:GLY:HA2	1.98	0.44
3:A:1420:A:N7	3:A:2211:A:C6	2.86	0.44
3:A:1450:G:C6	3:A:1451:C:N4	2.86	0.44
3:A:1972:G:H2'	3:A:1973:G:H8	1.82	0.44
3:A:2292:U:H2'	3:A:2293:G:C8	2.52	0.44
9:G:117:LEU:HD13	9:G:121:ILE:HG22	1.99	0.44
10:H:100:ALA:O	10:H:104:THR:HG23	2.17	0.44
13:K:65:THR:O	13:K:68:LYS:HB2	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:89:ARG:HB3	19:Q:113:ARG:NH1	2.32	0.44
3:A:239:C:HO2'	3:A:622:G:HO2'	1.60	0.44
3:A:630:G:N2	3:A:633:A:OP2	2.43	0.44
3:A:1177:G:H2'	3:A:1178:C:C6	2.51	0.44
19:Q:62:ARG:NH2	19:Q:101:ARG:HG2	2.33	0.44
21:S:27:ILE:HG22	21:S:28:ALA:O	2.18	0.44
22:T:46:LEU:HD23	22:T:46:LEU:HA	1.82	0.44
3:A:356:G:H2'	3:A:357:C:O4'	2.17	0.44
14:L:99:ILE:HG12	14:L:118:LEU:HB2	1.98	0.44
22:T:28:LYS:HB2	22:T:28:LYS:HE2	1.41	0.44
3:A:57:C:H2'	3:A:58:G:O4'	2.18	0.44
3:A:1082:U:H4'	11:I:46:ARG:NH1	2.32	0.44
3:A:1198:U:H2'	3:A:1199:U:C6	2.52	0.44
3:A:1591:A:H2'	3:A:1592:C:C6	2.53	0.44
3:A:2318:G:C6	3:A:2319:G:N1	2.85	0.44
3:A:2489:U:C4	3:A:2490:G:C6	3.06	0.44
3:A:2569:G:C2	3:A:2570:G:C8	3.05	0.44
5:C:141:VAL:HG12	5:C:192:LEU:HA	1.98	0.44
7:E:121:VAL:O	7:E:189:THR:HA	2.18	0.44
9:G:148:LEU:HD23	9:G:148:LEU:HA	1.71	0.44
16:N:90:GLU:HB3	16:N:91:TYR:CD1	2.53	0.44
26:X:36:ILE:HG23	26:X:58:THR:HG23	2.00	0.44
3:A:181:A:H1'	3:A:435:C:O4'	2.17	0.44
3:A:997:G:H5"	20:R:92:ARG:NH1	2.33	0.44
3:A:1230:A:H2'	3:A:1231:U:O4'	2.17	0.44
3:A:2387:U:H1'	26:X:41:ARG:NH1	2.33	0.44
3:A:2654:A:OP1	3:A:2654:A:H8	2.01	0.44
3:A:2776:A:C8	3:A:2782:G:C5	3.05	0.44
8:F:147:ASP:OD1	8:F:150:ARG:NH2	2.51	0.44
9:G:42:GLU:HG3	9:G:55:ARG:HH21	1.83	0.44
25:W:21:ARG:HE	25:W:87:GLN:HA	1.83	0.44
28:Z:56:LEU:HD22	28:Z:56:LEU:HA	1.82	0.44
3:A:2024:G:H2'	3:A:2025:C:C6	2.53	0.44
3:A:2377:A:H2'	3:A:2378:A:C8	2.53	0.44
3:A:2683:C:H4'	6:D:13:ARG:NH1	2.33	0.44
3:A:2704:C:H2'	3:A:2705:A:O4'	2.17	0.44
8:F:67:ILE:HD12	8:F:84:PRO:HB3	2.00	0.44
17:O:86:ARG:HD3	17:O:121:LYS:HG3	1.99	0.44
27:Y:59:ILE:HG12	27:Y:67:VAL:HG21	2.00	0.44
3:A:149:A:C2	3:A:150:U:C2	3.06	0.44
3:A:277:G:H4'	3:A:278:A:N7	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:677:A:O2'	3:A:2071:A:H5'	2.17	0.44
3:A:1301:A:H2'	3:A:1301:A:N3	2.33	0.44
3:A:2230:G:H1'	27:Y:32:ASN:HB2	1.99	0.44
23:U:24:MET:CG	23:U:93:LEU:CD1	2.96	0.44
3:A:870:U:OP1	16:N:6:ARG:NH1	2.51	0.44
3:A:1266:G:N2	3:A:2012:G:H2'	2.33	0.44
3:A:1853:A:N6	3:A:1888:G:O2'	2.51	0.44
5:C:205:LEU:HD23	5:C:205:LEU:HA	1.68	0.44
9:G:44:LYS:HE3	9:G:44:LYS:HB2	1.80	0.44
16:N:95:LEU:HA	16:N:95:LEU:HD23	1.77	0.44
19:Q:53:ARG:HB2	19:Q:56:HIS:HB2	1.99	0.44
3:A:11:C:H2'	3:A:12:U:H5'	2.00	0.43
3:A:973:A:OP2	21:S:81:LYS:HE3	2.18	0.43
3:A:1082:U:O2'	11:I:39:THR:HG23	2.18	0.43
3:A:1266:G:O2'	3:A:2012:G:O6	2.34	0.43
3:A:1614:A:C2	22:T:93:ALA:HB2	2.52	0.43
3:A:2678:C:H2'	3:A:2679:A:O4'	2.18	0.43
8:F:48:LYS:HE2	8:F:48:LYS:HB2	1.85	0.43
19:Q:25:THR:HB	19:Q:88:ARG:HG2	1.99	0.43
23:U:31:VAL:O	23:U:32:LEU:HD23	2.18	0.43
3:A:463:G:N1	3:A:467:G:C6	2.86	0.43
3:A:566:U:H5"	15:M:29:LYS:HE3	1.99	0.43
3:A:834:G:C2	3:A:835:C:C2	3.06	0.43
3:A:1287:A:H5'	17:O:103:ARG:HD2	1.98	0.43
3:A:1735:A:H2'	3:A:1736:U:O4'	2.18	0.43
3:A:1962:C:H4'	3:A:1963:U:C5	2.52	0.43
3:A:2172:U:H4'	3:A:2173:A:H5'	2.01	0.43
8:F:138:PHE:HA	8:F:139:PRO:HD3	1.90	0.43
8:F:170:LEU:HD23	8:F:170:LEU:HA	1.75	0.43
10:H:26:ALA:HA	10:H:30:LEU:HB2	1.99	0.43
18:P:52:SER:O	18:P:58:ILE:HD12	2.18	0.43
3:A:380:G:H2'	3:A:381:G:O4'	2.18	0.43
3:A:1068:G:N2	3:A:1095:A:O3'	2.44	0.43
3:A:1354:A:H2'	3:A:1355:G:O4'	2.19	0.43
3:A:1627:G:C2	3:A:1628:G:C8	3.07	0.43
3:A:2443:C:H2'	3:A:2444:G:H8	1.82	0.43
8:F:128:TYR:CE2	8:F:130:MET:HG2	2.53	0.43
10:H:46:PHE:HD1	10:H:50:ARG:NH2	2.16	0.43
12:J:90:SER:HB2	12:J:136:MET:O	2.18	0.43
3:A:33:C:N4	3:A:446:G:O2'	2.45	0.43
3:A:1056:G:H1'	3:A:1103:A:N6	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1205:A:H2'	7:E:165:HIS:HE1	1.83	0.43
3:A:1667:G:N2	3:A:1992:G:OP2	2.44	0.43
3:A:1710:G:H2'	3:A:1711:A:C8	2.53	0.43
3:A:2114:A:C2	3:A:2166:U:H2'	2.53	0.43
3:A:2847:U:H2'	3:A:2848:G:O4'	2.18	0.43
15:M:80:SER:O	15:M:84:LYS:HE3	2.19	0.43
16:N:26:VAL:HB	16:N:133:LYS:HB2	2.00	0.43
18:P:18:LEU:HA	18:P:18:LEU:HD23	1.71	0.43
22:T:47:VAL:HG22	22:T:103:ILE:HD13	2.00	0.43
3:A:475:C:N4	3:A:476:G:C6	2.86	0.43
3:A:969:G:H2'	3:A:970:U:C6	2.53	0.43
3:A:1093:G:H1'	3:A:1099:G:N1	2.32	0.43
3:A:1515:A:H3'	3:A:1516:G:H8	1.84	0.43
3:A:2647:U:H2'	3:A:2648:G:C8	2.54	0.43
3:A:2786:U:H2'	3:A:2787:C:C6	2.53	0.43
4:B:114:C:H2'	4:B:115:A:H8	1.83	0.43
5:C:153:GLN:O	5:C:156:ARG:HG3	2.18	0.43
6:D:131:ASP:O	6:D:140:HIS:HD2	2.01	0.43
20:R:24:TYR:O	20:R:29:SER:HB3	2.19	0.43
20:R:117:LEU:HD23	20:R:117:LEU:HA	1.77	0.43
3:A:783:A:C5	3:A:785:G:H1'	2.53	0.43
3:A:1351:C:H4'	3:A:1572:A:O4'	2.18	0.43
3:A:1542:U:H2'	3:A:1543:G:O4'	2.18	0.43
3:A:1858:A:H2'	3:A:1859:U:O4'	2.17	0.43
5:C:33:LEU:HA	5:C:33:LEU:HD23	1.58	0.43
12:J:110:ALA:O	12:J:114:ALA:HB2	2.18	0.43
20:R:9:ILE:H	20:R:9:ILE:HD12	1.84	0.43
21:S:91:GLN:NE2	21:S:92:TRP:H	2.16	0.43
1:1:72:A:H2'	1:1:73:G:H8	1.82	0.43
3:A:674:G:H2'	3:A:804:A:H61	1.83	0.43
3:A:1434:A:C2	3:A:1435:G:C5	3.07	0.43
3:A:1517:G:C2	3:A:1732:C:N3	2.86	0.43
3:A:1759:A:H2'	3:A:1760:C:C6	2.54	0.43
3:A:1922:G:H2'	3:A:1923:U:O4'	2.18	0.43
3:A:2144:G:N2	3:A:2148:G:O6	2.52	0.43
3:A:2512:C:H5"	3:A:2513:A:OP2	2.17	0.43
8:F:145:LYS:HA	8:F:145:LYS:HD3	1.89	0.43
16:N:133:LYS:HE3	16:N:133:LYS:HB3	1.42	0.43
21:S:4:VAL:HG12	21:S:39:LEU:HB2	2.00	0.43
23:U:34:VAL:HG11	23:U:43:ILE:HD13	2.01	0.43
3:A:14:A:C6	3:A:526:A:C2	3.07	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:93:G:H2'	3:A:94:A:H8	1.84	0.43
3:A:112:U:H5'	28:Z:58:ASN:ND2	2.34	0.43
3:A:141:G:C8	3:A:142:A:O4'	2.72	0.43
3:A:1736:U:H2'	3:A:1737:G:O4'	2.18	0.43
3:A:2292:U:H2'	3:A:2293:G:H8	1.84	0.43
3:A:2588:G:O6	3:A:2607:G:C6	2.72	0.43
3:A:2646:C:OP2	3:A:2732:G:O2'	2.35	0.43
4:B:49:C:H2'	4:B:50:A:C8	2.54	0.43
5:C:90:ASN:ND2	5:C:197:ASN:HB2	2.34	0.43
7:E:108:ILE:O	7:E:112:LEU:HG	2.18	0.43
15:M:41:ARG:H	15:M:41:ARG:HG2	1.62	0.43
3:A:195:A:H5"	15:M:47:ARG:HH22	1.84	0.43
3:A:461:C:H2'	3:A:462:C:H6	1.84	0.43
3:A:1494:A:H2'	3:A:1495:A:H8	1.84	0.43
6:D:109:VAL:HG12	6:D:201:LEU:HD22	2.01	0.43
6:D:148:GLN:OE1	6:D:148:GLN:N	2.51	0.43
7:E:29:HIS:O	7:E:32:VAL:HG22	2.19	0.43
7:E:181:ILE:H	7:E:181:ILE:HG13	1.69	0.43
14:L:3:GLN:HE21	14:L:3:GLN:HB3	1.66	0.43
17:O:72:ASP:OD1	17:O:73:ASN:N	2.51	0.43
20:R:74:ILE:HG12	20:R:75:SER:N	2.34	0.43
26:X:47:ALA:HB1	26:X:51:VAL:O	2.19	0.43
1:1:33:C:H6	1:1:33:C:O5'	2.02	0.43
3:A:76:C:H6	3:A:76:C:O5'	2.02	0.43
3:A:493:G:H2'	3:A:494:G:O4'	2.19	0.43
3:A:1088:A:H61	12:J:135:SER:HB3	1.83	0.43
3:A:1590:A:H2'	3:A:1591:A:C8	2.54	0.43
3:A:2038:G:H2'	3:A:2039:U:O4'	2.17	0.43
3:A:2130:U:O2'	3:A:2133:G:O2'	2.32	0.43
3:A:2843:G:H2'	3:A:2844:G:C8	2.54	0.43
5:C:8:PRO:HB3	5:C:14:ARG:HG3	1.99	0.43
5:C:245:VAL:HA	5:C:252:THR:HG22	2.01	0.43
7:E:128:ALA:O	7:E:130:LYS:N	2.51	0.43
20:R:17:ILE:HD13	20:R:17:ILE:HA	1.62	0.43
3:A:464:U:C2	3:A:788:A:C6	3.06	0.42
3:A:1501:G:H2'	3:A:1502:A:H8	1.84	0.42
3:A:1614:A:H8	3:A:1614:A:O5'	2.02	0.42
3:A:2138:G:C6	3:A:2154:A:C2	3.06	0.42
3:A:2518:A:H2'	3:A:2518:A:N3	2.34	0.42
4:B:66:A:H61	4:B:107:G:H2'	1.84	0.42
5:C:200:HIS:CD2	5:C:200:HIS:C	2.92	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:79:ILE:HG21	8:F:85:ILE:HD11	2.01	0.42
10:H:62:LEU:HD22	10:H:137:GLU:OE1	2.19	0.42
10:H:104:THR:HA	10:H:108:VAL:O	2.19	0.42
16:N:33:LEU:HD11	16:N:128:THR:HB	2.00	0.42
19:Q:40:LEU:HD23	19:Q:40:LEU:HA	1.75	0.42
3:A:5:A:H2'	3:A:6:A:C8	2.54	0.42
3:A:307:G:N1	3:A:310:A:OP2	2.52	0.42
3:A:653:U:C1'	3:A:654:A:H5"	2.49	0.42
3:A:1044:C:O2'	3:A:1111:A:N1	2.45	0.42
3:A:1141:U:H4'	3:A:1142:A:O4'	2.19	0.42
3:A:1387:A:H2'	3:A:1388:G:O4'	2.18	0.42
5:C:133:ARG:HD2	10:H:123:ARG:NH1	2.35	0.42
8:F:4:LEU:HD23	8:F:4:LEU:HA	1.73	0.42
13:K:26:GLY:O	13:K:30:THR:HG23	2.18	0.42
14:L:11:ALA:O	14:L:100:PHE:N	2.46	0.42
3:A:729:G:H2'	3:A:1775:U:H1'	2.01	0.42
3:A:819:A:N3	3:A:819:A:H2'	2.34	0.42
3:A:1637:A:H2'	3:A:1638:C:C6	2.54	0.42
3:A:1751:U:H2'	3:A:1752:C:C6	2.54	0.42
3:A:1798:U:OP2	5:C:271:ARG:NH2	2.52	0.42
3:A:2184:A:H2'	3:A:2185:U:C6	2.53	0.42
3:A:2304:G:H22	3:A:2312:U:H3	1.67	0.42
3:A:2533:U:OP1	3:A:2665:A:O2'	2.34	0.42
3:A:2771:C:H2'	3:A:2772:C:C6	2.54	0.42
9:G:149:ARG:HG3	9:G:162:VAL:O	2.20	0.42
11:I:15:VAL:HG11	11:I:60:LEU:CD2	2.50	0.42
11:I:118:ILE:HA	11:I:119:PRO:HD2	1.84	0.42
15:M:6:LEU:HD23	15:M:6:LEU:HA	1.82	0.42
16:N:36:VAL:HG13	25:W:82:TYR:CD2	2.55	0.42
25:W:29:ILE:O	25:W:91:PHE:HB2	2.19	0.42
3:A:543:G:H5'	3:A:544:C:OP2	2.18	0.42
3:A:729:G:C5	5:C:207:LYS:HB2	2.55	0.42
3:A:987:C:O2'	3:A:1000:A:N3	2.44	0.42
3:A:1064:C:H5"	12:J:88:SER:HB2	2.01	0.42
3:A:1327:A:H2'	3:A:1328:A:O4'	2.19	0.42
3:A:1463:C:H2'	3:A:1464:G:H8	1.84	0.42
3:A:1524:G:H2'	3:A:1525:A:O4'	2.20	0.42
3:A:2322:A:C4	3:A:2323:G:C8	3.07	0.42
3:A:2776:A:C2	3:A:2778:A:C4	3.07	0.42
3:A:2790:U:H5'	3:A:2893:A:N7	2.34	0.42
4:B:57:A:C4	8:F:26:MET:HB3	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:210:ALA:HA	5:C:213:TRP:CE3	2.53	0.42
12:J:33:VAL:HG13	12:J:67:PHE:CD2	2.54	0.42
12:J:113:LYS:HA	12:J:116:ASP:HB2	2.01	0.42
19:Q:106:LYS:O	19:Q:109:ARG:HD3	2.20	0.42
20:R:24:TYR:N	20:R:24:TYR:HD1	2.17	0.42
3:A:1039:A:H2'	3:A:1040:A:O4'	2.19	0.42
3:A:1047:G:OP1	11:I:56:ARG:NH1	2.52	0.42
3:A:1324:G:C4	3:A:1328:A:N6	2.88	0.42
3:A:1473:G:H2'	3:A:1474:U:O4'	2.19	0.42
3:A:1780:A:H3'	3:A:1781:U:H2'	2.01	0.42
4:B:106:G:H2'	4:B:107:G:O4'	2.19	0.42
24:V:61:LYS:HG2	24:V:62:GLU:H	1.85	0.42
1:1:72:A:H2'	1:1:73:G:C8	2.55	0.42
3:A:794:A:H2'	3:A:795:C:C6	2.55	0.42
3:A:1400:U:H2'	3:A:1401:G:O4'	2.19	0.42
3:A:2700:A:H2'	3:A:2701:U:C6	2.54	0.42
7:E:109:LEU:HA	7:E:109:LEU:HD23	1.79	0.42
9:G:97:ALA:HB3	9:G:104:ASN:HB2	2.01	0.42
12:J:22:PRO:HB2	12:J:23:PRO:HD3	2.02	0.42
14:L:65:THR:HB	14:L:68:GLY:H	1.84	0.42
3:A:647:G:H2'	3:A:648:G:C8	2.55	0.42
3:A:669:G:N2	3:A:670:A:C2	2.88	0.42
3:A:1597:A:C5'	3:A:1598:A:H5'	2.47	0.42
3:A:1759:A:C2	3:A:2697:G:H1'	2.54	0.42
3:A:2433:A:H5'	3:A:2434:A:OP2	2.19	0.42
5:C:24:LEU:HA	5:C:24:LEU:HD12	1.66	0.42
16:N:42:THR:N	16:N:45:GLN:OE1	2.47	0.42
25:W:2:PHE:HE1	25:W:53:LYS:HD2	1.84	0.42
3:A:123:G:N2	3:A:129:C:C2	2.87	0.42
3:A:812:C:C2	3:A:1250:G:N1	2.87	0.42
3:A:910:A:C6	3:A:911:A:C6	3.08	0.42
3:A:1065:U:H2'	3:A:1066:U:O4'	2.19	0.42
3:A:2119:A:H62	3:A:2167:U:H1'	1.85	0.42
6:D:73:VAL:HG11	6:D:93:GLY:HA2	2.01	0.42
12:J:38:PHE:CD1	12:J:59:ILE:HD11	2.54	0.42
12:J:103:ARG:H	12:J:103:ARG:HD2	1.83	0.42
13:K:96:ARG:HA	13:K:97:PRO:HD2	1.92	0.42
3:A:565:C:H4'	3:A:1253:A:C6	2.55	0.42
3:A:571:U:H3'	21:S:80:ARG:NH2	2.34	0.42
3:A:1482:G:H2'	3:A:1483:G:H8	1.84	0.42
3:A:1877:A:H2'	3:A:1878:G:O4'	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:34:ILE:HB	8:F:96:MET:HG3	2.02	0.42
10:H:94:ILE:HG23	10:H:98:ASP:HB2	2.01	0.42
17:O:103:ARG:HB3	17:O:106:ASP:OD1	2.20	0.42
20:R:31:VAL:HG12	20:R:34:VAL:H	1.85	0.42
3:A:1449:G:N2	3:A:1463:C:C2	2.88	0.42
3:A:1902:C:H4'	5:C:242:LYS:O	2.19	0.42
3:A:1946:U:H2'	3:A:1947:C:H6	1.84	0.42
3:A:2209:G:C2	3:A:2216:G:C2	3.08	0.42
4:B:48:U:H4'	18:P:100:HIS:HD2	1.84	0.42
8:F:79:ILE:HD12	8:F:79:ILE:O	2.20	0.42
10:H:1:MET:O	10:H:20:ASN:HA	2.20	0.42
3:A:335:C:H5"	24:V:82:ARG:HD2	2.02	0.41
3:A:1509:A:O2'	3:A:1510:G:H8	2.03	0.41
3:A:2339:C:O3'	4:B:41:G:N2	2.52	0.41
12:J:74:PRO:HA	12:J:75:PRO:HD3	1.89	0.41
22:T:33:LEU:HD23	22:T:33:LEU:HA	1.66	0.41
27:Y:26:LYS:HD3	27:Y:26:LYS:HA	1.88	0.41
3:A:53:A:H2'	3:A:54:G:O4'	2.20	0.41
3:A:877:A:C6	3:A:899:A:C6	3.08	0.41
3:A:1417:C:H2'	3:A:1418:G:C8	2.55	0.41
3:A:1463:C:H2'	3:A:1464:G:C8	2.55	0.41
3:A:2796:U:HO2'	3:A:2797:U:H6	1.63	0.41
3:A:2812:G:H2'	3:A:2813:A:O4'	2.20	0.41
8:F:57:LEU:HD12	8:F:87:CYS:SG	2.61	0.41
8:F:70:ALA:HB3	8:F:81:GLN:HA	2.02	0.41
25:W:2:PHE:HB3	25:W:50:MET:HE3	2.02	0.41
3:A:118:A:N3	3:A:178:G:H1'	2.36	0.41
3:A:297:G:H2'	3:A:298:G:O4'	2.20	0.41
3:A:848:C:H42	3:A:930:G:H1	1.68	0.41
3:A:1056:G:H5'	11:I:35:VAL:HG21	2.02	0.41
3:A:1432:G:H2'	3:A:1433:A:C8	2.55	0.41
3:A:1499:C:H2'	3:A:1500:G:H8	1.85	0.41
3:A:1709:U:H2'	3:A:1710:G:C8	2.55	0.41
3:A:1821:A:H2'	3:A:1822:C:C6	2.55	0.41
3:A:1825:U:O2	5:C:253:LYS:NZ	2.31	0.41
3:A:2267:A:H5"	3:A:2268:A:C5'	2.50	0.41
3:A:2286:G:C8	3:A:2287:A:N6	2.88	0.41
3:A:2365:G:H4'	26:X:60:PHE:CE2	2.55	0.41
3:A:2706:A:C2	3:A:2707:U:C2	3.08	0.41
5:C:176:LEU:HB2	5:C:180:GLU:O	2.20	0.41
8:F:130:MET:HE3	8:F:130:MET:HB2	1.94	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:43:LYS:HE2	12:J:118:THR:HA	2.01	0.41
3:A:75:G:H4'	28:Z:48:ARG:NH2	2.35	0.41
3:A:393:C:H2'	3:A:394:C:H6	1.85	0.41
3:A:799:G:C6	3:A:800:A:C6	3.08	0.41
3:A:1484:U:H2'	3:A:1485:U:C6	2.55	0.41
3:A:1880:U:H2'	3:A:1881:C:C6	2.55	0.41
9:G:83:PHE:HB2	9:G:135:GLY:O	2.21	0.41
13:K:58:ASN:ND2	13:K:128:ASN:OD1	2.42	0.41
3:A:648:G:C2	3:A:649:G:C5	3.08	0.41
3:A:1078:U:O2	3:A:1088:A:H3'	2.21	0.41
3:A:1110:G:HO2'	3:A:1111:A:P	2.44	0.41
3:A:1607:C:O2'	3:A:1608:A:OP1	2.37	0.41
3:A:2102:G:C2	3:A:2187:U:O2	2.73	0.41
3:A:2838:G:H2'	3:A:2839:G:O4'	2.20	0.41
3:A:2860:A:H5"	3:A:2861:U:OP2	2.21	0.41
27:Y:3:ARG:NE	27:Y:30:LEU:HD13	2.35	0.41
3:A:328:U:H4'	24:V:66:GLN:HE21	1.86	0.41
3:A:1005:C:H2'	3:A:1006:C:H6	1.84	0.41
3:A:1057:A:N7	3:A:1086:A:H2'	2.35	0.41
3:A:1073:A:H2'	3:A:1074:G:O4'	2.21	0.41
3:A:1366:A:H2'	3:A:1367:A:O4'	2.21	0.41
3:A:1770:G:C6	3:A:1983:G:C6	3.07	0.41
3:A:1972:G:H2'	3:A:1973:G:C8	2.55	0.41
4:B:71:C:C2	4:B:106:G:C2	3.08	0.41
7:E:170:ARG:HD3	7:E:170:ARG:HA	1.91	0.41
14:L:71:ARG:HA	14:L:71:ARG:HD3	1.81	0.41
14:L:93:GLN:HA	14:L:94:PRO:HD3	1.88	0.41
16:N:65:ILE:HG12	16:N:103:TYR:HD2	1.85	0.41
3:A:528:A:C8	3:A:2042:A:C2	3.09	0.41
3:A:2895:G:H2'	3:A:2896:C:C6	2.55	0.41
4:B:95:U:H2'	4:B:96:G:C8	2.56	0.41
9:G:73:ASN:O	9:G:77:ILE:HG13	2.20	0.41
9:G:76:VAL:O	9:G:80:THR:HG23	2.20	0.41
3:A:561:G:H4'	20:R:48:ARG:HH22	1.86	0.41
3:A:678:C:H2'	3:A:679:C:H6	1.84	0.41
3:A:681:G:C2	3:A:797:G:C2	3.09	0.41
3:A:779:U:H2'	3:A:780:G:C8	2.56	0.41
3:A:948:C:H2'	3:A:949:G:H8	1.85	0.41
3:A:981:A:N1	3:A:2027:G:O2'	2.42	0.41
3:A:1789:A:H2'	3:A:1790:C:O4'	2.21	0.41
8:F:36:LEU:HA	8:F:153:ASP:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:154:PRO:HA	9:G:160:LYS:O	2.21	0.41
10:H:128:HIS:O	10:H:143:ILE:HA	2.20	0.41
15:M:3:LEU:HD23	15:M:3:LEU:HA	1.77	0.41
15:M:78:ARG:HG2	15:M:113:ALA:HB3	2.03	0.41
1:1:98:U:H2'	1:1:99:G:C8	2.55	0.41
3:A:31:C:O3'	3:A:1238:G:H5'	2.21	0.41
3:A:449:A:C4	3:A:450:G:C8	3.08	0.41
3:A:520:G:H2'	3:A:521:U:C6	2.56	0.41
3:A:601:C:O2'	3:A:605:G:H5"	2.21	0.41
3:A:776:G:HO2'	3:A:777:G:P	2.41	0.41
3:A:807:U:H2'	3:A:808:G:H8	1.85	0.41
3:A:1024:G:C6	3:A:1025:G:C6	3.09	0.41
3:A:1869:G:C2	3:A:1873:G:C6	3.09	0.41
3:A:2061:G:H2'	3:A:2501:C:O2'	2.21	0.41
3:A:2352:A:N1	26:X:34:GLY:HA3	2.35	0.41
3:A:2578:G:OP2	3:A:2578:G:H4'	2.20	0.41
3:A:2627:G:H1'	3:A:2777:G:N2	2.36	0.41
3:A:2785:C:H2'	3:A:2786:U:H6	1.85	0.41
8:F:13:VAL:O	8:F:17:MET:HB2	2.21	0.41
9:G:9:VAL:HG23	9:G:52:PHE:HE1	1.86	0.41
16:N:6:ARG:CZ	16:N:6:ARG:HB2	2.50	0.41
17:O:72:ASP:O	17:O:76:VAL:HG13	2.21	0.41
22:T:109:ASP:OD1	22:T:110:ARG:N	2.54	0.41
27:Y:54:LYS:O	27:Y:58:VAL:HG23	2.19	0.41
3:A:64:A:C6	3:A:65:U:C4	3.09	0.41
3:A:465:G:C6	3:A:466:A:N6	2.89	0.41
3:A:811:U:C2	3:A:1251:C:C5	3.09	0.41
3:A:1341:G:C2	3:A:1398:C:H4'	2.56	0.41
3:A:1374:G:H8	3:A:1374:G:OP2	2.04	0.41
3:A:1423:G:N2	3:A:1576:U:O2	2.54	0.41
3:A:1672:A:N6	3:A:1673:G:C6	2.89	0.41
3:A:2343:U:H2'	3:A:2344:U:C6	2.55	0.41
3:A:2394:C:H42	3:A:2422:C:N4	2.19	0.41
3:A:2550:G:C6	3:A:2551:C:C4	3.09	0.41
3:A:2682:A:C2	6:D:23:PRO:HB3	2.56	0.41
3:A:2847:U:C5	3:A:2848:G:C5	3.09	0.41
4:B:7:G:H5"	18:P:29:HIS:CE1	2.56	0.41
14:L:17:ARG:HA	14:L:17:ARG:HD3	1.77	0.41
27:Y:3:ARG:O	27:Y:12:PRO:HD3	2.21	0.41
28:Z:21:LEU:HD23	28:Z:21:LEU:HA	1.82	0.41
28:Z:38:GLN:HG3	28:Z:39:GLN:H	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:74:C:O5'	2:2:74:C:H6	2.04	0.40
3:A:141:G:C8	3:A:141:G:C3'	3.04	0.40
3:A:277:G:H4'	3:A:278:A:C5	2.56	0.40
3:A:501:A:H2'	3:A:502:A:C8	2.56	0.40
3:A:778:G:H5"	3:A:779:U:OP2	2.21	0.40
3:A:997:G:OP1	20:R:92:ARG:HD2	2.21	0.40
3:A:1332:G:N7	3:A:1609:A:O2'	2.46	0.40
3:A:1365:A:N3	3:A:1365:A:H2'	2.36	0.40
3:A:1818:U:C5	5:C:156:ARG:NH2	2.90	0.40
3:A:2663:G:H2'	3:A:2664:G:O4'	2.21	0.40
5:C:34:LEU:HD21	5:C:63:ARG:HG3	2.03	0.40
5:C:176:LEU:HA	5:C:176:LEU:HD23	1.80	0.40
7:E:67:ARG:HE	7:E:67:ARG:HB3	1.61	0.40
8:F:65:PRO:HA	8:F:89:VAL:HG22	2.02	0.40
11:I:99:PHE:HD2	11:I:106:PHE:HZ	1.69	0.40
16:N:38:ARG:HB2	16:N:98:PRO:HD3	2.03	0.40
18:P:115:LEU:HD23	18:P:117:PHE:CE2	2.56	0.40
18:P:115:LEU:HD23	18:P:117:PHE:HE2	1.86	0.40
21:S:85:LYS:HE2	21:S:85:LYS:HB3	1.80	0.40
23:U:49:LYS:HG3	23:U:50:LEU:HD23	2.03	0.40
27:Y:72:ARG:HG3	27:Y:78:TYR:HE2	1.86	0.40
28:Z:42:LEU:HA	28:Z:42:LEU:HD23	1.81	0.40
3:A:396:G:H1'	27:Y:29:PHE:HB3	2.02	0.40
3:A:729:G:C6	5:C:207:LYS:HB2	2.56	0.40
3:A:743:A:OP1	6:D:135:GLY:HA2	2.21	0.40
3:A:863:A:H2'	3:A:864:G:H8	1.86	0.40
3:A:2423:U:H2'	3:A:2424:C:C1'	2.51	0.40
3:A:2431:U:O2	3:A:2431:U:O4'	2.39	0.40
3:A:2600:A:H2'	3:A:2601:C:C6	2.56	0.40
8:F:28:VAL:HA	8:F:29:PRO:HD3	1.91	0.40
12:J:42:PHE:CE1	12:J:57:VAL:HB	2.56	0.40
1:1:68:A:H2'	1:1:69:G:C8	2.56	0.40
3:A:42:A:C6	3:A:43:G:C5	3.10	0.40
3:A:118:A:C8	3:A:119:A:C8	3.09	0.40
3:A:199:A:N6	3:A:2434:A:C5	2.89	0.40
3:A:353:C:H2'	3:A:354:A:O4'	2.22	0.40
3:A:717:C:C5	3:A:718:A:C8	3.10	0.40
3:A:719:C:H2'	3:A:720:U:C6	2.57	0.40
3:A:871:U:H4'	16:N:68:PHE:CD2	2.56	0.40
3:A:2143:C:H2'	3:A:2144:G:O4'	2.21	0.40
3:A:2229:U:H2'	3:A:2230:G:H8	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2421:G:H4'	3:A:2421:G:OP1	2.21	0.40
4:B:68:C:H2'	4:B:69:G:O4'	2.22	0.40
11:I:13:ALA:O	11:I:17:GLU:HB2	2.22	0.40
11:I:48:ALA:HB3	11:I:50:VAL:HG23	2.03	0.40
11:I:61:ARG:HG2	11:I:73:LYS:HG2	2.02	0.40
14:L:103:VAL:HB	14:L:107:LEU:HD12	2.02	0.40
15:M:79:LEU:HB2	15:M:113:ALA:O	2.21	0.40
17:O:65:LEU:HA	17:O:65:LEU:HD12	1.85	0.40
26:X:70:GLU:HG3	26:X:72:LYS:HE2	2.04	0.40
3:A:1:G:H2'	3:A:2:G:C8	2.56	0.40
3:A:445:C:H2'	3:A:446:G:O4'	2.22	0.40
3:A:1071:G:O2'	3:A:1089:A:OP2	2.36	0.40
3:A:1127:A:N7	3:A:2488:G:O2'	2.54	0.40
3:A:1275:A:OP2	3:A:1646:C:N4	2.52	0.40
3:A:1807:G:N2	3:A:1811:G:C5	2.89	0.40
3:A:2365:G:P	26:X:55:ARG:HG2	2.61	0.40
3:A:2388:A:H5'	3:A:2389:G:OP2	2.21	0.40
5:C:251:GLN:HE21	5:C:251:GLN:HB2	1.58	0.40
9:G:90:VAL:HG21	9:G:163:ARG:NH1	2.37	0.40
11:I:100:ALA:HB2	11:I:106:PHE:CE1	2.56	0.40
15:M:81:ASP:HB3	15:M:100:ILE:HD13	2.02	0.40
17:O:22:ARG:HG3	17:O:70:THR:HA	2.03	0.40
3:A:362:A:H3'	3:A:363:G:C8	2.48	0.40
3:A:447:A:C5	3:A:473:G:C5	3.10	0.40
3:A:863:A:H2'	3:A:864:G:C8	2.57	0.40
3:A:1139:G:H8	3:A:1139:G:OP2	2.05	0.40
3:A:1234:U:H2'	3:A:1235:G:O4'	2.21	0.40
3:A:1945:G:C5	3:A:1946:U:C4	3.09	0.40
3:A:2283:C:C2	3:A:2389:G:C2	3.09	0.40
3:A:2563:U:O2	3:A:2566:A:C5	2.75	0.40
3:A:2603:G:C6	3:A:2604:U:C4	3.10	0.40
6:D:13:ARG:HD2	6:D:15:PHE:CE2	2.56	0.40
10:H:60:GLU:HA	10:H:63:ALA:HB3	2.04	0.40
12:J:97:LYS:HE2	12:J:139:VAL:HG12	2.03	0.40
18:P:25:ARG:O	18:P:25:ARG:HG3	2.22	0.40
28:Z:46:VAL:O	28:Z:50:VAL:HG23	2.21	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	
5	C	269/271 (99%)	261 (97%)	8 (3%)	0	100	100
6	D	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
7	E	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
8	F	175/177 (99%)	166 (95%)	9 (5%)	0	100	100
9	G	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
10	H	147/149 (99%)	137 (93%)	9 (6%)	1 (1%)	22	62
11	I	123/125 (98%)	113 (92%)	9 (7%)	1 (1%)	19	59
12	J	132/134 (98%)	126 (96%)	6 (4%)	0	100	100
13	K	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
14	L	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
15	M	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
16	N	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
17	O	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
18	P	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
19	Q	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
20	R	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
21	S	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
22	T	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
23	U	93/95 (98%)	89 (96%)	3 (3%)	1 (1%)	14	51
24	V	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
25	W	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
26	X	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
27	Y	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
28	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
29	a	56/58 (97%)	55 (98%)	1 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	b	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
31	c	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
32	d	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
33	e	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
34	f	36/38 (95%)	36 (100%)	0	0	100	100
35	g	414/416 (100%)	402 (97%)	12 (3%)	0	100	100
36	h	54/56 (96%)	54 (100%)	0	0	100	100
37	i	408/450 (91%)	397 (97%)	10 (2%)	1 (0%)	47	81
38	j	69/71 (97%)	67 (97%)	2 (3%)	0	100	100
39	k	21/23 (91%)	18 (86%)	3 (14%)	0	100	100
40	l	269/271 (99%)	265 (98%)	4 (2%)	0	100	100
All	All	4667/4779 (98%)	4520 (97%)	143 (3%)	4 (0%)	54	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
37	i	97	ALA
23	U	89	GLU
10	H	118	PRO
11	I	108	VAL

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	
5	C	216/216 (100%)	192 (89%)	24 (11%)	6	25
6	D	164/164 (100%)	154 (94%)	10 (6%)	18	46
7	E	165/165 (100%)	152 (92%)	13 (8%)	12	38
8	F	148/148 (100%)	130 (88%)	18 (12%)	5	22
9	G	137/137 (100%)	129 (94%)	8 (6%)	20	47

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	H	114/114 (100%)	100 (88%)	14 (12%)	4 21
11	I	95/95 (100%)	90 (95%)	5 (5%)	22 49
12	J	104/104 (100%)	93 (89%)	11 (11%)	6 26
13	K	116/116 (100%)	105 (90%)	11 (10%)	8 29
14	L	104/104 (100%)	94 (90%)	10 (10%)	8 29
15	M	103/103 (100%)	94 (91%)	9 (9%)	10 33
16	N	109/109 (100%)	100 (92%)	9 (8%)	11 36
17	O	102/102 (100%)	95 (93%)	7 (7%)	15 42
18	P	87/87 (100%)	75 (86%)	12 (14%)	3 19
19	Q	99/99 (100%)	90 (91%)	9 (9%)	9 32
20	R	89/89 (100%)	82 (92%)	7 (8%)	12 38
21	S	84/84 (100%)	76 (90%)	8 (10%)	8 29
22	T	93/93 (100%)	88 (95%)	5 (5%)	22 49
23	U	82/82 (100%)	77 (94%)	5 (6%)	18 46
24	V	83/83 (100%)	76 (92%)	7 (8%)	11 36
25	W	78/78 (100%)	72 (92%)	6 (8%)	13 39
26	X	57/58 (98%)	51 (90%)	6 (10%)	7 26
27	Y	67/67 (100%)	63 (94%)	4 (6%)	19 46
28	Z	54/54 (100%)	47 (87%)	7 (13%)	4 20
29	a	48/48 (100%)	46 (96%)	2 (4%)	30 55
30	b	47/47 (100%)	35 (74%)	12 (26%)	0 4
31	c	45/46 (98%)	40 (89%)	5 (11%)	6 25
32	d	38/38 (100%)	32 (84%)	6 (16%)	2 15
33	e	51/51 (100%)	47 (92%)	4 (8%)	12 38
34	f	34/34 (100%)	31 (91%)	3 (9%)	10 33
37	i	336/338 (99%)	334 (99%)	2 (1%)	86 92
39	k	16/16 (100%)	16 (100%)	0	100 100
40	l	217/217 (100%)	217 (100%)	0	100 100
All	All	3382/3386 (100%)	3123 (92%)	259 (8%)	16 39

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	C	3	VAL
5	C	24	LEU
5	C	35	GLU
5	C	51	THR
5	C	72	ASP
5	C	74	ILE
5	C	120	VAL
5	C	130	LEU
5	C	134	ASN
5	C	156	ARG
5	C	180	GLU
5	C	185	GLU
5	C	189	ARG
5	C	195	VAL
5	C	203	ARG
5	C	204	VAL
5	C	228	VAL
5	C	242	LYS
5	C	250	VAL
5	C	251	GLN
5	C	257	THR
5	C	261	LYS
5	C	265	LYS
5	C	271	ARG
6	D	12	THR
6	D	13	ARG
6	D	18	ASP
6	D	28	GLU
6	D	73	VAL
6	D	84	LEU
6	D	128	ARG
6	D	139	SER
6	D	160	LYS
6	D	168	GLU
7	E	84	THR
7	E	85	PHE
7	E	94	GLN
7	E	97	ASN
7	E	105	LEU
7	E	115	GLN
7	E	119	ILE
7	E	127	GLU
7	E	148	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	E	173	THR
7	E	179	SER
7	E	184	ASP
7	E	196	VAL
8	F	3	LYS
8	F	4	LEU
8	F	14	LYS
8	F	25	VAL
8	F	49	LEU
8	F	51	ASP
8	F	52	ASN
8	F	72	LYS
8	F	81	GLN
8	F	104	ILE
8	F	106	ILE
8	F	130	MET
8	F	141	ILE
8	F	144	ASP
8	F	149	VAL
8	F	150	ARG
8	F	153	ASP
8	F	162	SER
9	G	10	VAL
9	G	11	VAL
9	G	49	THR
9	G	87	LEU
9	G	114	ASP
9	G	125	CYS
9	G	127	THR
9	G	153	ARG
10	H	15	LEU
10	H	17	ASP
10	H	25	TYR
10	H	37	VAL
10	H	58	LEU
10	H	60	GLU
10	H	76	GLU
10	H	77	THR
10	H	78	VAL
10	H	86	ASP
10	H	87	GLU
10	H	110	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	H	112	LYS
10	H	116	ARG
11	I	16	SER
11	I	36	ASP
11	I	58	THR
11	I	96	PHE
11	I	109	LYS
12	J	9	VAL
12	J	21	SER
12	J	28	LEU
12	J	31	GLN
12	J	55	ILE
12	J	66	SER
12	J	111	GLN
12	J	112	THR
12	J	113	LYS
12	J	116	ASP
12	J	128	SER
13	K	5	THR
13	K	7	LYS
13	K	34	ARG
13	K	40	HIS
13	K	44	TYR
13	K	69	ARG
13	K	70	THR
13	K	88	THR
13	K	103	ILE
13	K	122	LEU
13	K	131	ASN
14	L	1	MET
14	L	21	CYS
14	L	42	THR
14	L	49	ARG
14	L	56	ASP
14	L	58	LEU
14	L	65	THR
14	L	84	CYS
14	L	106	GLU
14	L	116	ILE
15	M	2	ARG
15	M	14	LYS
15	M	46	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	M	47	ARG
15	M	55	MET
15	M	59	ARG
15	M	86	GLU
15	M	91	ASP
15	M	126	ARG
16	N	6	ARG
16	N	7	THR
16	N	12	MET
16	N	25	ASP
16	N	54	THR
16	N	58	LYS
16	N	115	GLU
16	N	133	LYS
16	N	135	VAL
17	O	2	ARG
17	O	14	SER
17	O	36	THR
17	O	69	ARG
17	O	74	GLU
17	O	75	ILE
17	O	100	CYS
18	P	2	ASP
18	P	5	SER
18	P	19	GLN
18	P	20	GLU
18	P	31	THR
18	P	36	TYR
18	P	43	ASN
18	P	55	GLU
18	P	61	GLN
18	P	69	ASP
18	P	78	VAL
18	P	98	GLN
19	Q	3	ASN
19	Q	7	GLN
19	Q	21	ARG
19	Q	26	VAL
19	Q	51	ARG
19	Q	65	SER
19	Q	68	GLU
19	Q	92	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	Q	115	ASN
20	R	6	ARG
20	R	13	ARG
20	R	17	ILE
20	R	24	TYR
20	R	51	ARG
20	R	52	GLN
20	R	109	LEU
21	S	20	VAL
21	S	25	LEU
21	S	38	VAL
21	S	45	GLU
21	S	71	LYS
21	S	72	VAL
21	S	83	TYR
21	S	101	ILE
22	T	12	SER
22	T	28	LYS
22	T	74	ILE
22	T	95	ARG
22	T	98	LYS
23	U	7	LEU
23	U	16	VAL
23	U	17	SER
23	U	48	GLN
23	U	72	GLN
24	V	7	ARG
24	V	34	VAL
24	V	41	LEU
24	V	42	VAL
24	V	68	SER
24	V	83	VAL
24	V	102	THR
25	W	7	GLU
25	W	12	GLN
25	W	61	LEU
25	W	78	GLN
25	W	90	ASP
25	W	92	VAL
26	X	11	ARG
26	X	12	ASN
26	X	21	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	X	35	SER
26	X	41	ARG
26	X	56	ASP
27	Y	2	SER
27	Y	4	VAL
27	Y	42	SER
27	Y	74	ARG
28	Z	2	LYS
28	Z	16	THR
28	Z	28	LEU
28	Z	44	LYS
28	Z	45	GLN
28	Z	48	ARG
28	Z	56	LEU
29	a	36	VAL
29	a	56	LYS
30	b	4	GLN
30	b	9	THR
30	b	15	MET
30	b	18	SER
30	b	25	VAL
30	b	26	THR
30	b	28	LEU
30	b	32	LYS
30	b	36	GLU
30	b	40	ARG
30	b	46	ASP
30	b	52	ARG
31	c	5	ILE
31	c	6	ARG
31	c	10	LYS
31	c	22	THR
31	c	47	VAL
32	d	1	MET
32	d	12	ARG
32	d	24	THR
32	d	25	LYS
32	d	34	ARG
32	d	41	ARG
33	e	8	ARG
33	e	31	HIS
33	e	32	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	e	51	SER
34	f	2	LYS
34	f	12	ARG
34	f	36	ARG
37	i	23	THR
37	i	27	VAL

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

Mol	Chain	Res	Type
5	C	86	ASN
5	C	90	ASN
5	C	200	HIS
5	C	251	GLN
6	D	136	ASN
6	D	140	HIS
7	E	165	HIS
8	F	63	GLN
8	F	81	GLN
8	F	127	ASN
10	H	11	ASN
10	H	33	GLN
10	H	43	ASN
10	H	66	ASN
12	J	31	GLN
13	K	80	HIS
13	K	86	GLN
14	L	3	GLN
14	L	89	ASN
15	M	104	GLN
16	N	3	GLN
17	O	18	GLN
18	P	100	HIS
19	Q	52	ASN
19	Q	66	ASN
20	R	81	ASN
21	S	82	HIS
22	T	7	HIS
23	U	48	GLN
23	U	59	ASN
23	U	91	GLN
26	X	46	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	Z	39	GLN
28	Z	58	ASN
32	d	26	ASN
32	d	29	GLN
37	i	91	GLN
40	l	161	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	103/104 (99%)	22 (21%)	0
2	2	2/3 (66%)	1 (50%)	0
3	A	2878/2903 (99%)	518 (17%)	19 (0%)
4	B	119/120 (99%)	13 (10%)	0
All	All	3102/3130 (99%)	554 (17%)	19 (0%)

All (554) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	27	G
1	1	29	U
1	1	30	A
1	1	33	C
1	1	34	U
1	1	37	U
1	1	38	U
1	1	39	A
1	1	41	C
1	1	42	A
1	1	46	C
1	1	57	G
1	1	75	U
1	1	76	G
1	1	83	G
1	1	87	C
1	1	88	G
1	1	90	G
1	1	94	U
1	1	95	A
1	1	102	A
1	1	107	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	76	A
3	A	10	A
3	A	12	U
3	A	33	C
3	A	34	U
3	A	35	G
3	A	45	G
3	A	46	G
3	A	49	A
3	A	50	U
3	A	51	G
3	A	62	U
3	A	63	A
3	A	65	U
3	A	71	A
3	A	72	U
3	A	74	A
3	A	75	G
3	A	84	A
3	A	93	G
3	A	96	C
3	A	101	A
3	A	102	U
3	A	103	A
3	A	110	G
3	A	118	A
3	A	119	A
3	A	120	U
3	A	136	G
3	A	137	U
3	A	138	U
3	A	139	U
3	A	142	A
3	A	156	A
3	A	162	U
3	A	181	A
3	A	188	G
3	A	196	A
3	A	199	A
3	A	215	G
3	A	216	A
3	A	220	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	221	A
3	A	222	A
3	A	226	A
3	A	248	G
3	A	266	G
3	A	272	A
3	A	275	C
3	A	276	U
3	A	285	G
3	A	291	G
3	A	302	C
3	A	311	A
3	A	329	G
3	A	330	A
3	A	335	C
3	A	349	U
3	A	353	C
3	A	356	G
3	A	361	G
3	A	362	A
3	A	372	G
3	A	386	G
3	A	396	G
3	A	399	U
3	A	411	G
3	A	419	U
3	A	424	G
3	A	454	A
3	A	455	C
3	A	475	C
3	A	477	A
3	A	479	A
3	A	480	A
3	A	481	G
3	A	491	G
3	A	504	A
3	A	505	A
3	A	509	C
3	A	510	C
3	A	513	A
3	A	518	G
3	A	529	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	531	C
3	A	532	A
3	A	533	G
3	A	543	G
3	A	544	C
3	A	550	C
3	A	552	U
3	A	558	U
3	A	563	A
3	A	567	U
3	A	568	U
3	A	573	U
3	A	575	A
3	A	586	A
3	A	603	A
3	A	613	A
3	A	614	A
3	A	615	U
3	A	627	A
3	A	632	A
3	A	634	C
3	A	637	A
3	A	645	C
3	A	646	U
3	A	647	G
3	A	653	U
3	A	654	A
3	A	655	A
3	A	668	A
3	A	685	A
3	A	686	U
3	A	711	G
3	A	712	G
3	A	713	G
3	A	718	A
3	A	730	A
3	A	747	U
3	A	753	A
3	A	757	G
3	A	763	G
3	A	764	A
3	A	765	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	775	G
3	A	777	G
3	A	782	A
3	A	784	G
3	A	785	G
3	A	788	A
3	A	789	A
3	A	790	U
3	A	791	C
3	A	793	A
3	A	794	A
3	A	801	G
3	A	805	G
3	A	812	C
3	A	827	U
3	A	828	U
3	A	831	G
3	A	846	U
3	A	859	G
3	A	865	C
3	A	869	G
3	A	878	A
3	A	896	A
3	A	897	C
3	A	899	A
3	A	907	G
3	A	910	A
3	A	914	G
3	A	915	C
3	A	932	U
3	A	933	A
3	A	946	C
3	A	953	G
3	A	957	C
3	A	961	C
3	A	974	G
3	A	983	A
3	A	990	A
3	A	996	A
3	A	999	U
3	A	1005	C
3	A	1009	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	1012	U
3	A	1013	C
3	A	1022	G
3	A	1023	U
3	A	1027	A
3	A	1033	U
3	A	1040	A
3	A	1046	A
3	A	1056	G
3	A	1057	A
3	A	1070	A
3	A	1071	G
3	A	1073	A
3	A	1083	U
3	A	1087	G
3	A	1088	A
3	A	1090	A
3	A	1101	U
3	A	1111	A
3	A	1112	G
3	A	1116	G
3	A	1129	A
3	A	1130	U
3	A	1132	U
3	A	1133	A
3	A	1135	C
3	A	1136	G
3	A	1139	G
3	A	1142	A
3	A	1143	A
3	A	1155	A
3	A	1173	U
3	A	1179	G
3	A	1182	G
3	A	1206	G
3	A	1212	G
3	A	1218	G
3	A	1236	G
3	A	1238	G
3	A	1247	A
3	A	1249	U
3	A	1252	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	1253	A
3	A	1256	G
3	A	1262	A
3	A	1271	G
3	A	1272	A
3	A	1294	U
3	A	1300	G
3	A	1301	A
3	A	1302	A
3	A	1308	A
3	A	1329	U
3	A	1332	G
3	A	1337	G
3	A	1338	G
3	A	1345	C
3	A	1346	G
3	A	1365	A
3	A	1379	U
3	A	1383	A
3	A	1395	A
3	A	1403	A
3	A	1416	G
3	A	1417	C
3	A	1424	G
3	A	1428	C
3	A	1434	A
3	A	1437	C
3	A	1449	G
3	A	1451	C
3	A	1452	G
3	A	1453	A
3	A	1482	G
3	A	1489	C
3	A	1491	G
3	A	1493	C
3	A	1494	A
3	A	1495	A
3	A	1497	U
3	A	1498	C
3	A	1509	A
3	A	1510	G
3	A	1515	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	1524	G
3	A	1529	G
3	A	1533	C
3	A	1535	A
3	A	1536	C
3	A	1537	G
3	A	1554	U
3	A	1560	G
3	A	1566	A
3	A	1569	A
3	A	1576	U
3	A	1578	U
3	A	1581	G
3	A	1583	A
3	A	1585	C
3	A	1606	C
3	A	1607	C
3	A	1608	A
3	A	1616	A
3	A	1634	A
3	A	1639	C
3	A	1647	U
3	A	1648	U
3	A	1649	G
3	A	1660	G
3	A	1674	G
3	A	1677	A
3	A	1715	G
3	A	1722	A
3	A	1725	U
3	A	1729	U
3	A	1730	C
3	A	1738	G
3	A	1744	A
3	A	1757	A
3	A	1764	C
3	A	1773	A
3	A	1782	U
3	A	1786	A
3	A	1791	A
3	A	1800	C
3	A	1801	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	1802	A
3	A	1808	A
3	A	1809	A
3	A	1811	G
3	A	1816	C
3	A	1829	A
3	A	1847	A
3	A	1849	G
3	A	1850	G
3	A	1870	C
3	A	1871	A
3	A	1872	A
3	A	1876	A
3	A	1896	G
3	A	1906	G
3	A	1920	C
3	A	1927	A
3	A	1929	G
3	A	1930	G
3	A	1931	U
3	A	1934	C
3	A	1936	A
3	A	1937	A
3	A	1939	U
3	A	1955	U
3	A	1956	U
3	A	1960	A
3	A	1962	C
3	A	1966	A
3	A	1967	C
3	A	1970	A
3	A	1971	U
3	A	1972	G
3	A	1974	C
3	A	1982	U
3	A	1991	U
3	A	1992	G
3	A	1993	U
3	A	1997	C
3	A	2021	C
3	A	2023	C
3	A	2030	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	2031	A
3	A	2033	A
3	A	2043	C
3	A	2050	C
3	A	2054	A
3	A	2055	C
3	A	2056	G
3	A	2060	A
3	A	2061	G
3	A	2062	A
3	A	2069	G
3	A	2072	C
3	A	2093	G
3	A	2097	A
3	A	2101	A
3	A	2103	C
3	A	2104	C
3	A	2105	U
3	A	2106	U
3	A	2111	U
3	A	2112	G
3	A	2113	U
3	A	2116	G
3	A	2117	A
3	A	2118	U
3	A	2119	A
3	A	2120	G
3	A	2123	G
3	A	2126	A
3	A	2128	G
3	A	2131	U
3	A	2132	U
3	A	2133	G
3	A	2134	A
3	A	2145	C
3	A	2146	C
3	A	2147	A
3	A	2148	G
3	A	2159	G
3	A	2160	C
3	A	2161	C
3	A	2163	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	2164	C
3	A	2165	C
3	A	2167	U
3	A	2168	G
3	A	2169	A
3	A	2170	A
3	A	2171	A
3	A	2172	U
3	A	2173	A
3	A	2174	C
3	A	2177	C
3	A	2178	C
3	A	2185	U
3	A	2187	U
3	A	2190	G
3	A	2198	A
3	A	2203	U
3	A	2204	G
3	A	2211	A
3	A	2212	A
3	A	2225	A
3	A	2238	G
3	A	2239	G
3	A	2250	G
3	A	2268	A
3	A	2278	A
3	A	2280	G
3	A	2283	C
3	A	2287	A
3	A	2288	A
3	A	2297	A
3	A	2305	U
3	A	2308	G
3	A	2322	A
3	A	2325	G
3	A	2331	G
3	A	2336	A
3	A	2345	G
3	A	2347	C
3	A	2350	C
3	A	2354	C
3	A	2357	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	2366	A
3	A	2383	G
3	A	2385	C
3	A	2402	U
3	A	2403	C
3	A	2406	A
3	A	2420	C
3	A	2421	G
3	A	2422	C
3	A	2423	U
3	A	2424	C
3	A	2425	A
3	A	2427	C
3	A	2429	G
3	A	2430	A
3	A	2431	U
3	A	2432	A
3	A	2434	A
3	A	2435	A
3	A	2440	C
3	A	2441	U
3	A	2445	G
3	A	2448	A
3	A	2464	G
3	A	2475	C
3	A	2476	A
3	A	2478	A
3	A	2491	U
3	A	2492	U
3	A	2497	A
3	A	2502	G
3	A	2504	U
3	A	2505	G
3	A	2506	U
3	A	2507	C
3	A	2513	A
3	A	2514	U
3	A	2518	A
3	A	2520	C
3	A	2529	G
3	A	2566	A
3	A	2567	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	2578	G
3	A	2582	G
3	A	2585	U
3	A	2586	U
3	A	2602	A
3	A	2603	G
3	A	2609	U
3	A	2613	U
3	A	2615	U
3	A	2621	G
3	A	2623	G
3	A	2624	G
3	A	2629	U
3	A	2630	G
3	A	2636	C
3	A	2638	G
3	A	2669	G
3	A	2682	A
3	A	2689	U
3	A	2690	U
3	A	2714	G
3	A	2716	C
3	A	2726	A
3	A	2733	A
3	A	2739	U
3	A	2744	G
3	A	2748	A
3	A	2757	A
3	A	2765	A
3	A	2778	A
3	A	2779	U
3	A	2780	G
3	A	2791	G
3	A	2792	A
3	A	2798	U
3	A	2799	A
3	A	2801	G
3	A	2820	A
3	A	2821	A
3	A	2825	G
3	A	2833	U
3	A	2835	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	2836	U
3	A	2849	U
3	A	2860	A
3	A	2861	U
3	A	2867	G
3	A	2870	C
3	A	2873	A
3	A	2879	A
3	A	2880	C
3	A	2883	A
3	A	2884	U
3	A	2885	G
3	A	2886	A
3	A	2888	C
3	A	2891	U
4	B	24	G
4	B	25	U
4	B	35	C
4	B	41	G
4	B	45	A
4	B	56	G
4	B	66	A
4	B	67	G
4	B	71	C
4	B	88	C
4	B	89	U
4	B	90	C
4	B	109	A

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	A	100	U
3	A	613	A
3	A	645	C
3	A	653	U
3	A	784	G
3	A	827	U
3	A	830	G
3	A	1110	G
3	A	1344	U
3	A	1494	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	1721	G
3	A	1939	U
3	A	2127	G
3	A	2158	A
3	A	2422	C
3	A	2424	C
3	A	2430	A
3	A	2602	A
3	A	2756	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
42	ALF	l	1001	-	0,4,4	-	-	-		
42	ALF	i	1001	-	0,4,4	-	-	-		
44	GDP	i	1003	43	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
44	GDP	l	1003	43	24,30,30	0.96	1 (4%)	30,47,47	1.30	4 (13%)

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
44	GDP	i	1003	43	-	4/12/32/32	0/3/3/3
44	GDP	l	1003	43	-	7/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	l	1003	GDP	C6-N1	-2.44	1.34	1.37
44	i	1003	GDP	C6-N1	-2.35	1.34	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	i	1003	GDP	PA-O3A-PB	-3.78	119.86	132.83
44	l	1003	GDP	PA-O3A-PB	-3.67	120.23	132.83
44	i	1003	GDP	C3'-C2'-C1'	3.00	105.49	100.98
44	l	1003	GDP	C3'-C2'-C1'	2.94	105.40	100.98
44	l	1003	GDP	C8-N7-C5	2.37	107.50	102.99
44	i	1003	GDP	C8-N7-C5	2.36	107.50	102.99
44	l	1003	GDP	C5-C6-N1	2.35	118.11	113.95
44	i	1003	GDP	C5-C6-N1	2.33	118.07	113.95

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	i	1003	GDP	C5'-O5'-PA-O3A
44	i	1003	GDP	O4'-C4'-C5'-O5'
44	i	1003	GDP	C3'-C4'-C5'-O5'
44	l	1003	GDP	PA-O3A-PB-O2B
44	l	1003	GDP	C5'-O5'-PA-O1A
44	l	1003	GDP	C5'-O5'-PA-O2A
44	l	1003	GDP	O4'-C4'-C5'-O5'
44	l	1003	GDP	C3'-C4'-C5'-O5'
44	i	1003	GDP	C5'-O5'-PA-O1A
44	l	1003	GDP	PA-O3A-PB-O1B
44	l	1003	GDP	C5'-O5'-PA-O3A

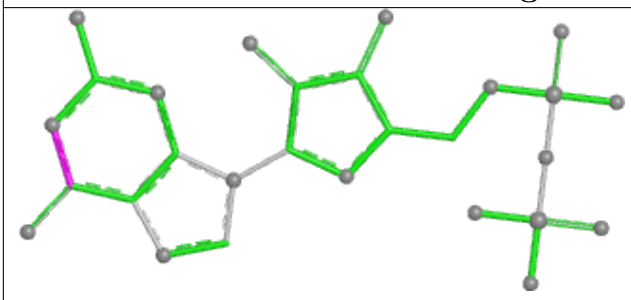
There are no ring outliers.

No monomer is involved in short contacts.

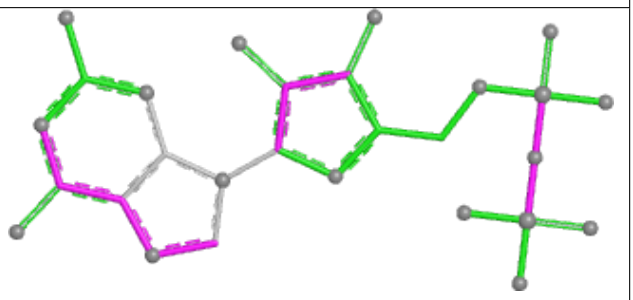
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

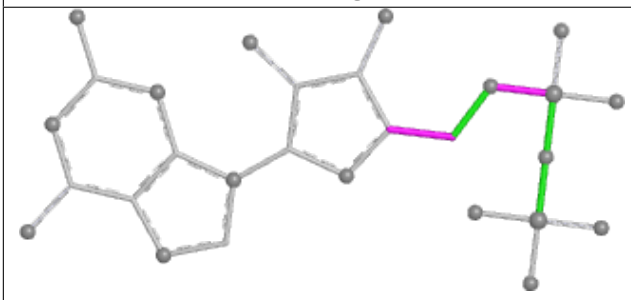
Ligand GDP i 1003



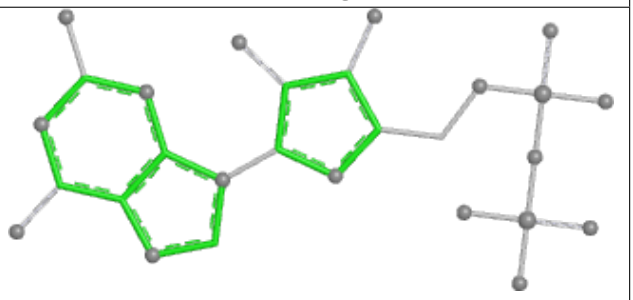
Bond lengths



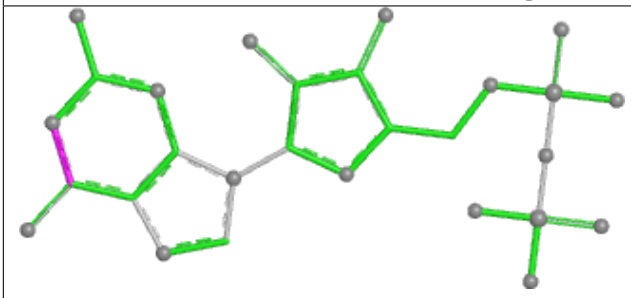
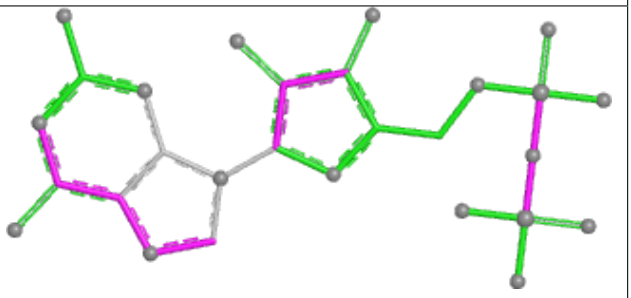
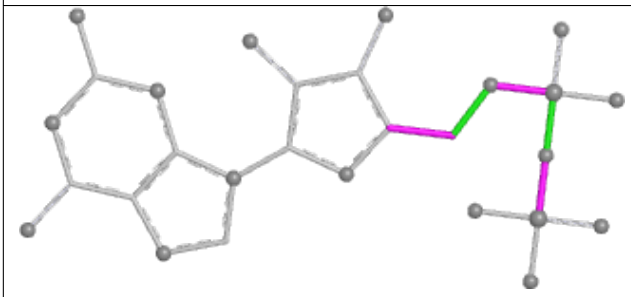
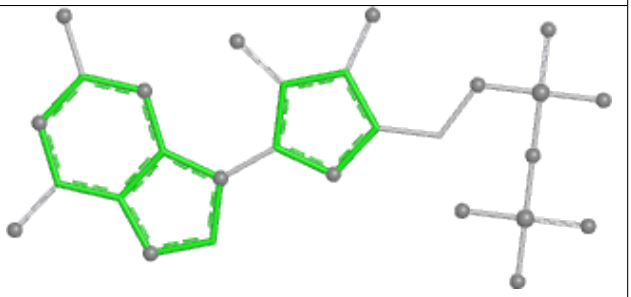
Bond angles



Torsions



Rings

Ligand GDP l 1003	
 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.

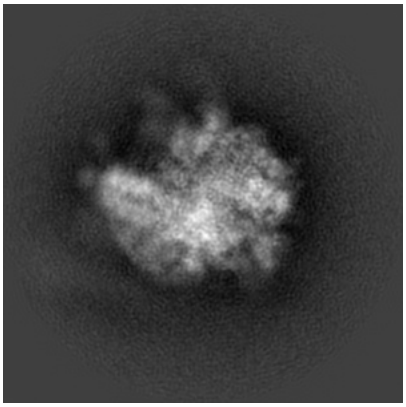
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3617. These allow visual inspection of the internal detail of the map and identification of artifacts.

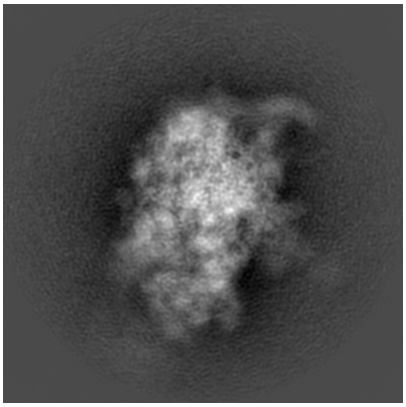
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

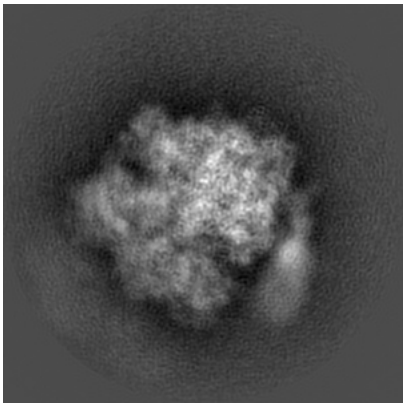
6.1.1 Primary map



X



Y

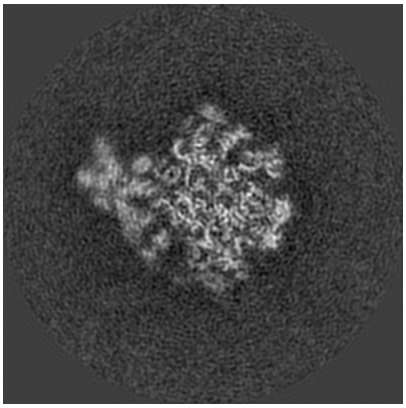


Z

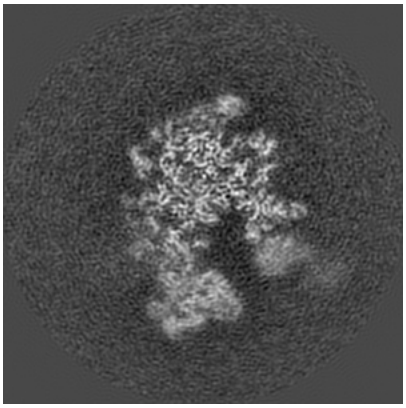
The images above show the map projected in three orthogonal directions.

6.2 Central slices

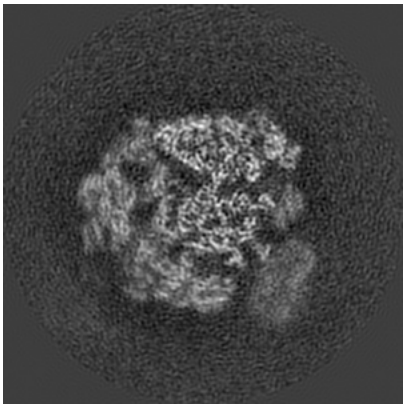
6.2.1 Primary map



X Index: 160



Y Index: 160

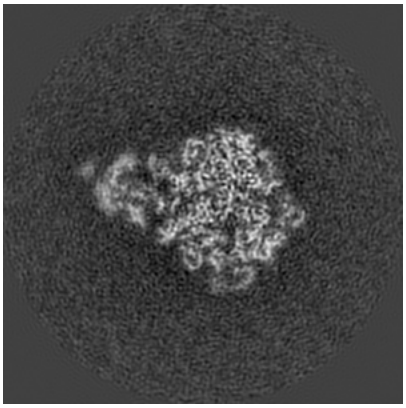


Z Index: 160

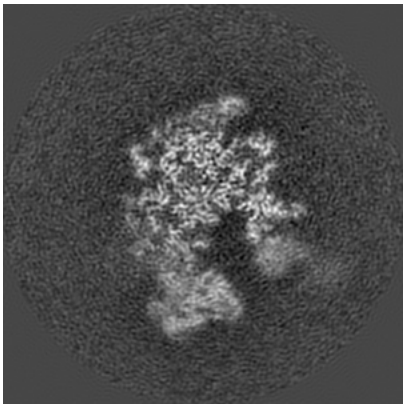
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

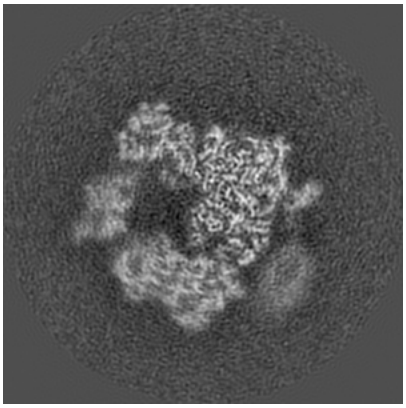
6.3.1 Primary map



X Index: 170



Y Index: 159



Z Index: 175

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

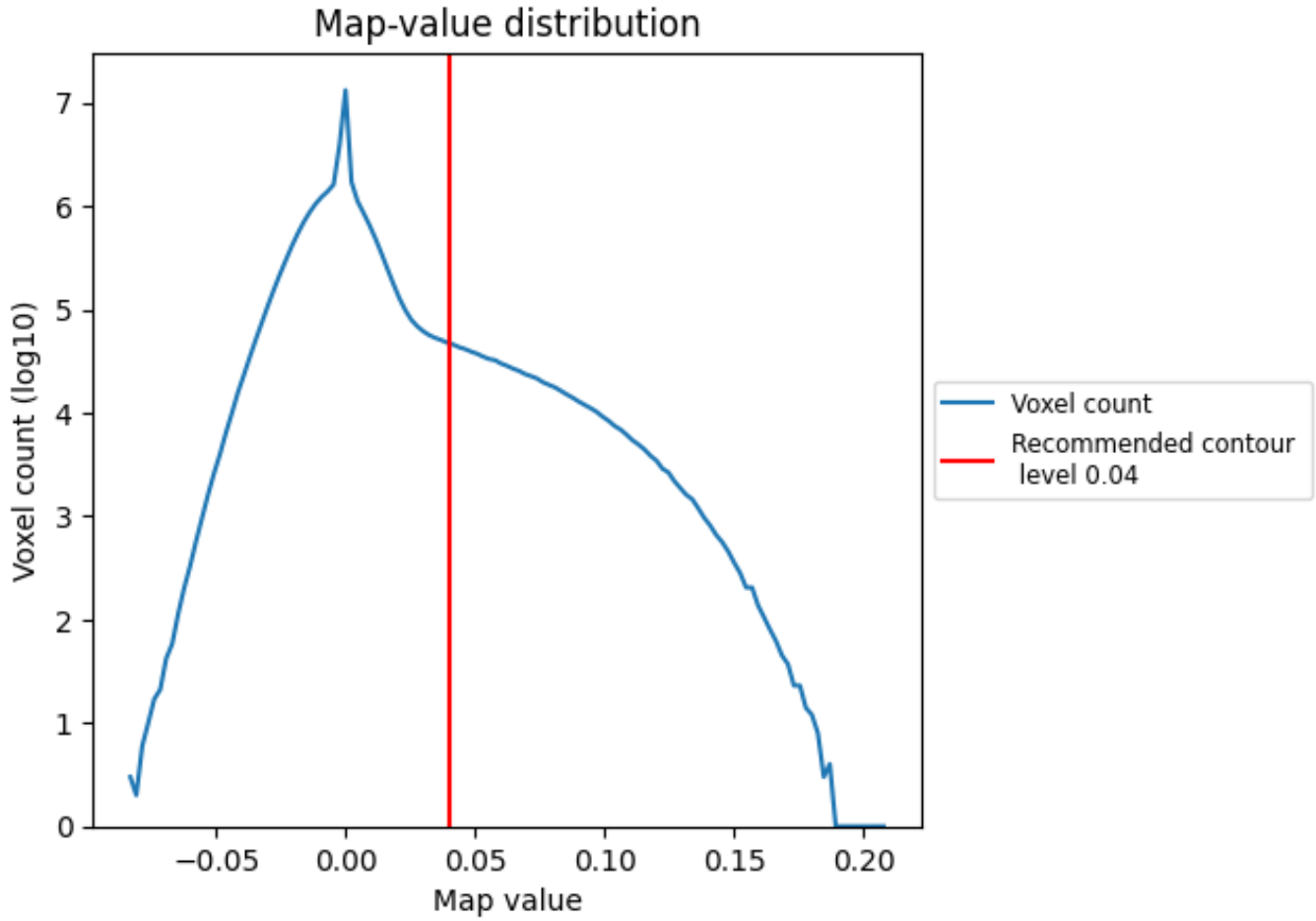
6.5 Mask visualisation (i)

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

7 Map analysis

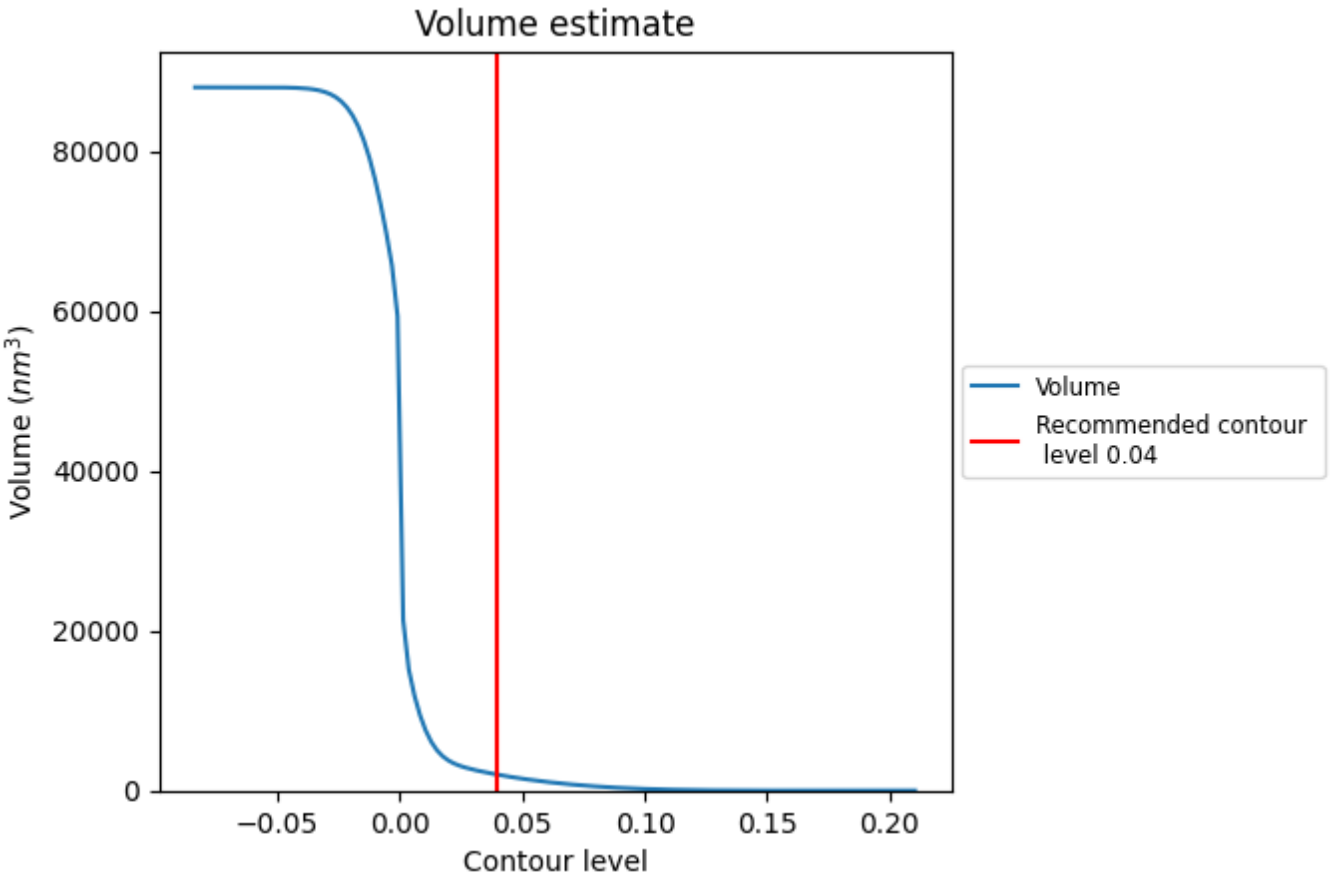
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

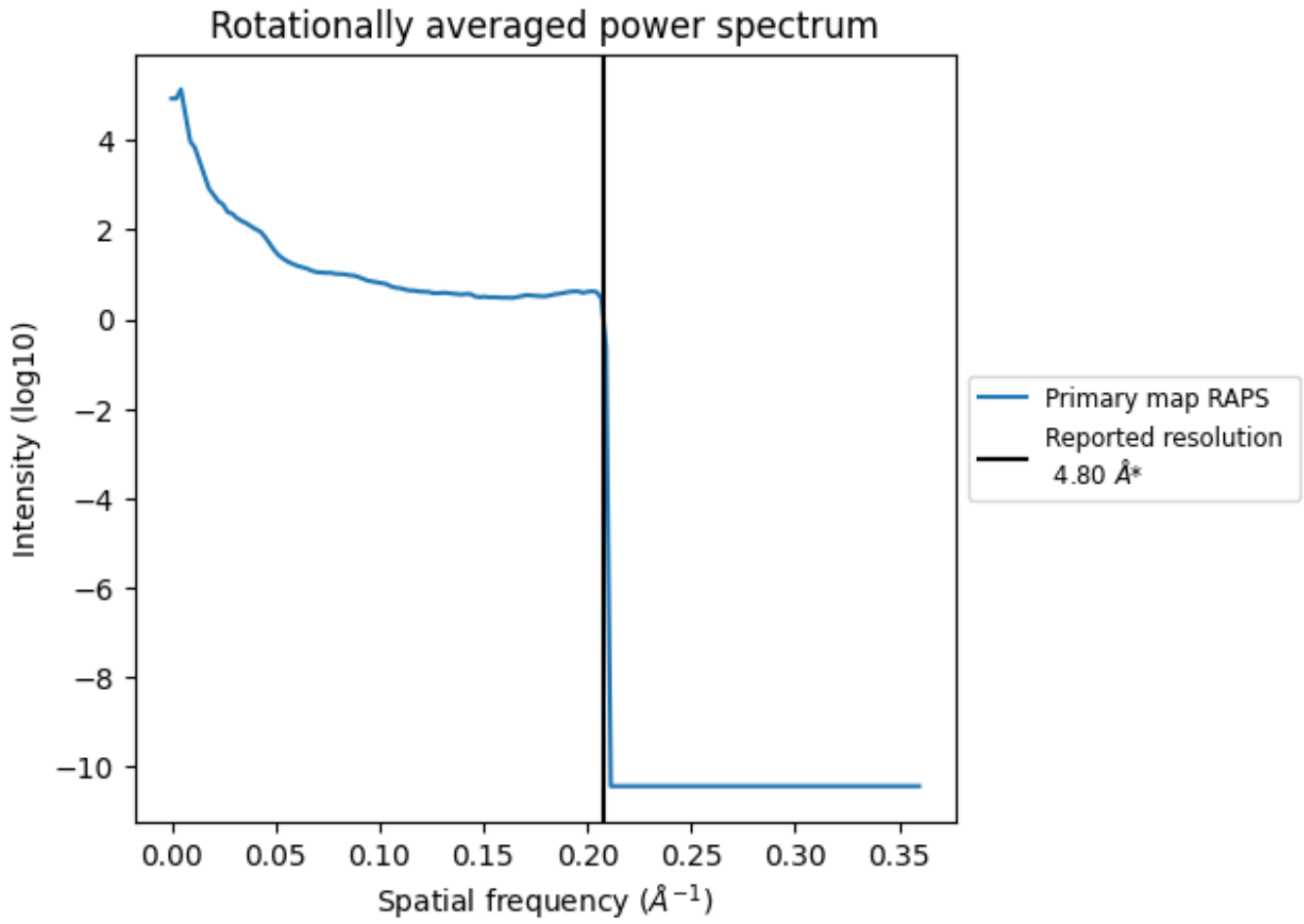
7.2 Volume estimate



The volume at the recommended contour level is 1992 nm^3; this corresponds to an approximate mass of 1799 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 0.208 Å^{-1}

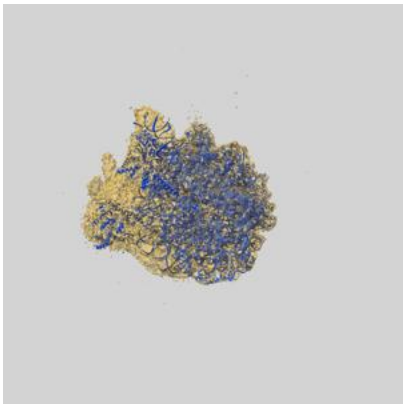
8 Fourier-Shell correlation (i)

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

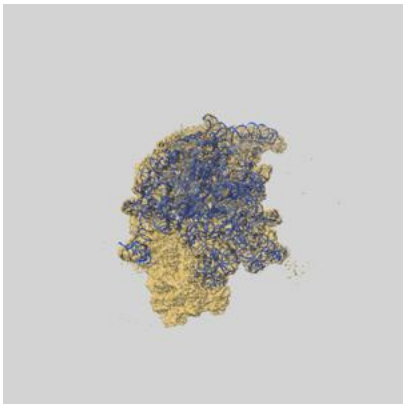
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3617 and PDB model 5NCO. Per-residue inclusion information can be found in section 3 on page 13.

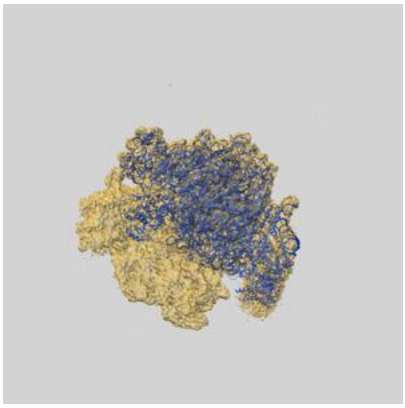
9.1 Map-model overlay



X



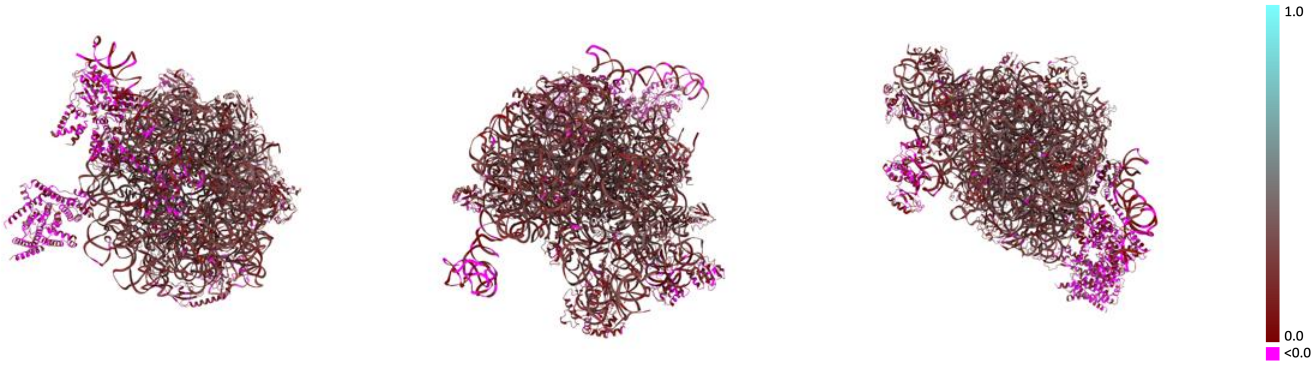
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

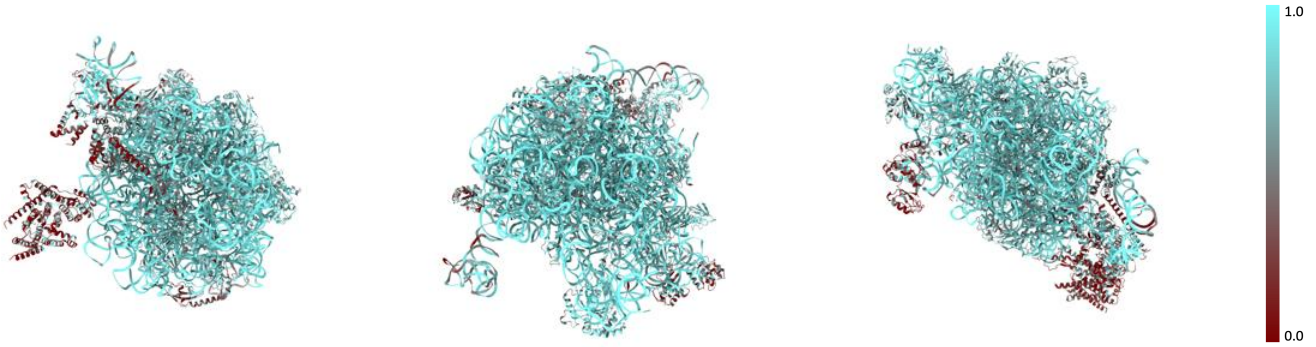
9.2 Q-score mapped to coordinate model (i)



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.

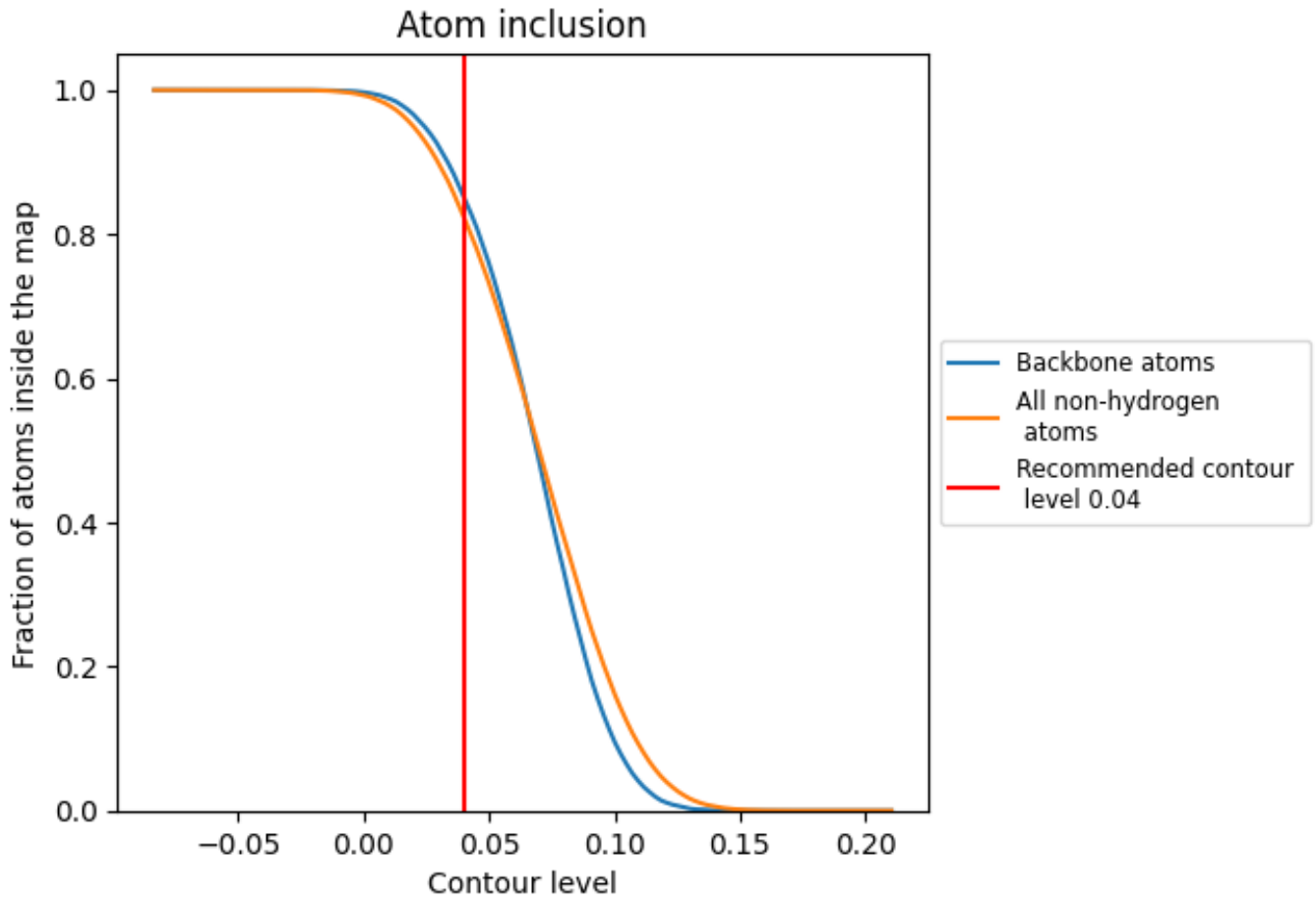
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 82% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8235	0.2180
1	0.7473	0.0820
2	0.9032	0.2770
A	0.9267	0.2540
B	0.9513	0.2450
C	0.6996	0.2090
D	0.7159	0.2310
E	0.7211	0.2080
F	0.6907	0.1350
G	0.7309	0.2130
H	0.4338	0.1410
I	0.4082	0.0570
J	0.3230	0.0500
K	0.7273	0.2280
L	0.6254	0.2120
M	0.7441	0.2090
N	0.7418	0.2380
O	0.6565	0.2170
P	0.7796	0.1880
Q	0.6836	0.2320
R	0.7885	0.2280
S	0.7340	0.2260
T	0.6675	0.2230
U	0.6865	0.2060
V	0.7083	0.2070
W	0.7127	0.2120
X	0.7500	0.1850
Y	0.7005	0.2080
Z	0.6912	0.1640
a	0.7735	0.2340
b	0.7243	0.2260
c	0.6675	0.1380
d	0.7155	0.2070
e	0.6925	0.2100
f	0.7747	0.1990

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
g	0.2909	0.0050
h	0.1562	-0.0410
i	0.5009	0.0590
j	0.2817	0.0170
k	0.6667	0.1140
l	0.6437	0.0390