wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:46 PM BST

PDB ID	:	3J79
EMDB ID:	:	EMD-2660
Title	:	Cryo-EM structure of the Plasmodium falciparum 80S ribosome bound to the anti-protozoan drug emetine, large subunit
Authors	:	Wong, W.; Bai, X.C.; Brown, A.; Fernandez, I.S.; Hanssen, E.; Condron, M.; Tan, Y.H.; Baum, J.; Scheres, S.H.W.
Deposited on	:	2014-06-02
Resolution	:	3.20 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

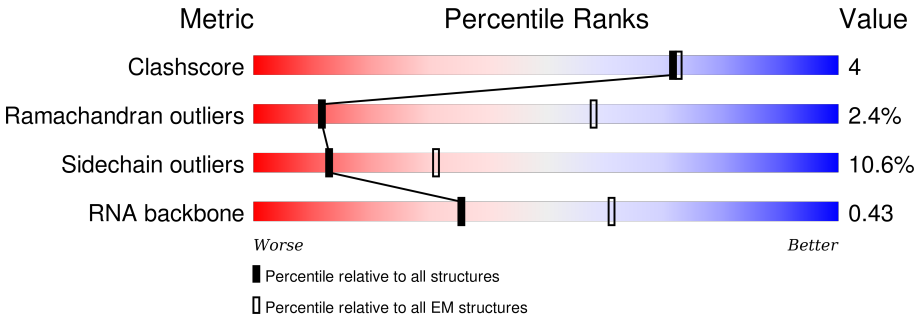
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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%

Mol	Chain	Length	Quality of chain
1	A	3788	53% 27% 5% 16%
2	B	119	75% 20% • •
3	C	159	55% 33% 6% • 5%
4	D	260	79% 13% • 5%
5	E	386	79% 17% • •
6	F	411	76% 16% • 5%
7	G	173	52% 17% • 28%
8	H	190	70% 25% • • •

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Mol	Chain	Length	Quality of chain
9	I	221	72% 19% • 6%
10	J	283	67% 13% • 19%
11	K	202	79% 19% •
12	L	215	76% 18% • •
13	M	139	68% 24% • • 5%
14	N	165	58% 25% 5% • 12%
15	O	148	82% 16% ••
16	P	205	73% 22% •
17	Q	219	74% 11% • 14%
18	R	294	67% 17% • 14%
19	S	187	77% 21% • •
20	T	182	81% 18% ••
21	U	184	75% 22% • •
22	V	161	84% 12% • •
23	W	203	69% 13% • 16%
24	X	139	59% 11% 30%
25	Y	190	43% 10% • 47%
26	Z	126	77% 17% •• •
27	0	162	28% 10% 62%
28	1	146	80% 15% • •
29	2	127	72% 8% • 18%
30	3	124	75% 17% • •
31	4	67	82% 16% •
32	5	257	67% 19% • 13%
33	6	108	62% 26% • 9%

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Mol	Chain	Length	Quality of chain
34	7	120	58% 17% 6% 20%
35	8	131	71% 22% 5%
36	9	140	51% 16% 5% 26%
37	a	150	63% 8% 29%
38	b	112	79% 5% 15%
39	c	92	83% 14%
40	d	87	75% 8% 17%
41	e	51	71% 14% 16%
42	f	128	36% 60%
43	g	39	90% 5% 5%
44	h	96	83% 5% 11%
45	i	104	81% 11% 9%

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 124514 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 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	3191	67935	30426	12044	22274	3191	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	118	2525	1128	461	818	118	0	0

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C	151	3224	1444	589	1040	151	0	0

- Molecule 4 is a protein called 60S ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	247	1866	1166	374	317	9	0	0

- Molecule 5 is a protein called 60S ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	380	3061	1948	575	521	17	0	0

- Molecule 6 is a protein called 60S ribosomal protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	390	3094	1962	594	527	11	0	0

- Molecule 7 is a protein called 60S ribosomal protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	124	Total	C	N	O	S	0	0
			1010	636	197	171	6		

- Molecule 8 is a protein called 60S ribosomal protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	185	Total	C	N	O	S	0	0
			1460	938	261	255	6		

- Molecule 9 is a protein called 60S ribosomal protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	207	Total	C	N	O	S	0	0
			1684	1096	298	285	5		

- Molecule 10 is a protein called 60S ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	229	Total	C	N	O	S	0	0
			1873	1210	337	319	7		

- Molecule 11 is a protein called 60S ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	201	Total	C	N	O	S	0	0
			1659	1064	311	276	8		

- Molecule 12 is a protein called 60S ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	211	Total	C	N	O	S	0	0
			1761	1119	349	290	3		

- Molecule 13 is a protein called 60S ribosomal protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	132	Total	C	N	O	S	0	0
			996	631	179	178	8		

- Molecule 14 is a protein called 60S ribosomal protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	146	Total	C	N	O	S	0	0
			1197	779	210	202	6		

- Molecule 15 is a protein called 60S ribosomal protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	147	Total	C	N	O	S	0	0
			1172	747	232	189	4		

- Molecule 16 is a protein called 60S ribosomal protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	204	Total	C	N	O	S	0	0
			1697	1075	351	267	4		

- Molecule 17 is a protein called 60S ribosomal protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	189	Total	C	N	O	S	0	0
			1544	984	291	261	8		

- Molecule 18 is a protein called 60S ribosomal protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	252	Total	C	N	O	S	0	0
			2045	1297	384	358	6		

- Molecule 19 is a protein called 60S ribosomal protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	186	Total	C	N	O	S	0	0
			1502	958	299	240	5		

- Molecule 20 is a protein called 60S ribosomal protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	181	Total	C	N	O	S	0	0
			1505	949	308	244	4		

- Molecule 21 is a protein called 60S ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	180	Total	C	N	O	S	0	0
			1496	946	289	254	7		

- Molecule 22 is a protein called 60S ribosomal protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	155	Total	C	N	O	S	0	0
			1275	814	241	214	6		

- Molecule 23 is a protein called 60S ribosomal protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	170	Total	C	N	O	S	0	0
			1318	824	266	221	7		

- Molecule 24 is a protein called 60S ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	97	Total	C	N	O	S	0	0
			824	548	135	139	2		

- Molecule 25 is a protein called 60S ribosomal protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	101	Total	C	N	O	S	0	0
			796	502	144	144	6		

- Molecule 26 is a protein called 60S ribosomal protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	121	Total	C	N	O	S	0	0
			1000	626	206	165	3		

- Molecule 27 is a protein called 60S ribosomal protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	62	Total	C	N	O	S	0	0
			521	336	97	87	1		

- Molecule 28 is a protein called 60S ribosomal protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	140	Total	C	N	O	S	0	0
			1134	736	204	191	3		

- Molecule 29 is a protein called 60S ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	104	Total	C	N	O	S	0	0
			830	529	151	147	3		

- Molecule 30 is a protein called 60S ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	119	Total	C	N	O	S	0	0
			994	635	194	163	2		

- Molecule 31 is a protein called 60S ribosomal protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	66	Total	C	N	O	S	0	0
			555	347	116	90	2		

- Molecule 32 is a protein called 60S ribosomal protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	223	Total	C	N	O	S	0	0
			1879	1211	357	306	5		

- Molecule 33 is a protein called 60S ribosomal protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	98	Total	C	N	O	S	0	0
			740	462	132	139	7		

- Molecule 34 is a protein called 60S ribosomal protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	7	96	Total	C	N	O	S	0	0
			793	508	151	129	5		

- Molecule 35 is a protein called 60S ribosomal protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	8	125	Total	C	N	O	S	0	0
			1036	660	206	163	7		

- Molecule 36 is a protein called 60S ribosomal protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	9	103	Total	C	N	O	S	0	0
			844	543	163	135	3		

- Molecule 37 is a protein called 60S ribosomal protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	a	106	Total	C	N	O	S	0	0
			858	530	184	138	6		

- Molecule 38 is a protein called 60S ribosomal protein eL36.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	b	95	Total	C	N	O	0	0
			756	477	150	129		

- Molecule 39 is a protein called 60S ribosomal protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	c	89	Total	C	N	O	S	0	0
			705	439	150	111	5		

- Molecule 40 is a protein called 60S ribosomal protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	d	72	Total	C	N	O	S	0	0
			603	395	107	99	2		

- Molecule 41 is a protein called 60S ribosomal protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	e	43	Total	C	N	O	S	0	0
			388	243	92	52	1		

- Molecule 42 is a protein called 60S ribosomal protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	f	51	Total	C	N	O	S	0	0
			413	255	87	66	5		

- Molecule 43 is a protein called 60S ribosomal protein eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	g	37	Total	C	N	O	S	0	0
			342	210	86	44	2		

- Molecule 44 is a protein called 60S ribosomal protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	h	85	Total	C	N	O	S	0	0
			658	417	127	107	7		

- Molecule 45 is a protein called 60S ribosomal protein eL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	i	95	Total	C	N	O	S	0	0
			778	490	152	127	9		

- Molecule 46 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
46	B	3	Total	Mg	0
			3	3	
46	A	153	Total	Mg	0
			153	153	
46	Q	1	Total	Mg	0
			1	1	
46	C	5	Total	Mg	0
			5	5	
46	M	1	Total	Mg	0
			1	1	

- Molecule 47 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
47	h	1	Total	Zn	0
			1	1	
47	a	1	Total	Zn	0
			1	1	

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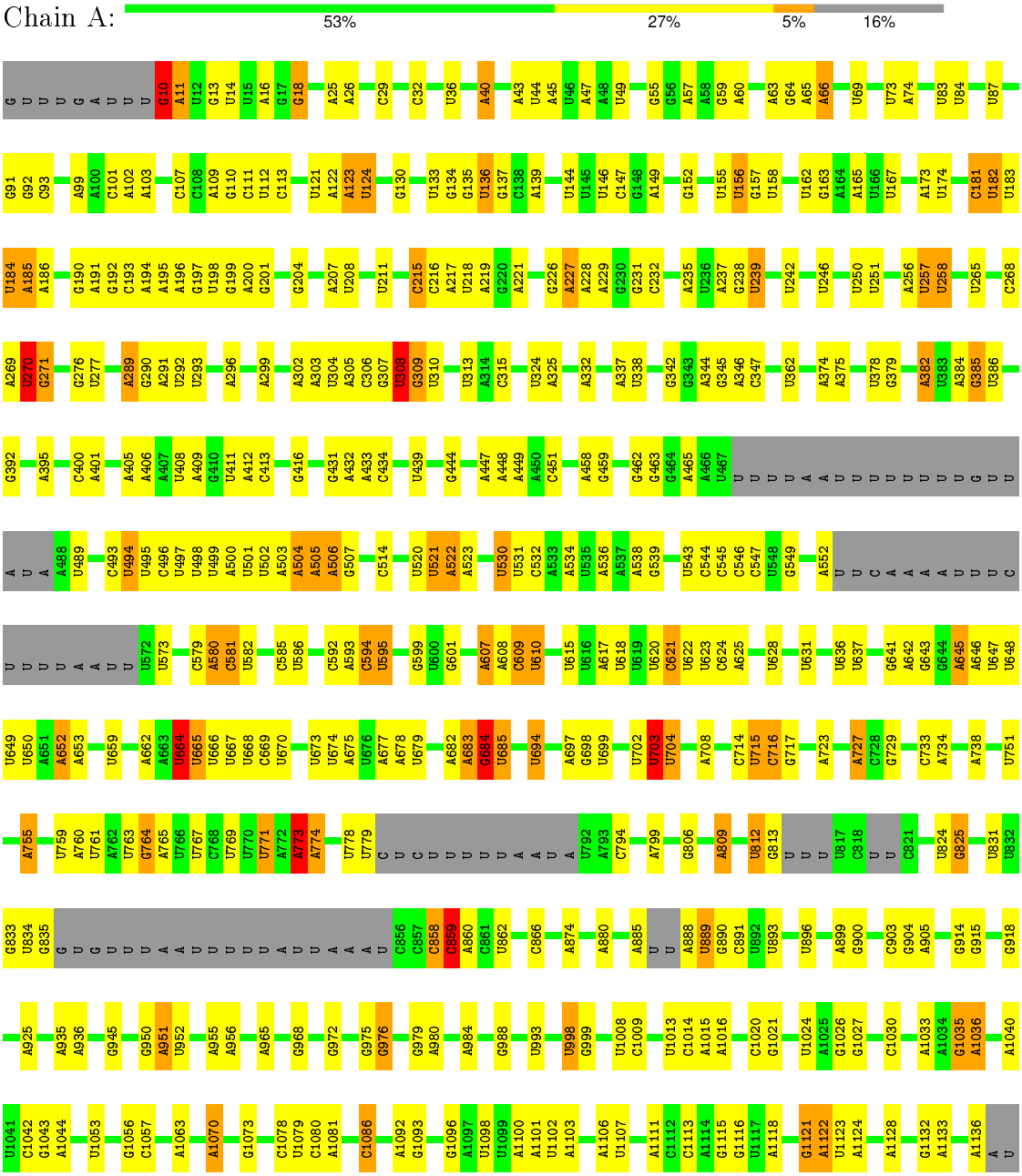
Mol	Chain	Residues	Atoms	AltConf
47	c	1	Total Zn 1 1	0
47	f	1	Total Zn 1 1	0
47	i	1	Total Zn 1 1	0

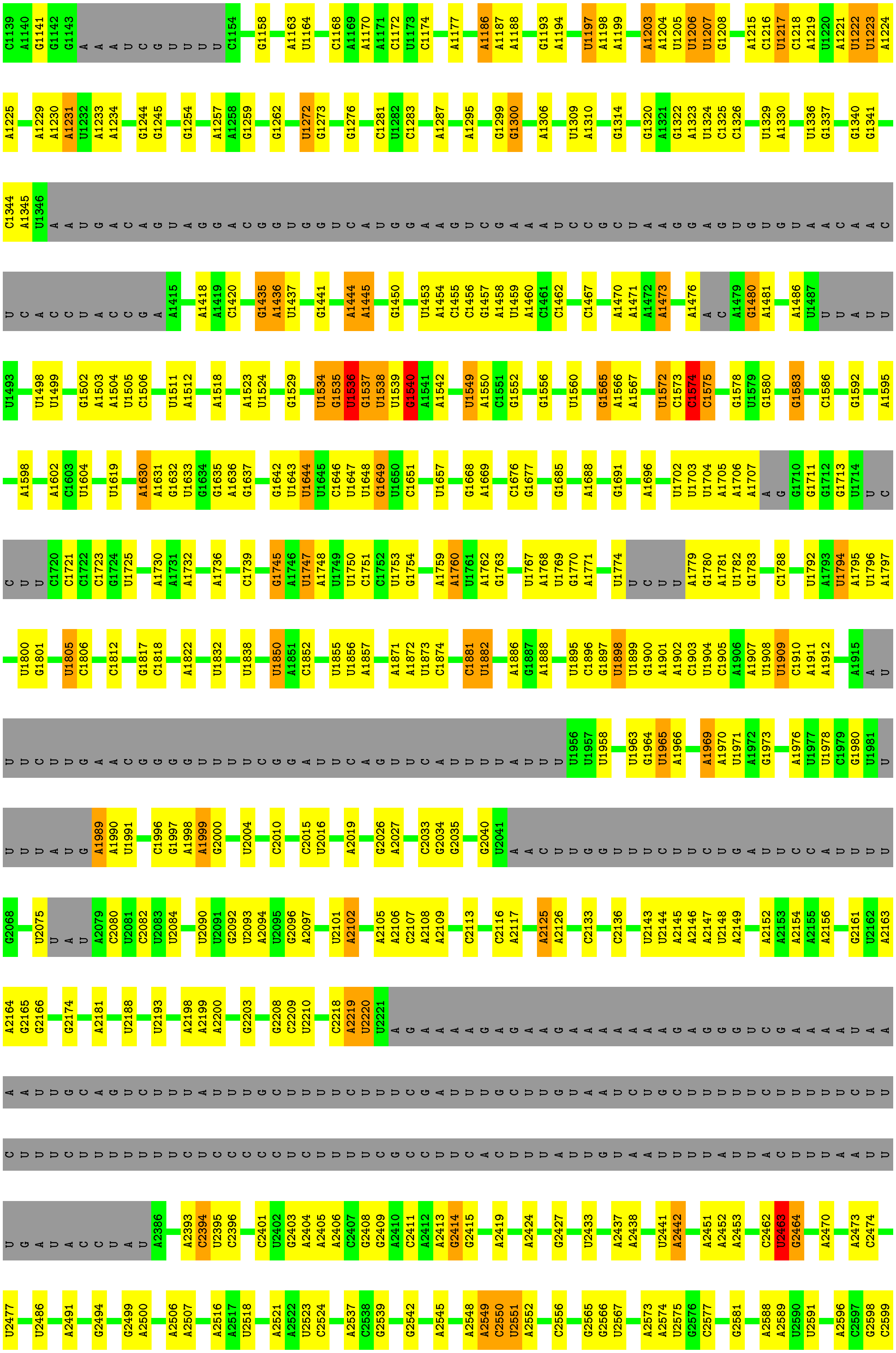
3 Residue-property plots (i)

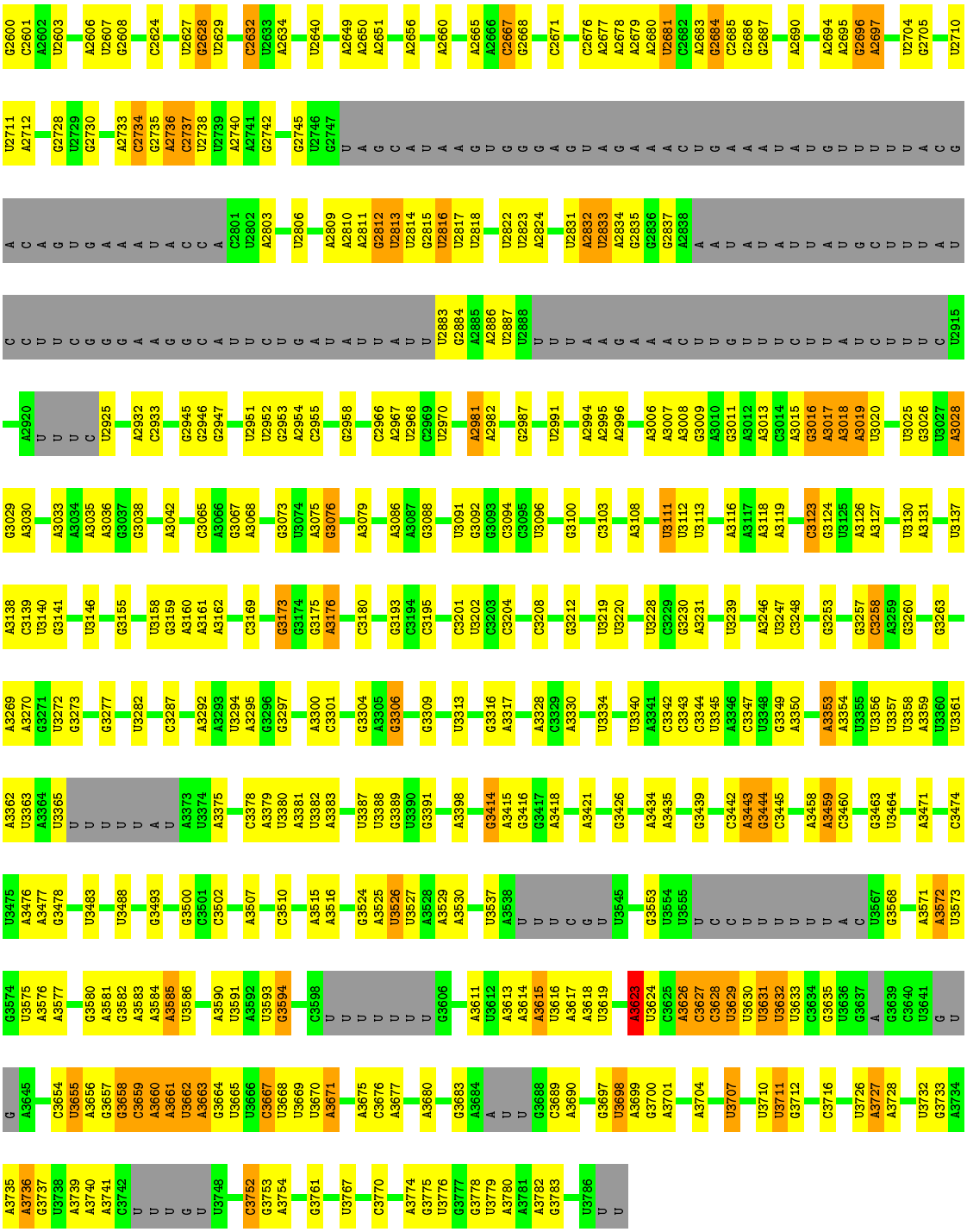
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. 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: 28S ribosomal RNA

Chain A:

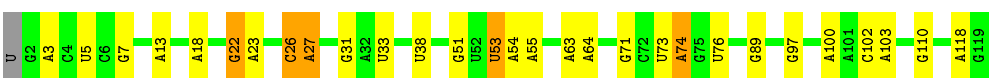



C1139 A1140 G1141 G1142 G1143 A A A U C G U U U U C1154 G1158 A1163 U1164 C1168 A1169 A1170 A1171 C1172 U1173 C1174 A1177 A1186 A1187 A1188 G1193 A1194 U1197 A1198 A1199 A1203 A1204 U1205 U1206 U1207 G1208 A1215 C1216 U1217 C1218 A1219 U1220 A1221 U1222 U1223 A1224
A1225 A1229 A1230 A1231 U1232 A1233 A1234 G1244 G1245 G1254 A1257 A1258 G1259 G1262 U1272 G1273 G1276 C1281 U1282 C1283 A1287 A1295 G1299 G1300 A1306 U1309 A1310 G1314 G1320 A1321 G1322 A1323 U1324 C1325 C1326 U1329 A1330 U1336 G1337 G1340 G1341
C1344 A1345 U1346 A A U G A C A G G U A G G A C G G U G G U C A U G G A A G U C G G A A A U C C G C U A A G G A G U G U G U A A C A A C
U C A C C U A C C G A A1415 A1418 A1419 C1420 G1435 A1436 U1437 G1441 A1444 A1445 G1450 U1453 A1454 C1455 C1456 G1457 A1458 U1459 A1460 C1461 C1462 C1467 A1470 A1471 A1472 A1473 A1476 A C A1479 G1480 A1481 A1486 U1487 U U A U U
U1493 U1498 U1499 G1502 A1503 A1504 U1505 C1506 U1511 A1512 A1518 A1523 U1524 G1529 U1534 G1535 U1536 G1537 U1538 U1539 G1540 A1541 A1542 U1549 A1550 C1551 G1552 G1556 U1560 G1565 A1566 A1567 U1572 C1573 C1574 C1575 G1578 U1579 G1580 G1583 C1586 G1592 A1595
A1598 A1602 C1603 U1604 U1619 A1630 A1631 G1632 U1633 G1634 G1635 A1636 G1637 G1642 U1643 U1644 U1645 C1646 U1647 U1648 G1649 U1650 C1651 U1657 G1668 A1669 C1676 G1677 G1685 A1688 G1691 A1696 U1702 U1703 U1704 A1705 A1706 A1707 A G G1710 G1711 G1712 G1713 U1714 U C
C U U C1720 C1721 C1722 C1723 G1724 U1725 A1730 A1731 A1732 A1736 C1739 G1745 A1746 U1747 A1748 U1749 U1750 C1751 C1752 U1753 G1754 A1759 A1760 U1761 A1762 G1763 U1767 A1768 U1769 G1770 A1771 U1774 U C U U A1779 G1780 A1781 U1782 G1783 C1788 U1792 A1793 U1794 A1795 U1796 A1797
U1800 G1801 U1805 C1806 C1812 G1817 C1818 A1822 U1832 U1838 U1850 A1851 C1852 U1855 U1856 A1857 A1871 A1872 U1873 C1874 C1881 U1882 A1886 G1887 A1888 U1895 C1896 G1897 U1898 U1899 G1900 A1901 A1902 C1903 U1904 C1905 A1906 A1907 U1908 U1909 C1910 A1911 A1912 A1915 A U
U U C U U G A A C G G G G U U U C G G A U U C A G U U C A U U U U A U U U U1956 U1957 U1958 U1963 G1964 U1965 A1966 A1969 A1970 U1971 A1972 G1973 A1976 U1977 U1978 C1979 G1980 U1981 U
U U U A U G A1989 A1990 U1991 C1996 G1997 A1998 A1999 G2000 U2004 C2010 C2015 U2016 A2019 G2026 A2027 C2033 G2034 G2035 G2040 U2041 A A C U U G G U U U C U U C U G A U U C C A U U U U
G2068 U2075 U A U A2079 C2080 U2081 C2082 U2083 U2084 U2090 U2091 G2092 U2093 A2094 U2095 G2096 A2097 U2101 A2102 A2105 A2106 C2107 A2108 A2109 C2113 C2116 A2117 A2125 A2126 C2133 C2136 U2143 U2144 A2145 A2146 A2147 U2148 A2149 A2152 A2153 A2154 A2155 A2156 G2161 U2162 A2163
A2164 G2165 G2166 G2174 A2181 U2188 U2193 A2198 A2199 A2200 G2203 G2208 C2209 U2210 C2218 A2219 U2220 U2221 A G A A A A G A G A A G A A A A A G A G G G U C G A A A A U A A
A A U U G C A G U C U U U A U U U G C U U U U C U U U C G A U U U G C U U G U A A U C U G C U U U U C U U U U C U U
C U U U C U U U U U U U C U C C C C C U C U U U U C G C C U U C A C U U U A U U G U A A U U U U A U U A C U U U A A U U
U G A U A C C U A U A2386 A2393 C2394 U2395 C2396 C2401 U2402 G2403 A2404 A2405 A2406 C2407 G2408 G2409 A2410 C2411 A2412 A2413 G2414 G2415 A2419 A2424 G2427 U2433 A2437 A2438 U2441 A2442 A2451 A2452 A2453 C2462 U2463 G2464 A2470 A2473 C2474
U2477 U2486 A2491 G2494 G2499 A2500 A2506 A2507 A2516 A2517 U2518 A2521 A2522 U2523 C2524 A2537 C2538 G2539 G2542 A2545 A2548 A2549 C2550 U2551 A2552 C2556 G2565 G2566 U2567 A2573 A2574 U2575 G2576 C2577 G2581 A2588 A2589 U2590 U2591 A2596 C2597 G2598 C2599



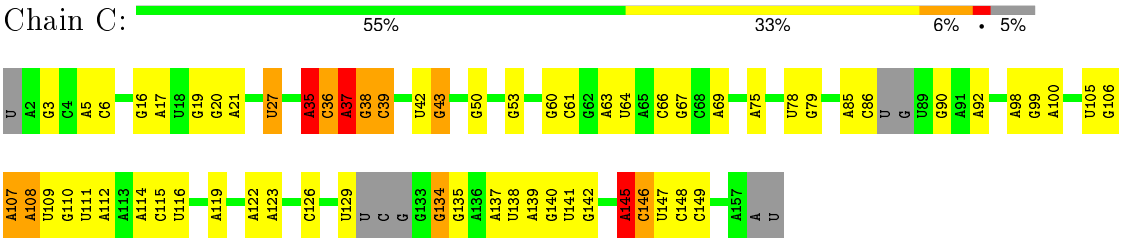
• Molecule 2: 5S ribosomal RNA

Chain B:



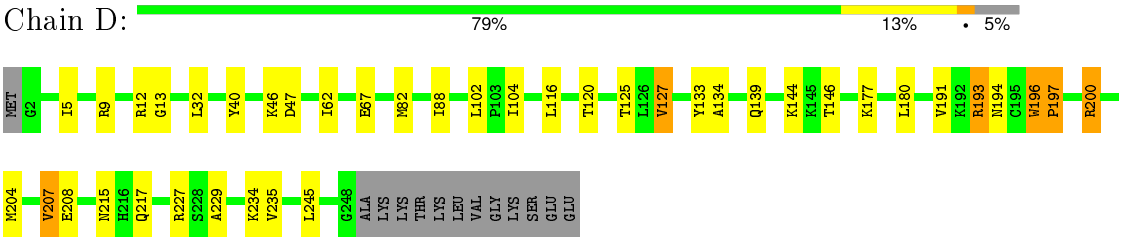
• Molecule 3: 5.8S ribosomal RNA

Chain C:



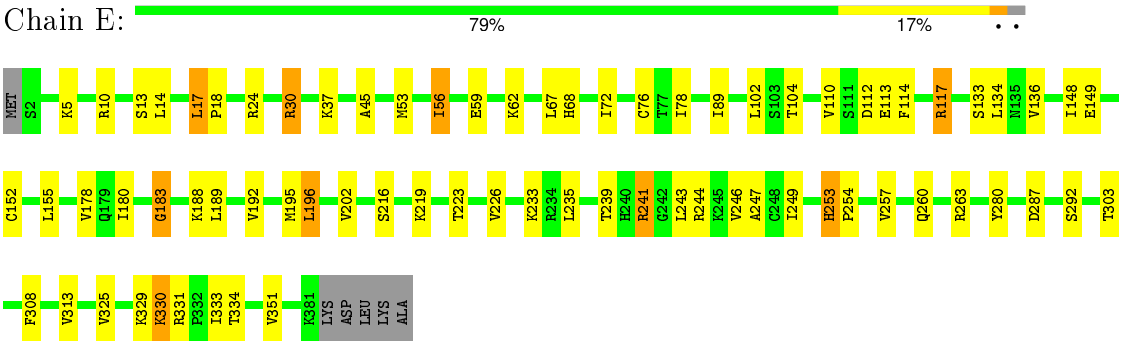
- Molecule 4: 60S ribosomal protein uL2

Chain D:



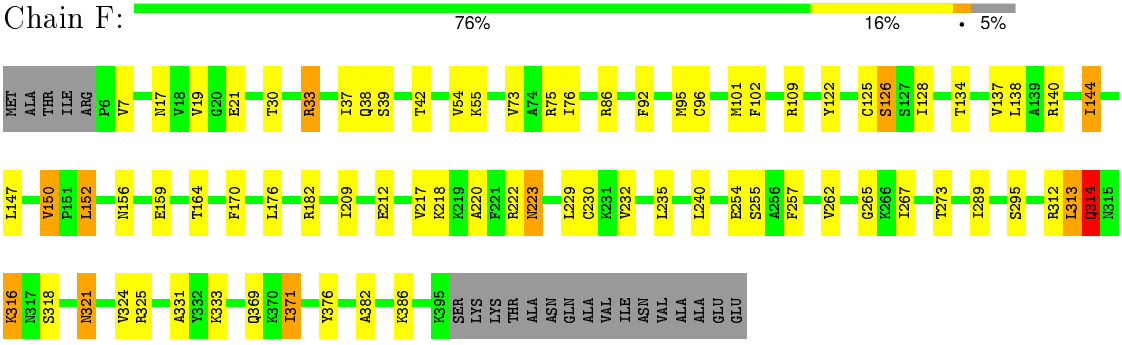
- Molecule 5: 60S ribosomal protein uL3

Chain E:



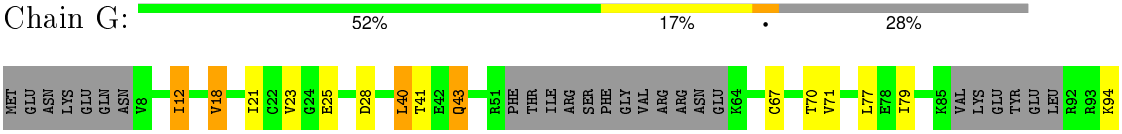
- Molecule 6: 60S ribosomal protein uL4

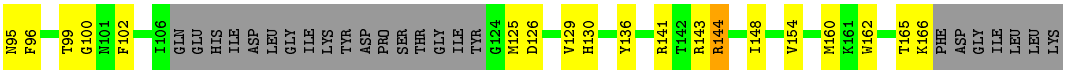
Chain F:



- Molecule 7: 60S ribosomal protein uL5

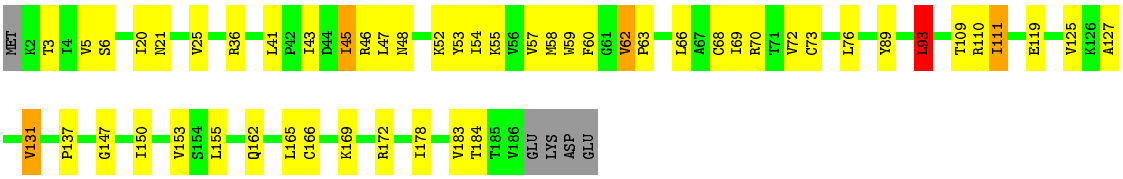
Chain G:





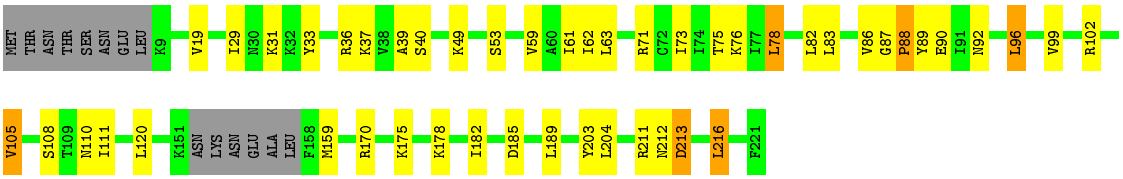
- Molecule 8: 60S ribosomal protein uL6

Chain H:



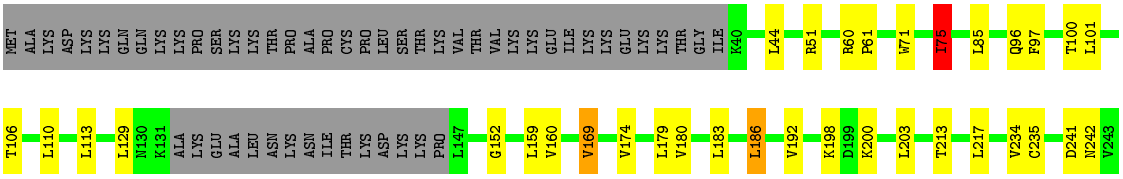
- Molecule 9: 60S ribosomal protein eL6

Chain I:



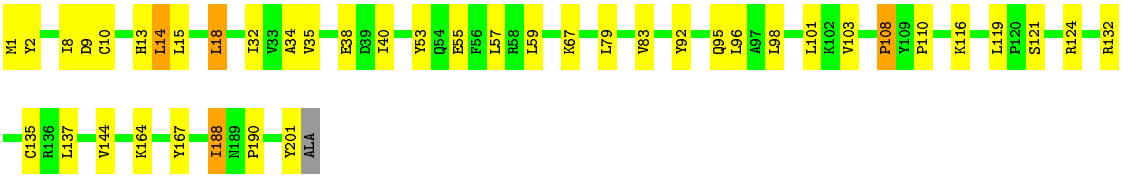
- Molecule 10: 60S ribosomal protein eL8

Chain J:



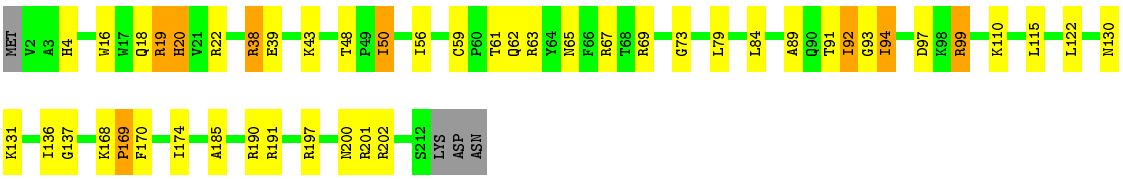
- Molecule 11: 60S ribosomal protein uL13

Chain K:



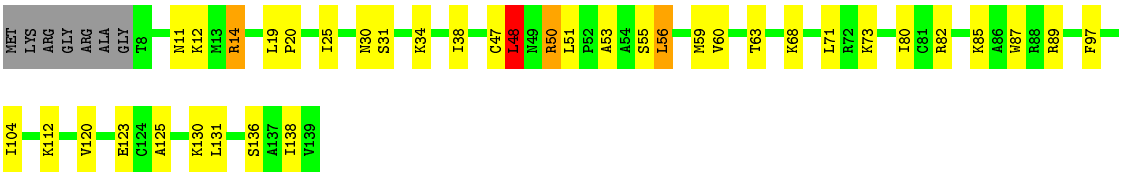
- Molecule 12: 60S ribosomal protein eL13

Chain L:



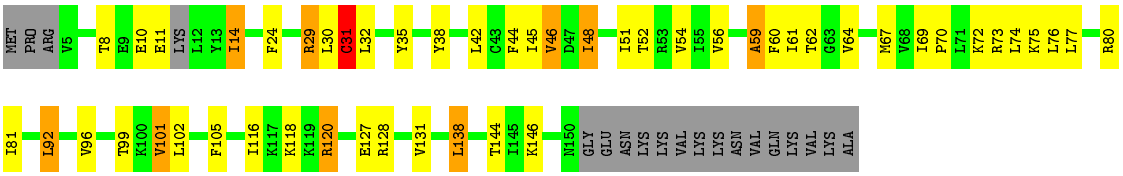
• Molecule 13: 60S ribosomal protein uL14

Chain M:



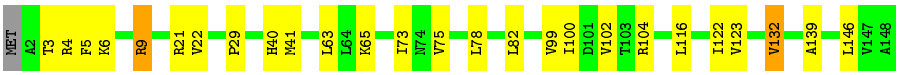
• Molecule 14: 60S ribosomal protein eL14

Chain N:



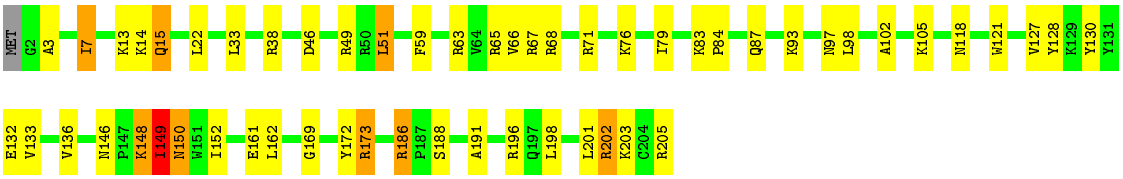
• Molecule 15: 60S ribosomal protein uL15

Chain O:



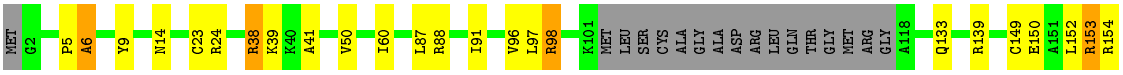
• Molecule 16: 60S ribosomal protein eL15

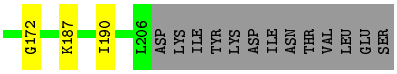
Chain P:



• Molecule 17: 60S ribosomal protein uL16

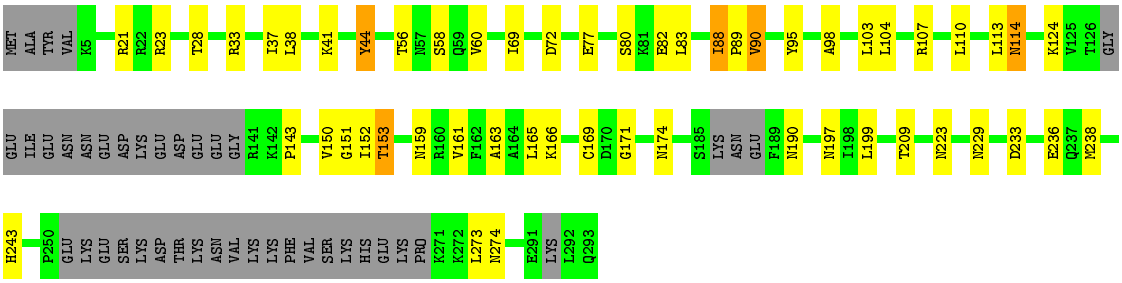
Chain Q:





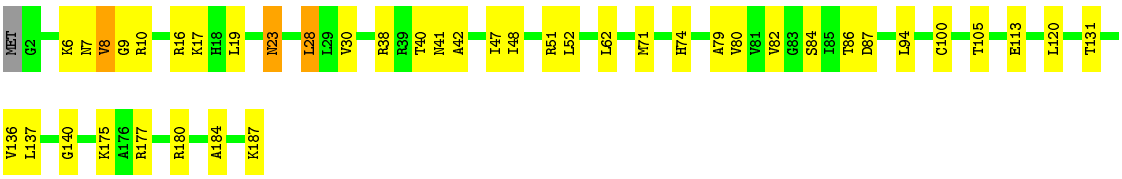
- Molecule 18: 60S ribosomal protein uL18

Chain R:



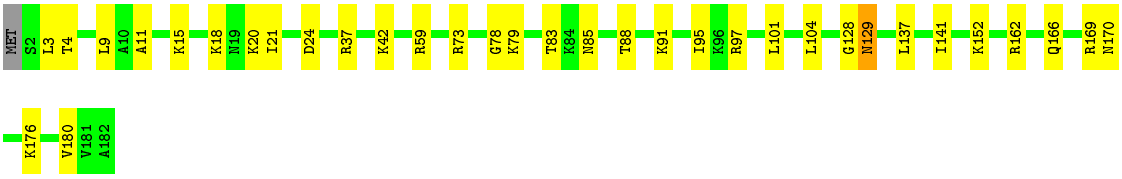
- Molecule 19: 60S ribosomal protein eL18

Chain S:



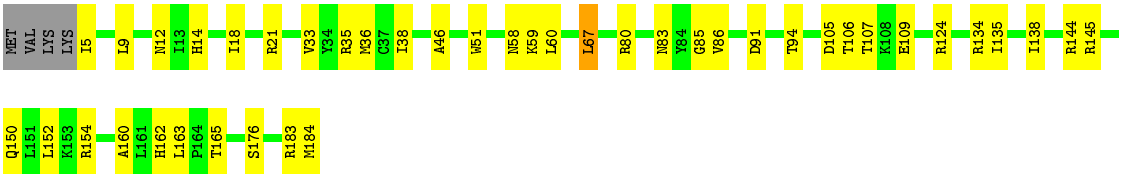
- Molecule 20: 60S ribosomal protein eL19

Chain T:



- Molecule 21: 60S ribosomal protein eL20

Chain U:

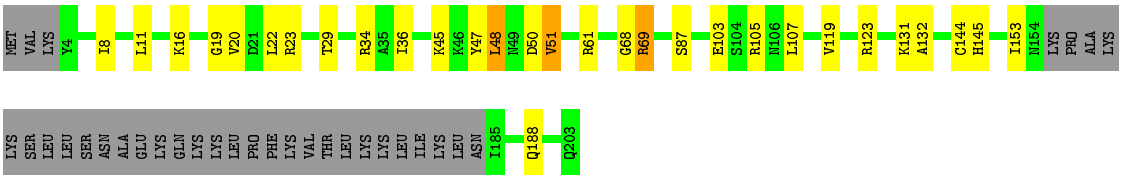


- Molecule 22: 60S ribosomal protein eL21

Chain V:

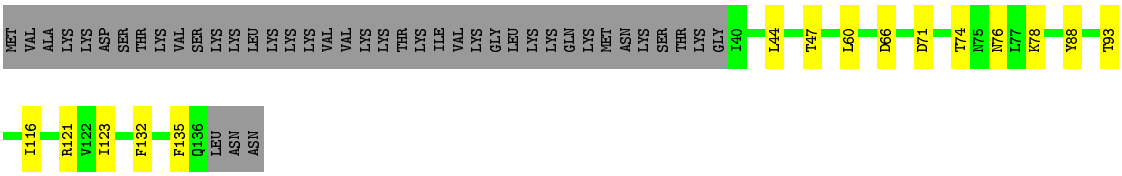
• Molecule 23: 60S ribosomal protein uL22

Chain W:



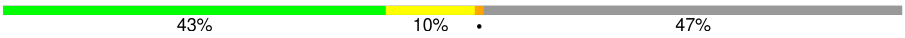
• Molecule 24: 60S ribosomal protein eL22

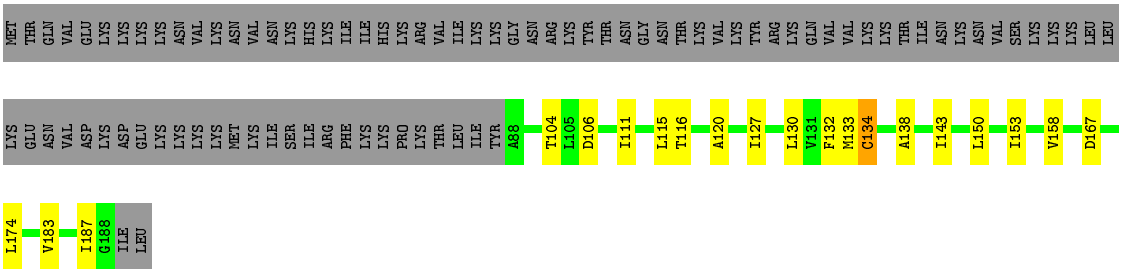
Chain X:



• Molecule 25: 60S ribosomal protein uL23

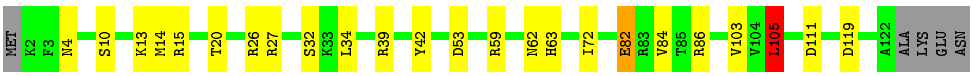
Chain Y:





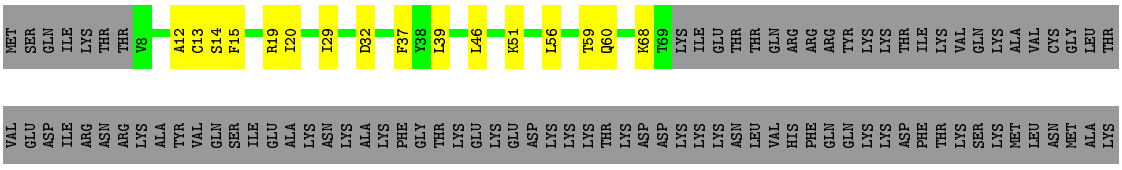
• Molecule 26: 60S ribosomal protein uL24

Chain Z:



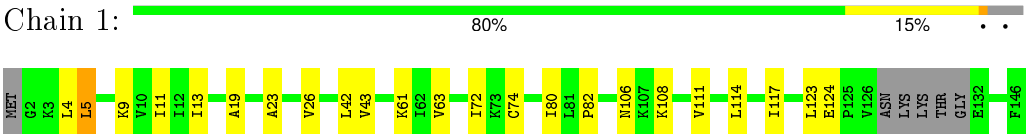
• Molecule 27: 60S ribosomal protein eL24

Chain 0:



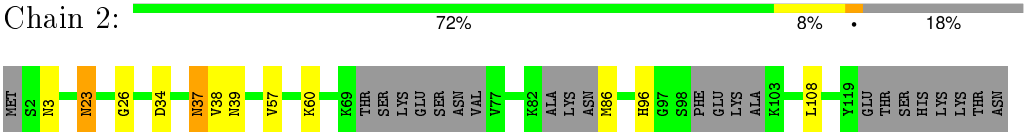
- Molecule 28: 60S ribosomal protein eL27

Chain 1:



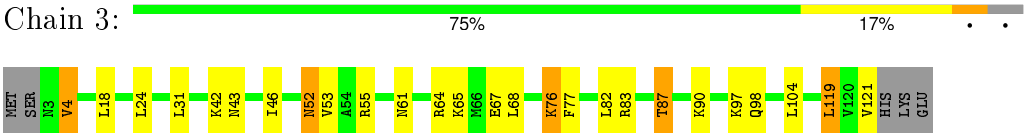
- Molecule 29: 60S ribosomal protein eL28

Chain 2:



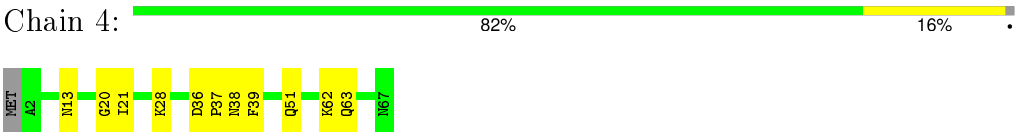
- Molecule 30: 60S ribosomal protein uL29

Chain 3:



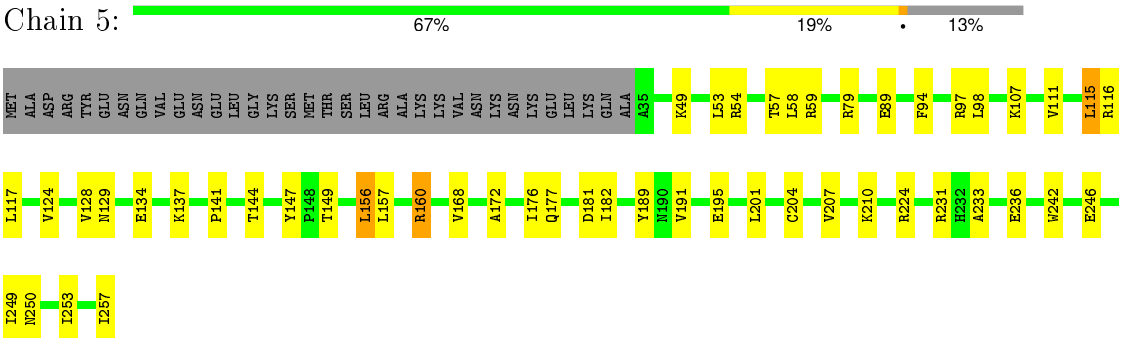
- Molecule 31: 60S ribosomal protein eL29

Chain 4:



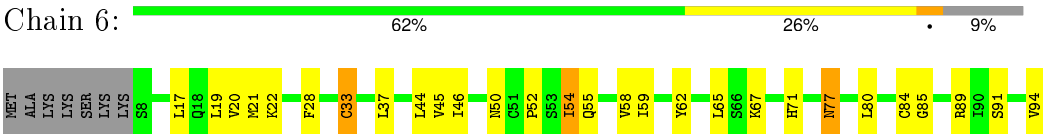
- Molecule 32: 60S ribosomal protein uL30

Chain 5:



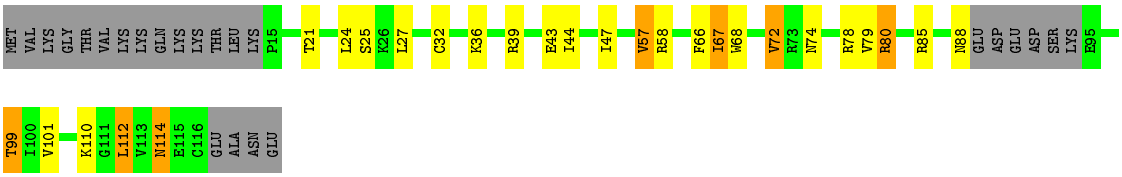
- Molecule 33: 60S ribosomal protein eL30

Chain 6:



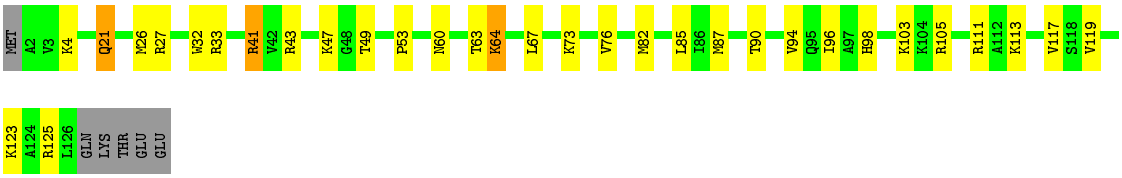
- Molecule 34: 60S ribosomal protein eL31

Chain 7:



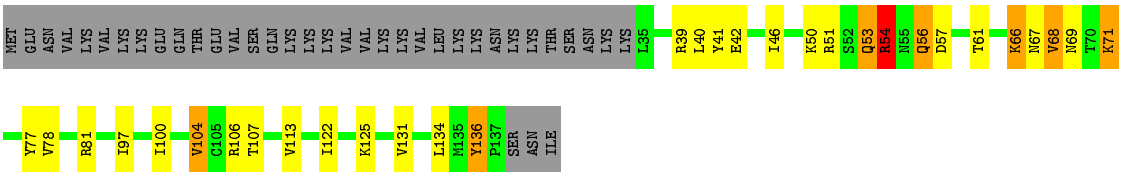
- Molecule 35: 60S ribosomal protein eL32

Chain 8:



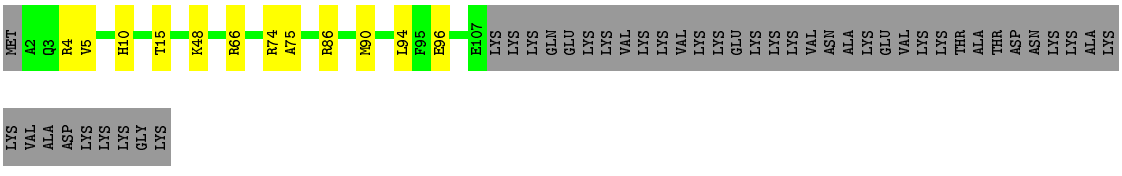
- Molecule 36: 60S ribosomal protein eL33

Chain 9:



- Molecule 37: 60S ribosomal protein eL34

Chain a:

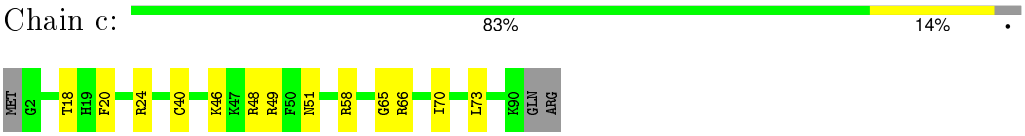


- Molecule 38: 60S ribosomal protein eL36

Chain b:

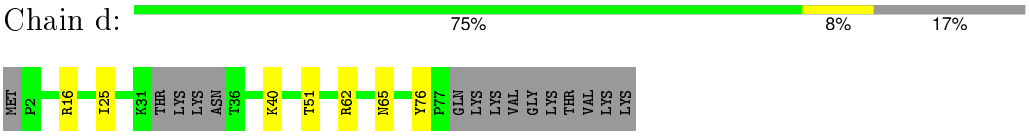
- Molecule 39: 60S ribosomal protein eL37

Chain c:



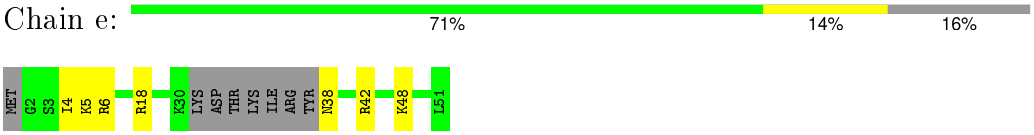
• Molecule 40: 60S ribosomal protein eL38

Chain d:



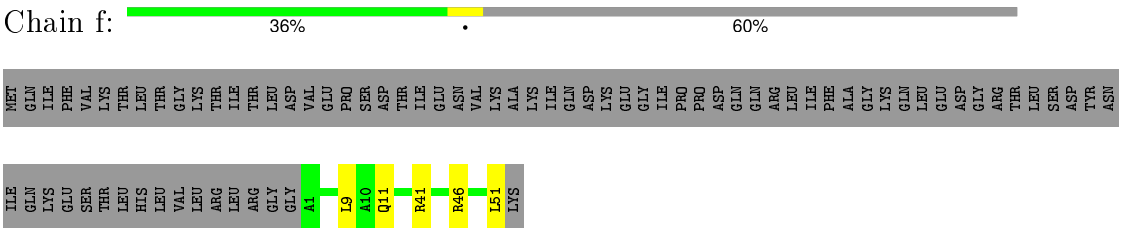
• Molecule 41: 60S ribosomal protein eL39

Chain e:



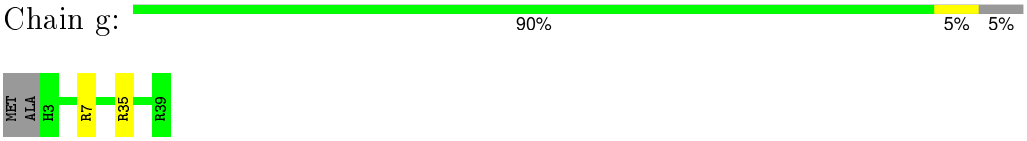
• Molecule 42: 60S ribosomal protein eL40

Chain f:



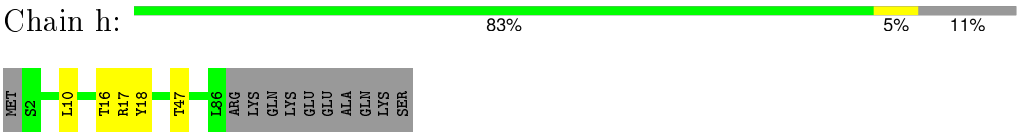
• Molecule 43: 60S ribosomal protein eL41

Chain g:



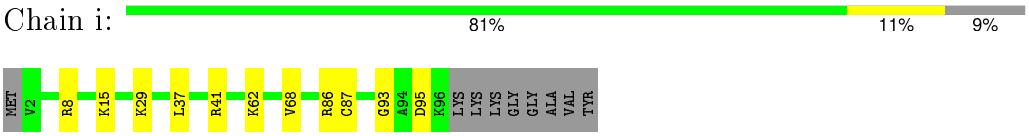
• Molecule 44: 60S ribosomal protein eL43

Chain h:



• Molecule 45: 60S ribosomal protein eL44

Chain i:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	105247	Depositor
Resolution determination method	FSC 0.143 gold-standard	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	78000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.30	1/75991 (0.0%)	0.73	35/118299 (0.0%)
10	J	0.41	0/1901	0.74	0/2537
11	K	0.45	0/1689	0.81	0/2260
12	L	0.44	0/1793	0.80	0/2387
13	M	0.45	0/1012	0.73	0/1363
14	N	0.45	0/1213	0.81	0/1616
15	O	0.44	0/1199	0.76	0/1597
16	P	0.44	0/1735	0.83	2/2320 (0.1%)
17	Q	0.41	0/1579	0.73	0/2113
18	R	0.43	0/2074	0.79	0/2773
19	S	0.43	0/1530	0.80	0/2040
2	B	0.26	0/2826	0.69	0/4404
20	T	0.46	0/1521	0.80	0/2012
21	U	0.43	0/1526	0.73	0/2043
22	V	0.40	0/1300	0.70	0/1732
23	W	0.45	0/1338	0.78	0/1793
24	X	0.40	0/841	0.66	0/1125
25	Y	0.41	0/805	0.74	0/1074
26	Z	0.39	0/1012	0.78	1/1339 (0.1%)
27	0	0.46	0/533	0.76	0/711
28	1	0.37	0/1151	0.68	0/1531
29	2	0.41	0/839	0.64	0/1114
3	C	0.28	0/3608	0.74	4/5615 (0.1%)
30	3	0.44	0/1004	0.82	0/1329
31	4	0.43	0/564	0.77	0/737
32	5	0.45	0/1917	0.83	0/2562
33	6	0.42	0/748	0.83	0/1001
34	7	0.44	0/805	0.82	0/1073
35	8	0.45	0/1053	0.79	0/1399
36	9	0.48	0/864	0.87	0/1160
37	a	0.38	0/871	0.77	0/1161
38	b	0.46	0/762	0.83	0/1008

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
39	c	0.47	0/718	0.84	0/946
4	D	0.48	0/1901	0.82	1/2544 (0.0%)
40	d	0.42	0/611	0.71	0/812
41	e	0.48	0/396	0.84	0/521
42	f	0.45	0/418	0.83	0/556
43	g	0.45	0/347	0.95	0/448
44	h	0.43	0/667	0.73	0/887
45	i	0.41	0/788	0.71	0/1032
5	E	0.43	0/3129	0.74	0/4195
6	F	0.42	0/3144	0.80	2/4205 (0.0%)
7	G	0.43	0/1020	0.80	0/1349
8	H	0.42	0/1485	0.77	1/2009 (0.0%)
9	I	0.41	0/1707	0.75	0/2274
All	All	0.36	1/133935 (0.0%)	0.75	46/197006 (0.0%)

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
11	K	0	1
14	N	0	1
23	W	0	1
32	5	0	1
33	6	0	1
36	9	0	1
39	c	0	1
4	D	0	1
5	E	0	3
6	F	0	1
9	I	0	1
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2463	U	O3'-P	-5.46	1.54	1.61

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1805	U	C2'-C3'-O3'	8.69	128.62	109.50
1	A	289	A	C2'-C3'-O3'	8.40	127.98	109.50
3	C	145	A	C2'-C3'-O3'	8.31	127.79	109.50
3	C	37	A	C2'-C3'-O3'	8.03	127.16	109.50
1	A	652	A	C2'-C3'-O3'	7.52	126.05	109.50
1	A	215	C	C2'-C3'-O3'	7.44	125.86	109.50
1	A	1536	U	C2'-C3'-O3'	7.09	125.10	109.50
1	A	703	U	C2'-C3'-O3'	6.89	124.73	113.70
1	A	505	A	C2'-C3'-O3'	6.85	124.66	113.70
1	A	1197	U	C2'-C3'-O3'	6.71	124.43	113.70
1	A	1999	A	C2'-C3'-O3'	6.70	124.41	113.70
26	Z	105	LEU	CA-CB-CG	6.39	129.99	115.30
1	A	1540	G	N9-C1'-C2'	6.31	122.20	114.00
1	A	683	A	C4'-C3'-O3'	6.30	125.61	113.00
3	C	134	G	C2'-C3'-O3'	6.26	123.72	113.70
8	H	93	LEU	CA-CB-CG	6.13	129.40	115.30
1	A	859	C	C2'-C3'-O3'	6.11	123.47	113.70
1	A	581	C	C2'-C3'-O3'	6.09	123.44	113.70
1	A	3623	A	C2'-C3'-O3'	6.03	123.34	113.70
1	A	504	A	C2'-C3'-O3'	5.97	123.26	113.70
1	A	621	C	C2'-C3'-O3'	5.86	123.08	113.70
16	P	173	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	A	91	G	C2'-C3'-O3'	5.79	122.96	113.70
1	A	3414	G	C2'-C3'-O3'	5.79	122.96	113.70
1	A	1989	A	C2'-C3'-O3'	5.77	122.94	113.70
1	A	514	C	C2'-C3'-O3'	5.72	122.85	113.70
1	A	607	A	C2'-C3'-O3'	5.71	122.83	113.70
1	A	10	G	C2'-C3'-O3'	5.59	122.64	113.70
1	A	1540	G	O4'-C1'-C2'	-5.51	100.29	105.80
6	F	313	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	3444	G	C2'-C3'-O3'	5.38	122.32	113.70
1	A	1747	U	N1-C1'-C2'	5.35	120.95	114.00
1	A	270	U	C2'-C3'-O3'	5.31	122.19	113.70
1	A	1574	C	C4'-C3'-O3'	5.26	123.52	113.00
4	D	200	ARG	NE-CZ-NH2	5.25	122.93	120.30
1	A	2394	C	C2'-C3'-O3'	5.25	122.10	113.70
1	A	773	A	C4'-C3'-O3'	5.25	123.49	113.00
1	A	764	G	C2'-C3'-O3'	5.23	122.07	113.70
6	F	33	ARG	NE-CZ-NH2	5.15	122.87	120.30
1	A	664	U	C4'-C3'-O3'	5.13	123.25	113.00
1	A	308	U	C4'-C3'-O3'	5.11	123.23	113.00
16	P	173	ARG	NE-CZ-NH1	5.10	122.85	120.30
3	C	35	A	C2'-C3'-O3'	5.09	121.85	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2816	U	C2'-C3'-O3'	5.09	121.84	113.70
1	A	684	G	C4'-C3'-O3'	-5.08	98.72	109.40
1	A	580	A	C2'-C3'-O3'	5.03	121.75	113.70

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	5	89	GLU	Peptide
33	6	52	PRO	Peptide
36	9	136	TYR	Peptide
4	D	196	TRP	Peptide
5	E	17	LEU	Peptide
5	E	195	MET	Peptide
5	E	253	HIS	Peptide
6	F	150	VAL	Peptide
9	I	87	GLY	Peptide
11	K	108	PRO	Peptide
14	N	59	ALA	Peptide
23	W	131	LYS	Peptide
39	c	20	PHE	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	A	67935	0	34190	456	0
2	B	2525	0	1274	7	0
3	C	3224	0	1630	20	0
4	D	1866	0	1964	18	0
5	E	3061	0	3205	40	0
6	F	3094	0	3333	37	0
7	G	1010	0	1073	14	0
8	H	1460	0	1532	19	0
9	I	1684	0	1849	15	0
10	J	1873	0	2055	10	0
11	K	1659	0	1782	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	1761	0	1895	20	0
13	M	996	0	1044	17	0
14	N	1197	0	1312	28	0
15	O	1172	0	1230	16	0
16	P	1697	0	1802	30	0
17	Q	1544	0	1582	11	0
18	R	2045	0	2129	14	0
19	S	1502	0	1636	17	0
20	T	1505	0	1671	14	0
21	U	1496	0	1556	21	0
22	V	1275	0	1355	7	0
23	W	1318	0	1319	10	0
24	X	824	0	882	4	0
25	Y	796	0	850	12	0
26	Z	1000	0	1099	4	0
27	0	521	0	539	6	0
28	1	1134	0	1245	9	0
29	2	830	0	887	3	0
30	3	994	0	1121	9	0
31	4	555	0	599	1	0
32	5	1879	0	2005	21	0
33	6	740	0	763	9	0
34	7	793	0	869	10	0
35	8	1036	0	1139	12	0
36	9	844	0	886	14	0
37	a	858	0	911	0	0
38	b	756	0	842	0	0
39	c	705	0	754	0	0
40	d	603	0	686	0	0
41	e	388	0	421	0	0
42	f	413	0	449	0	0
43	g	342	0	388	0	0
44	h	658	0	724	0	0
45	i	778	0	857	0	0
46	A	153	0	0	0	0
46	B	3	0	0	0	0
46	C	5	0	0	0	0
46	M	1	0	0	0	0
46	Q	1	0	0	0	0
47	a	1	0	0	0	0
47	c	1	0	0	0	0
47	f	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	h	1	0	0	0	0
47	i	1	0	0	0	0
All	All	124514	0	91334	867	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 4.

All (867) 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)
1:A:3626:A:C6	1:A:3660:A:C6	2.12	1.37
1:A:3626:A:C2	1:A:3660:A:C2	2.31	1.19
1:A:3123:C:O2	12:L:202:ARG:NH2	1.80	1.14
1:A:3626:A:C5	1:A:3660:A:C6	2.38	1.12
1:A:3016:G:O6	1:A:3019:A:N6	1.87	1.07
1:A:2737:C:H2'	1:A:2738:U:C6	1.90	1.06
1:A:3626:A:C4	1:A:3660:A:N1	2.29	1.01
1:A:3626:A:C5	1:A:3660:A:N6	2.29	1.00
1:A:2733:A:C2'	1:A:2734:C:H5'	1.91	1.00
1:A:2812:G:C2	1:A:2813:U:C2	2.49	1.00
1:A:1574:C:O2'	1:A:1575:C:O5'	1.80	0.96
1:A:3654:C:C4	1:A:3655:U:O4	2.19	0.94
1:A:3626:A:C5	1:A:3660:A:N1	2.36	0.94
1:A:2733:A:H2'	1:A:2734:C:H5'	1.51	0.93
1:A:3629:U:H2'	1:A:3630:U:C6	2.03	0.93
1:A:3654:C:C5	1:A:3655:U:O4	2.21	0.93
1:A:3654:C:C4	1:A:3655:U:C4	2.59	0.90
1:A:2813:U:H2'	1:A:2814:U:C5	2.07	0.90
1:A:3626:A:C6	1:A:3660:A:N6	2.39	0.89
1:A:1630:A:O2'	1:A:2125:A:H1'	1.72	0.89
1:A:3630:U:H2'	1:A:3631:U:H5'	1.55	0.88
1:A:3632:U:O2'	1:A:3633:U:H5'	1.74	0.88
1:A:3626:A:N6	1:A:3659:C:N3	2.21	0.87
12:L:94:ILE:HD12	12:L:115:LEU:HD21	1.57	0.87
1:A:3626:A:C6	1:A:3660:A:C5	2.62	0.87
1:A:3629:U:H3	1:A:3656:A:H2	1.20	0.86
1:A:1910:C:H2'	1:A:1911:A:C8	2.11	0.85
1:A:3018:A:C8	1:A:3018:A:H5"	2.11	0.85
1:A:3629:U:O2'	1:A:3630:U:H5'	1.77	0.85
1:A:3016:G:H3'	1:A:3017:A:H5"	1.56	0.85
1:A:1534:U:O2'	1:A:1535:G:O5'	1.93	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3628:C:O2	1:A:3657:G:N2	2.09	0.84
1:A:3655:U:O2'	1:A:3656:A:H5'	1.79	0.83
1:A:2734:C:H2'	1:A:2735:G:O4'	1.80	0.82
1:A:1574:C:HO2'	1:A:1575:C:P	2.02	0.81
36:9:50:LYS:O	36:9:56:GLN:O	1.99	0.81
1:A:3626:A:N3	1:A:3660:A:C2	2.49	0.80
1:A:3018:A:H8	1:A:3018:A:H5"	1.44	0.80
1:A:3660:A:H2'	1:A:3661:A:C8	2.16	0.80
1:A:3655:U:H2'	1:A:3656:A:C8	2.17	0.80
1:A:2737:C:H6	1:A:2737:C:C5'	1.95	0.79
1:A:3629:U:N3	1:A:3656:A:H2	1.81	0.78
1:A:2812:G:O2'	1:A:2813:U:O5'	2.01	0.77
1:A:3629:U:H2'	1:A:3630:U:H6	1.45	0.77
22:V:120:ALA:HB2	22:V:127:ILE:HD12	1.65	0.77
1:A:3628:C:H2'	1:A:3629:U:C6	2.19	0.77
11:K:34:ALA:HB3	11:K:103:VAL:HG12	1.67	0.76
1:A:3628:C:H2'	1:A:3629:U:C5	2.19	0.76
1:A:3629:U:C2	1:A:3630:U:C5	2.74	0.76
1:A:2813:U:H2'	1:A:2814:U:C6	2.20	0.75
19:S:51:ARG:HB3	19:S:82:VAL:HG21	1.67	0.75
1:A:257:U:O2'	1:A:258:U:O4'	2.03	0.75
1:A:3629:U:N3	1:A:3630:U:C4	2.55	0.74
7:G:41:THR:HG21	7:G:71:VAL:HG11	1.69	0.74
1:A:3629:U:N3	1:A:3656:A:C2	2.51	0.73
1:A:3626:A:C2	1:A:3660:A:N1	2.57	0.73
1:A:257:U:H2'	1:A:258:U:C6	2.23	0.73
1:A:2736:A:N6	1:A:2813:U:O4	2.19	0.73
1:A:3626:A:C6	1:A:3660:A:N1	2.56	0.73
1:A:2685:C:O2'	5:E:263:ARG:NH2	2.21	0.73
1:A:3626:A:N6	1:A:3660:A:C6	2.58	0.72
1:A:3654:C:C5	1:A:3655:U:C4	2.77	0.72
36:9:78:VAL:O	36:9:104:VAL:O	2.08	0.72
19:S:51:ARG:HB2	19:S:82:VAL:HG11	1.71	0.71
1:A:2736:A:H2'	1:A:2737:C:C6	2.25	0.71
1:A:3626:A:N1	1:A:3660:A:C6	2.59	0.71
1:A:63:A:OP1	16:P:173:ARG:NH2	2.24	0.70
1:A:257:U:H4'	1:A:258:U:OP1	1.90	0.70
13:M:125:ALA:HB2	13:M:138:ILE:HD11	1.72	0.70
1:A:3631:U:H2'	1:A:3632:U:O4'	1.91	0.70
25:Y:143:ILE:HG21	25:Y:158:VAL:HG21	1.74	0.70
1:A:3660:A:O2'	1:A:3661:A:O4'	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:C:OP1	12:L:38:ARG:NH1	2.25	0.69
1:A:2736:A:C2'	1:A:2737:C:H5'	2.22	0.69
1:A:3658:G:N2	1:A:3659:C:H1'	2.08	0.68
1:A:998:U:H4'	23:W:132:ALA:HB2	1.76	0.68
1:A:3630:U:C2'	1:A:3631:U:H5'	2.24	0.68
1:A:2812:G:C6	1:A:2813:U:C4	2.81	0.68
16:P:121:TRP:O	16:P:130:TYR:O	2.12	0.68
1:A:3628:C:H3'	1:A:3629:U:C5	2.29	0.67
1:A:3656:A:O2'	1:A:3657:G:H5'	1.94	0.67
1:A:3613:A:N6	1:A:3614:A:N1	2.43	0.67
1:A:2812:G:N1	1:A:2813:U:C2	2.62	0.66
1:A:3658:G:H1'	1:A:3659:C:O5'	1.96	0.66
8:H:66:LEU:O	8:H:69:ILE:HG22	1.95	0.66
6:F:128:ILE:HD11	6:F:235:LEU:HD13	1.77	0.66
12:L:79:LEU:HD11	12:L:94:ILE:HD11	1.78	0.65
1:A:3655:U:H2'	1:A:3656:A:H8	1.60	0.65
1:A:1216:C:H2'	1:A:1217:U:H5'	1.78	0.65
1:A:3626:A:N1	1:A:3660:A:C5	2.64	0.65
28:1:11:ILE:HG21	28:1:80:ILE:HD13	1.78	0.65
8:H:3:THR:HG21	8:H:66:LEU:HD11	1.78	0.65
5:E:149:GLU:HG3	5:E:189:LEU:HD13	1.79	0.64
1:A:3654:C:N4	1:A:3655:U:O4	2.29	0.64
1:A:1262:G:O2'	1:A:2981:A:N3	2.25	0.64
5:E:89:ILE:HG22	5:E:155:LEU:HD22	1.78	0.64
1:A:3656:A:H2'	1:A:3657:G:C8	2.32	0.64
12:L:20:HIS:HB2	16:P:198:LEU:HD23	1.79	0.64
5:E:249:ILE:HG21	5:E:257:VAL:HG22	1.80	0.64
1:A:3018:A:H8	1:A:3018:A:C5'	2.10	0.63
14:N:96:VAL:HG23	14:N:101:VAL:HG12	1.80	0.63
1:A:2814:U:O2'	1:A:2815:G:O4'	2.16	0.63
5:E:67:LEU:HD21	5:E:72:ILE:HD12	1.79	0.63
14:N:31:CYS:SG	14:N:45:ILE:HD11	2.39	0.63
1:A:257:U:C2'	1:A:258:U:C6	2.82	0.63
5:E:303:THR:HG21	5:E:313:VAL:HG13	1.80	0.63
1:A:2814:U:O2'	1:A:2815:G:O5'	2.17	0.63
6:F:147:LEU:HD13	6:F:152:LEU:HD12	1.80	0.63
1:A:3626:A:N6	1:A:3660:A:N6	2.48	0.62
1:A:10:G:O2'	1:A:11:A:OP1	2.12	0.62
1:A:3613:A:N6	1:A:3614:A:C6	2.66	0.62
1:A:3628:C:C3'	1:A:3629:U:C6	2.83	0.62
32:5:57:THR:HG23	32:5:195:GLU:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3632:U:O5'	1:A:3632:U:H6	1.82	0.62
16:P:169:GLY:HA2	16:P:172:TYR:CE2	2.34	0.62
1:A:2463:U:H2'	1:A:2464:G:O4'	2.00	0.62
30:3:87:THR:HG23	30:3:90:LYS:HB2	1.82	0.62
1:A:2733:A:H2'	1:A:2734:C:C6	2.35	0.62
4:D:196:TRP:CE3	4:D:197:PRO:HD3	2.35	0.62
1:A:755:A:OP2	19:S:105:THR:HG21	1.99	0.62
27:0:13:CYS:O	27:0:15:PHE:N	2.33	0.62
1:A:3016:G:N3	1:A:3016:G:H2'	2.14	0.61
19:S:71:MET:SD	19:S:79:ALA:HB2	2.40	0.61
34:7:27:LEU:HD13	34:7:43:GLU:HB3	1.82	0.61
1:A:3018:A:H4'	1:A:3018:A:OP1	1.99	0.61
1:A:1480:G:O6	1:A:1502:G:O6	2.17	0.61
1:A:2733:A:O2'	1:A:2734:C:H5'	2.00	0.61
1:A:1908:U:H2'	1:A:1909:U:H5'	1.83	0.61
35:8:94:VAL:CG2	35:8:119:VAL:HG22	2.31	0.61
1:A:257:U:H2'	1:A:258:U:C5	2.34	0.60
8:H:127:ALA:HB1	8:H:131:VAL:HG13	1.83	0.60
1:A:1444:A:C5	21:U:163:LEU:HD11	2.36	0.60
32:5:189:TYR:HB3	32:5:207:VAL:HG21	1.82	0.60
36:9:56:GLN:HA	36:9:56:GLN:HE21	1.67	0.60
1:A:3626:A:N3	1:A:3660:A:N1	2.49	0.60
24:X:47:THR:HG22	24:X:88:TYR:HB3	1.84	0.60
1:A:3626:A:N6	1:A:3659:C:C2	2.70	0.59
1:A:1542:A:OP1	35:8:98:HIS:NE2	2.34	0.59
13:M:47:CYS:SG	13:M:50:ARG:NH1	2.74	0.59
5:E:226:VAL:HG11	5:E:246:VAL:HG23	1.84	0.59
1:A:2736:A:N6	1:A:2813:U:H3	2.01	0.59
1:A:3628:C:C2'	1:A:3629:U:C5	2.85	0.59
1:A:257:U:O2'	1:A:258:U:C6	2.52	0.59
21:U:160:ALA:HB1	21:U:162:HIS:CE1	2.37	0.59
1:A:3626:A:N6	1:A:3660:A:C5	2.70	0.59
1:A:2812:G:N1	1:A:2813:U:N3	2.51	0.59
1:A:257:U:O2'	1:A:258:U:OP1	2.21	0.59
16:P:161:GLU:HG2	16:P:162:LEU:HD22	1.83	0.59
1:A:2812:G:C6	1:A:2813:U:N3	2.71	0.59
1:A:308:U:O2'	1:A:309:G:H8	1.85	0.59
1:A:1462:C:O2'	32:5:160:ARG:NH1	2.36	0.59
7:G:102:PHE:CE2	7:G:129:VAL:HG21	2.37	0.59
1:A:3629:U:H3'	1:A:3629:U:OP2	2.03	0.59
14:N:69:ILE:HD11	14:N:74:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:150:VAL:HG23	18:R:161:VAL:HG21	1.85	0.58
1:A:2736:A:H2'	1:A:2737:C:H5'	1.85	0.58
1:A:2463:U:C2	1:A:2464:G:C8	2.91	0.58
33:6:45:VAL:HG22	33:6:94:VAL:HG22	1.85	0.58
18:R:89:PRO:O	18:R:90:VAL:HG22	2.02	0.58
34:7:24:LEU:HD23	34:7:27:LEU:HD12	1.85	0.58
1:A:99:A:OP1	16:P:196:ARG:HD2	2.03	0.58
19:S:40:THR:O	19:S:42:ALA:N	2.36	0.58
1:A:3654:C:C6	1:A:3655:U:C5	2.92	0.58
1:A:3613:A:C6	1:A:3614:A:N1	2.71	0.58
12:L:92:ILE:HG22	12:L:93:GLY:H	1.66	0.58
1:A:3657:G:H8	1:A:3657:G:O5'	1.86	0.58
1:A:2812:G:O2'	1:A:2813:U:O4'	2.17	0.58
1:A:3524:G:N7	5:E:30:ARG:NH2	2.51	0.58
1:A:3628:C:C2'	1:A:3629:U:C6	2.85	0.58
17:Q:150:GLU:O	17:Q:153:ARG:HG3	2.04	0.58
3:C:35:A:H2'	3:C:36:C:O4'	2.04	0.58
1:A:3306:G:C2	5:E:247:ALA:HB1	2.37	0.58
13:M:68:LYS:HB3	13:M:71:LEU:HD23	1.86	0.57
1:A:645:A:OP1	9:I:31:LYS:HG3	2.05	0.57
1:A:685:U:H2'	1:A:685:U:O2	2.03	0.57
5:E:102:LEU:HD12	5:E:152:CYS:SG	2.45	0.57
1:A:3658:G:H1'	1:A:3659:C:P	2.44	0.57
1:A:1909:U:H2'	1:A:1910:C:C2	2.39	0.57
1:A:2812:G:N2	1:A:2813:U:C2	2.73	0.57
1:A:1910:C:H2'	1:A:1911:A:H8	1.68	0.57
1:A:2737:C:H2'	1:A:2738:U:H6	1.59	0.57
1:A:2736:A:O2'	1:A:2737:C:H5'	2.03	0.57
6:F:316:LYS:HB3	6:F:324:VAL:HG21	1.86	0.57
5:E:14:LEU:HD23	5:E:17:LEU:HD11	1.85	0.57
1:A:2812:G:C2	1:A:2813:U:N1	2.73	0.57
1:A:2813:U:C2'	1:A:2814:U:C6	2.87	0.57
1:A:308:U:O2'	1:A:309:G:P	2.63	0.56
24:X:121:ARG:NE	24:X:123:ILE:HD11	2.20	0.56
8:H:89:TYR:CE1	8:H:183:VAL:HG13	2.40	0.56
6:F:371:ILE:HD13	32:5:79:ARG:HH11	1.70	0.56
1:A:3629:U:C2'	1:A:3630:U:H5'	2.34	0.56
1:A:2551:U:O5'	1:A:2551:U:H6	1.87	0.56
1:A:3658:G:O2'	1:A:3659:C:O5'	2.23	0.56
14:N:81:ILE:HG22	14:N:99:THR:HG21	1.86	0.56
1:A:3350:A:N3	23:W:69:ARG:NH2	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1630:A:HO2'	1:A:2125:A:H1'	1.71	0.56
35:8:85:LEU:HD21	35:8:94:VAL:HG12	1.87	0.56
1:A:101:C:H2'	1:A:102:A:O4'	2.05	0.56
1:A:3629:U:C2	1:A:3630:U:C6	2.93	0.56
1:A:2812:G:N2	1:A:2813:U:O2	2.38	0.56
1:A:3018:A:C8	1:A:3018:A:C5'	2.85	0.56
23:W:19:GLY:HA3	23:W:22:LEU:HD21	1.88	0.56
1:A:18:G:OP1	30:3:83:ARG:NH2	2.39	0.56
1:A:181:C:O2'	1:A:182:U:OP2	2.23	0.56
32:5:97:ARG:HB2	32:5:117:LEU:HD23	1.87	0.56
1:A:773:A:O2'	1:A:774:A:O5'	2.24	0.56
1:A:2696:G:H4'	1:A:2697:A:OP1	2.06	0.56
16:P:33:LEU:O	16:P:65:ARG:NH2	2.39	0.56
1:A:2812:G:C5	1:A:2813:U:C4	2.94	0.55
6:F:316:LYS:HG2	6:F:324:VAL:HG21	1.88	0.55
5:E:188:LYS:O	5:E:192:VAL:HG23	2.06	0.55
1:A:1552:G:OP1	35:8:64:LYS:O	2.24	0.55
1:A:1572:U:O2	1:A:1572:U:O5'	2.23	0.55
1:A:2679:A:C4	1:A:3353:A:C2	2.93	0.55
1:A:3628:C:C3'	1:A:3629:U:C5	2.89	0.55
32:5:147:TYR:CE2	32:5:246:GLU:HB2	2.42	0.55
4:D:104:ILE:HG22	4:D:146:THR:HG21	1.87	0.55
1:A:1444:A:C4	21:U:163:LEU:HD11	2.42	0.55
13:M:56:LEU:O	13:M:80:ILE:O	2.24	0.55
1:A:2577:C:O4'	1:A:2577:C:O2	2.25	0.55
1:A:3628:C:H3'	1:A:3629:U:H5	1.72	0.55
6:F:38:GLN:O	6:F:42:THR:HG23	2.07	0.55
1:A:256:A:C2	1:A:257:U:O2	2.59	0.55
1:A:3626:A:N1	1:A:3660:A:C2	2.74	0.55
1:A:1454:A:H2'	1:A:1455:C:O4'	2.07	0.55
14:N:30:LEU:HD12	14:N:44:PHE:CE2	2.42	0.55
1:A:3700:G:H2'	1:A:3701:A:H5"	1.88	0.55
20:T:128:GLY:O	20:T:129:ASN:CB	2.55	0.55
30:3:4:VAL:HB	30:3:52:ASN:HD21	1.72	0.55
1:A:2947:G:O2'	16:P:79:ILE:HG12	2.07	0.55
1:A:914:G:H2'	1:A:915:G:C8	2.41	0.55
4:D:196:TRP:CE3	4:D:197:PRO:CD	2.90	0.55
5:E:180:ILE:HD13	5:E:192:VAL:HG22	1.89	0.55
1:A:1572:U:C5	1:A:1573:C:C5	2.95	0.55
1:A:2181:A:N3	1:A:2413:A:H2'	2.21	0.55
29:2:23:ASN:ND2	29:2:26:GLY:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3629:U:C2	1:A:3630:U:C4	2.94	0.54
1:A:3626:A:N1	1:A:3660:A:C4	2.75	0.54
1:A:773:A:O2'	1:A:774:A:C8	2.61	0.54
4:D:200:ARG:NH1	4:D:217:GLN:OE1	2.40	0.54
9:I:61:ILE:HD12	9:I:71:ARG:HG2	1.89	0.54
1:A:3626:A:C2	1:A:3660:A:N3	2.73	0.54
32:5:156:LEU:HD12	32:5:257:ILE:HD13	1.90	0.54
1:A:684:G:H1'	6:F:314:GLN:HG2	1.90	0.54
7:G:18:VAL:CG1	7:G:70:THR:HG22	2.37	0.54
1:A:3628:C:C3'	1:A:3629:U:H6	2.20	0.54
1:A:3630:U:C2'	1:A:3631:U:C5'	2.86	0.54
1:A:3613:A:C6	1:A:3614:A:C6	2.96	0.54
18:R:150:VAL:HG22	18:R:153:THR:HG23	1.89	0.54
36:9:61:THR:HG21	36:9:122:ILE:HG12	1.90	0.54
1:A:2737:C:H5'	1:A:2737:C:H6	1.69	0.54
23:W:36:ILE:HD11	23:W:48:LEU:HD21	1.90	0.54
6:F:159:GLU:HA	6:F:217:VAL:HG13	1.90	0.54
1:A:64:G:OP1	16:P:186:ARG:NH2	2.42	0.53
19:S:47:ILE:HG21	19:S:137:LEU:HD13	1.89	0.53
1:A:1794:U:C2'	1:A:1794:U:O2	2.55	0.53
7:G:136:TYR:HA	7:G:148:ILE:HD11	1.90	0.53
16:P:13:LYS:O	16:P:15:GLN:N	2.38	0.53
33:6:84:CYS:SG	33:6:85:GLY:N	2.81	0.53
1:A:123:A:H3'	1:A:124:U:H5"	1.91	0.53
1:A:1549:U:O2	1:A:1549:U:O4'	2.27	0.53
28:1:5:LEU:HD23	28:1:80:ILE:HD11	1.91	0.53
27:0:13:CYS:O	27:0:13:CYS:SG	2.67	0.53
1:A:3735:A:N6	1:A:3753:G:C6	2.77	0.53
1:A:257:U:O2'	1:A:258:U:H5"	2.09	0.53
1:A:521:U:O2'	1:A:522:A:O5'	2.23	0.53
1:A:1203:A:N1	18:R:113:LEU:HD21	2.24	0.53
1:A:2737:C:C5'	1:A:2737:C:C6	2.85	0.53
6:F:314:GLN:HE21	6:F:314:GLN:HA	1.74	0.53
6:F:138:LEU:HG	6:F:144:ILE:HG22	1.91	0.53
1:A:3726:U:H4'	1:A:3727:A:H5"	1.90	0.53
10:J:174:VAL:HG11	10:J:213:THR:HG23	1.89	0.53
18:R:143:PRO:HB2	18:R:174:ASN:HB2	1.91	0.53
1:A:2188:U:O2'	1:A:2200:A:N7	2.41	0.52
13:M:82:ARG:HG2	13:M:97:PHE:CD2	2.45	0.52
23:W:29:THR:HG21	23:W:144:CYS:SG	2.49	0.52
1:A:3306:G:N3	5:E:247:ALA:HB1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:773:A:O2'	1:A:774:A:H8	1.93	0.52
23:W:20:VAL:O	23:W:145:HIS:ND1	2.43	0.52
6:F:30:THR:HG21	6:F:125:CYS:HB3	1.92	0.52
20:T:128:GLY:O	20:T:129:ASN:HB2	2.09	0.52
15:O:82:LEU:HD21	15:O:100:ILE:HD11	1.92	0.52
32:5:115:LEU:HB3	32:5:117:LEU:CD1	2.40	0.52
11:K:53:TYR:CD2	11:K:144:VAL:HG11	2.45	0.52
1:A:29:C:OP1	16:P:191:ALA:HB2	2.10	0.52
34:7:44:ILE:HD12	34:7:67:ILE:HD11	1.92	0.52
1:A:3258:C:O2'	1:A:3260:G:OP2	2.28	0.52
25:Y:111:ILE:HD11	25:Y:132:PHE:CG	2.44	0.52
14:N:70:PRO:HD3	21:U:9:LEU:HD21	1.92	0.52
32:5:191:VAL:HG23	32:5:191:VAL:O	2.10	0.52
6:F:134:THR:HG22	6:F:150:VAL:CG2	2.39	0.52
6:F:156:ASN:HD21	6:F:255:SER:H	1.58	0.52
28:1:11:ILE:HG22	28:1:82:PRO:HA	1.92	0.52
9:I:76:LYS:HD3	9:I:78:LEU:HD12	1.90	0.52
32:5:98:LEU:HD11	32:5:144:THR:CG2	2.39	0.52
34:7:66:PHE:HE2	34:7:79:VAL:HG12	1.75	0.52
6:F:289:ILE:HD11	19:S:28:LEU:HG	1.92	0.52
1:A:2737:C:O5'	1:A:2737:C:H6	1.92	0.51
14:N:69:ILE:CD1	14:N:74:LEU:HD21	2.40	0.51
3:C:141:U:H5'	25:Y:104:THR:HG21	1.90	0.51
10:J:160:VAL:HG13	10:J:192:VAL:HG11	1.91	0.51
1:A:544:C:O2	1:A:544:C:O4'	2.23	0.51
1:A:3015:A:O4'	1:A:3016:G:C6	2.63	0.51
1:A:1644:U:H5	1:A:2102:A:N1	2.08	0.51
1:A:3247:U:C6	1:A:3270:A:N6	2.79	0.51
1:A:1753:U:H2'	1:A:1754:G:O4'	2.11	0.51
4:D:5:ILE:HG22	4:D:208:GLU:O	2.10	0.51
8:H:62:VAL:HB	8:H:63:PRO:CD	2.40	0.51
1:A:771:U:O2	1:A:771:U:O4'	2.28	0.51
1:A:3627:C:C6	1:A:3627:C:C5'	2.94	0.51
6:F:147:LEU:HD11	6:F:176:LEU:HD21	1.93	0.51
8:H:5:VAL:HG22	8:H:59:TRP:CZ3	2.46	0.51
1:A:2832:A:N3	1:A:2832:A:H2'	2.26	0.51
1:A:3458:A:H2'	1:A:3459:A:O4'	2.10	0.51
4:D:104:ILE:HD11	4:D:116:LEU:HD21	1.93	0.51
1:A:3699:A:H2'	1:A:3700:G:O4'	2.11	0.51
19:S:175:LYS:O	19:S:180:ARG:NH1	2.42	0.51
1:A:3016:G:C3'	1:A:3017:A:H5"	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1133:A:C2	1:A:1163:A:C2	2.99	0.51
1:A:1092:A:H2'	1:A:1093:G:O4'	2.10	0.51
1:A:3629:U:C4	1:A:3630:U:C4	2.99	0.51
12:L:94:ILE:CD1	12:L:115:LEU:HD21	2.37	0.51
5:E:148:ILE:HG22	5:E:189:LEU:HD11	1.92	0.51
6:F:137:VAL:HG11	6:F:144:ILE:HD12	1.91	0.51
15:O:73:ILE:HD12	15:O:78:LEU:HD12	1.93	0.51
22:V:41:VAL:HG21	22:V:65:ILE:HD11	1.92	0.51
11:K:83:VAL:HG11	11:K:101:LEU:HD22	1.93	0.51
4:D:127:VAL:HG11	4:D:133:TYR:HA	1.93	0.51
1:A:3615:A:C2	14:N:32:LEU:HD11	2.46	0.51
1:A:3657:G:C2	1:A:3658:G:C6	2.99	0.51
25:Y:143:ILE:CG2	25:Y:158:VAL:HG21	2.40	0.51
1:A:3627:C:H2'	1:A:3627:C:O2	2.10	0.51
8:H:111:ILE:HG23	8:H:125:VAL:HG13	1.93	0.51
7:G:18:VAL:HG12	7:G:70:THR:HG22	1.93	0.50
8:H:62:VAL:HB	8:H:63:PRO:HD2	1.93	0.50
16:P:63:ARG:NH1	16:P:132:GLU:OE2	2.45	0.50
26:Z:32:SER:HB2	26:Z:105:LEU:HD12	1.92	0.50
1:A:1822:A:N1	1:A:2004:U:H5	2.08	0.50
14:N:116:ILE:HG22	14:N:120:ARG:HE	1.76	0.50
1:A:2814:U:H2'	1:A:2815:G:H8	1.76	0.50
1:A:3675:A:H2'	1:A:3676:C:O4'	2.12	0.50
17:Q:9:TYR:CD2	17:Q:97:LEU:HD13	2.46	0.50
5:E:133:SER:O	5:E:136:VAL:HG22	2.12	0.50
12:L:197:ARG:O	12:L:200:ASN:HB2	2.12	0.50
1:A:3699:A:O2'	1:A:3704:A:N1	2.39	0.50
1:A:1473:A:H8	1:A:1473:A:H5"	1.75	0.50
11:K:144:VAL:O	11:K:144:VAL:HG12	2.12	0.50
18:R:60:VAL:HG21	18:R:98:ALA:HA	1.93	0.50
1:A:2677:A:H61	11:K:95:GLN:HE22	1.60	0.50
1:A:3658:G:C1'	1:A:3659:C:P	3.00	0.50
1:A:976:G:OP2	20:T:91:LYS:NZ	2.44	0.50
1:A:3657:G:N2	1:A:3658:G:N1	2.60	0.49
32:5:141:PRO:HA	32:5:242:TRP:CD2	2.47	0.49
1:A:609:C:H3'	1:A:610:U:H5'	1.93	0.49
1:A:703:U:H2'	1:A:704:U:C6	2.46	0.49
9:I:88:PRO:O	9:I:90:GLU:N	2.46	0.49
1:A:2588:A:OP1	13:M:63:THR:HG21	2.11	0.49
27:0:12:ALA:HB2	27:0:19:ARG:HH12	1.77	0.49
1:A:66:A:OP2	12:L:99:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:11:GLU:O	14:N:14:ILE:HG13	2.12	0.49
10:J:100:THR:HG21	10:J:198:LYS:HA	1.93	0.49
1:A:257:U:C4'	1:A:258:U:OP1	2.60	0.49
1:A:1523:A:H2'	1:A:1524:U:O4'	2.13	0.49
7:G:21:ILE:HD11	7:G:125:MET:SD	2.51	0.49
1:A:3426:G:H5"	13:M:14:ARG:HB3	1.95	0.49
1:A:1908:U:C2'	1:A:1909:U:H5'	2.42	0.49
1:A:308:U:HO2'	1:A:309:G:P	2.36	0.49
1:A:3239:U:O2	5:E:247:ALA:HB3	2.13	0.49
1:A:723:A:N6	1:A:3228:U:OP1	2.43	0.49
1:A:3111:U:O4'	1:A:3111:U:O2	2.31	0.49
3:C:105:U:C4	3:C:106:G:C6	3.01	0.49
14:N:31:CYS:SG	14:N:74:LEU:HB3	2.52	0.49
3:C:37:A:H2'	3:C:38:G:H5"	1.95	0.49
1:A:237:A:H2'	1:A:238:G:O4'	2.12	0.49
1:A:217:A:H2'	6:F:164:THR:HG21	1.95	0.49
14:N:59:ALA:O	14:N:61:ILE:N	2.46	0.49
1:A:1881:C:O2'	1:A:1882:U:O5'	2.29	0.49
35:8:96:ILE:HG21	35:8:105:ARG:HG2	1.95	0.49
25:Y:153:ILE:HG23	25:Y:174:LEU:HD22	1.94	0.49
18:R:83:LEU:HB3	18:R:88:ILE:HG23	1.94	0.49
1:A:1534:U:HO2'	1:A:1535:G:P	2.33	0.48
23:W:29:THR:HG23	23:W:119:VAL:HG11	1.94	0.48
15:O:73:ILE:HD11	15:O:102:VAL:HG13	1.94	0.48
23:W:8:ILE:HG21	23:W:11:LEU:HG	1.95	0.48
7:G:102:PHE:CZ	7:G:129:VAL:HG21	2.48	0.48
4:D:104:ILE:CG2	4:D:146:THR:HG21	2.43	0.48
1:A:3387:U:H2'	1:A:3388:U:O4'	2.13	0.48
32:5:249:ILE:O	32:5:253:ILE:HG13	2.13	0.48
31:4:37:PRO:O	31:4:39:PHE:N	2.44	0.48
1:A:374:A:H2'	1:A:375:A:O4'	2.13	0.48
9:I:29:ILE:HD12	9:I:39:ALA:HB2	1.95	0.48
13:M:31:SER:HB2	13:M:104:ILE:HD11	1.95	0.48
9:I:61:ILE:HG12	9:I:105:VAL:HG23	1.94	0.48
8:H:20:ILE:HG22	8:H:25:VAL:HG12	1.96	0.48
1:A:2954:A:H2'	1:A:2955:C:O4'	2.13	0.48
36:9:53:GLN:O	36:9:54:ARG:HG2	2.14	0.48
1:A:2814:U:C2'	1:A:2815:G:H8	2.27	0.48
8:H:58:MET:HB2	8:H:69:ILE:HD12	1.96	0.48
12:L:16:TRP:CZ3	12:L:19:ARG:HD3	2.48	0.48
16:P:67:ARG:O	16:P:71:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100:A:H5”	30:3:65:LYS:HG3	1.94	0.48
1:A:2401:C:H1’	1:A:3736:A:C8	2.48	0.48
2:B:22:G:N7	2:B:53:U:H2’	2.28	0.48
5:E:67:LEU:HD21	5:E:72:ILE:CD1	2.43	0.48
15:O:100:ILE:HD12	15:O:122:ILE:HD11	1.94	0.48
10:J:257:LYS:O	10:J:261:LEU:HD22	2.14	0.48
18:R:60:VAL:HG22	18:R:80:SER:HB2	1.95	0.48
27:0:56:LEU:O	27:0:59:THR:HG22	2.14	0.48
1:A:3627:C:H6	1:A:3627:C:O5’	1.97	0.48
25:Y:130:LEU:HD11	25:Y:183:VAL:CG2	2.44	0.48
33:6:17:LEU:O	33:6:20:VAL:HG22	2.14	0.48
1:A:40:A:N7	15:O:29:PRO:O	2.47	0.48
1:A:2925:U:O4’	1:A:2925:U:O2	2.29	0.47
1:A:3711:U:O2	1:A:3711:U:O4’	2.29	0.47
1:A:3119:A:H5’	12:L:200:ASN:HB3	1.95	0.47
16:P:84:PRO:HA	16:P:87:GLN:HB2	1.96	0.47
18:R:95:TYR:CE1	18:R:163:ALA:HB2	2.50	0.47
1:A:239:U:O4’	1:A:239:U:O2	2.29	0.47
25:Y:134:CYS:HB3	25:Y:143:ILE:HD11	1.96	0.47
1:A:1511:U:H2’	1:A:1512:A:C8	2.50	0.47
19:S:30:VAL:HG12	19:S:52:LEU:HB3	1.96	0.47
27:0:20:ILE:HG12	27:0:39:LEU:HD23	1.95	0.47
1:A:3623:A:H4’	1:A:3623:A:OP1	2.14	0.47
8:H:54:ILE:HD11	8:H:76:LEU:HD13	1.96	0.47
1:A:2812:G:C4	1:A:2813:U:C6	3.03	0.47
1:A:257:U:HO2’	1:A:258:U:C1’	2.27	0.47
8:H:66:LEU:N	8:H:66:LEU:HD23	2.29	0.47
34:7:80:ARG:HD3	34:7:112:LEU:HD23	1.96	0.47
14:N:35:TYR:HB3	14:N:73:ARG:HG2	1.97	0.47
1:A:858:C:H3’	1:A:859:C:H5”	1.96	0.47
8:H:3:THR:HA	21:U:150:GLN:HE22	1.78	0.47
1:A:1747:U:H4’	1:A:2102:A:H4’	1.96	0.47
25:Y:116:THR:O	25:Y:120:ALA:HB3	2.14	0.47
1:A:2549:A:N3	1:A:2549:A:C2’	2.77	0.47
1:A:3631:U:H6	1:A:3631:U:H3’	1.79	0.47
6:F:235:LEU:HD22	6:F:240:LEU:HD11	1.96	0.47
14:N:30:LEU:HD23	14:N:77:LEU:HD23	1.96	0.47
11:K:8:ILE:HD12	11:K:32:ILE:HG23	1.95	0.47
1:A:3629:U:C4	1:A:3630:U:O4	2.67	0.47
1:A:1575:C:C5’	6:F:42:THR:HG21	2.45	0.47
1:A:1572:U:O2	1:A:1572:U:O4’	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1794:U:O2	1:A:1794:U:H2'	2.14	0.47
1:A:1598:A:C2	1:A:2649:A:C4	3.03	0.47
3:C:110:G:H4'	3:C:145:A:H5'	1.96	0.47
3:C:20:G:O2'	3:C:21:A:OP2	2.32	0.47
1:A:2634:A:OP2	5:E:244:ARG:NH2	2.48	0.47
25:Y:115:LEU:HD21	25:Y:133:MET:CE	2.44	0.47
16:P:136:VAL:HG11	16:P:152:ILE:HG21	1.97	0.47
6:F:218:LYS:HA	6:F:229:LEU:HD13	1.96	0.47
1:A:3347:C:O2	5:E:263:ARG:NH1	2.48	0.47
14:N:10:GLU:O	14:N:14:ILE:HG23	2.14	0.47
1:A:1444:A:H3'	1:A:1445:A:C5'	2.44	0.47
3:C:37:A:C2'	3:C:38:G:H5"	2.45	0.47
6:F:134:THR:HG22	6:F:150:VAL:HG21	1.97	0.47
14:N:128:ARG:O	14:N:131:VAL:HG22	2.14	0.47
1:A:3707:U:OP1	5:E:117:ARG:NH1	2.48	0.47
11:K:92:TYR:CE2	11:K:96:LEU:HD11	2.49	0.47
1:A:2812:G:N2	1:A:2813:U:H1'	2.30	0.47
14:N:81:ILE:CG2	14:N:99:THR:HG21	2.45	0.47
16:P:148:LYS:O	16:P:149:ILE:HG12	2.15	0.47
1:A:2812:G:HO2'	1:A:2813:U:C5'	2.27	0.46
5:E:226:VAL:HG11	5:E:246:VAL:CG2	2.44	0.46
1:A:1644:U:C5	1:A:2102:A:N1	2.83	0.46
25:Y:130:LEU:HD12	25:Y:174:LEU:HD21	1.97	0.46
17:Q:38:ARG:HG2	17:Q:41:ALA:HB2	1.97	0.46
1:A:751:U:O3'	6:F:33:ARG:NH1	2.48	0.46
1:A:2219:A:O2'	1:A:2220:U:O5'	2.30	0.46
1:A:1580:G:OP2	15:O:9:ARG:NH2	2.49	0.46
1:A:694:U:OP1	23:W:188:GLN:HA	2.14	0.46
1:A:3654:C:C5	1:A:3655:U:C5	3.03	0.46
13:M:120:VAL:HB	13:M:138:ILE:HD12	1.96	0.46
4:D:82:MET:SD	4:D:88:ILE:HD11	2.55	0.46
21:U:14:HIS:HA	21:U:109:GLU:HG2	1.97	0.46
11:K:18:LEU:HD23	11:K:119:LEU:HD12	1.97	0.46
1:A:227:A:N7	1:A:1538:U:H2'	2.29	0.46
20:T:18:LYS:HA	20:T:21:ILE:HD12	1.97	0.46
5:E:78:ILE:HD13	5:E:308:PHE:HZ	1.81	0.46
1:A:3016:G:H4'	1:A:3017:A:OP2	2.15	0.46
17:Q:50:VAL:HG11	17:Q:149:CYS:SG	2.55	0.46
16:P:127:VAL:HG23	16:P:128:TYR:CD2	2.51	0.46
32:5:107:LYS:O	32:5:111:VAL:HG23	2.16	0.46
1:A:2812:G:HO2'	1:A:2813:U:C4'	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:100:ILE:CD1	15:O:122:ILE:HD11	2.45	0.46
6:F:76:ILE:HG21	6:F:96:CYS:SG	2.55	0.46
1:A:107:C:O2'	1:A:332:A:N3	2.44	0.46
1:A:1322:G:H2'	1:A:1323:A:C8	2.50	0.46
1:A:1070:A:C4	1:A:1518:A:C2	3.03	0.46
1:A:1536:U:C2'	1:A:1537:G:OP1	2.64	0.46
1:A:664:U:H4'	1:A:665:U:OP1	2.16	0.46
2:B:5:U:OP1	7:G:144:ARG:NH2	2.47	0.46
1:A:1086:C:H5"	1:A:1086:C:H6	1.81	0.46
1:A:3629:U:O2	1:A:3630:U:C6	2.69	0.46
1:A:3654:C:C6	1:A:3655:U:H5	2.34	0.46
13:M:47:CYS:O	13:M:48:LEU:C	2.54	0.46
1:A:3627:C:C6	1:A:3627:C:O5'	2.69	0.46
11:K:8:ILE:HD12	11:K:32:ILE:CG2	2.46	0.46
1:A:3613:A:C6	1:A:3614:A:C2	3.04	0.46
1:A:1881:C:O2'	1:A:1882:U:C6	2.64	0.46
1:A:1118:A:C2	1:A:1177:A:C4	3.04	0.46
1:A:733:C:H2'	1:A:734:A:C8	2.51	0.46
6:F:222:ARG:O	6:F:223:ASN:CB	2.64	0.46
1:A:3028:A:H2'	1:A:3028:A:N3	2.31	0.46
26:Z:63:HIS:O	26:Z:63:HIS:ND1	2.48	0.46
11:K:9:ASP:HB2	11:K:116:LYS:HB3	1.96	0.46
3:C:42:U:H3'	3:C:43:G:H5'	1.98	0.46
16:P:146:ASN:O	16:P:150:ASN:HB2	2.16	0.46
2:B:26:C:H5'	2:B:27:A:OP2	2.16	0.46
26:Z:39:ARG:O	26:Z:42:TYR:O	2.34	0.46
1:A:1470:A:H2'	1:A:1471:A:O4'	2.16	0.46
1:A:3594:G:C2	1:A:3611:A:C2	3.04	0.46
7:G:43:GLN:N	7:G:43:GLN:HE21	2.14	0.46
14:N:72:LYS:O	21:U:165:THR:HG22	2.16	0.46
1:A:2628:G:N2	1:A:2632:C:O2'	2.49	0.46
1:A:3658:G:C2	1:A:3659:C:C2	3.04	0.45
11:K:10:CYS:HA	11:K:13:HIS:HD2	1.81	0.45
11:K:10:CYS:SG	11:K:34:ALA:HB1	2.56	0.45
1:A:3613:A:N1	1:A:3614:A:C2	2.84	0.45
28:1:23:ALA:HB1	28:1:43:VAL:HG12	1.99	0.45
18:R:95:TYR:CZ	18:R:163:ALA:HB2	2.51	0.45
1:A:270:U:O2'	1:A:271:G:OP2	2.31	0.45
1:A:103:A:O3'	12:L:67:ARG:NH2	2.49	0.45
17:Q:91:ILE:HD13	17:Q:133:GLN:OE1	2.16	0.45
10:J:169:VAL:HG22	10:J:203:LEU:HD21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:U:O2	1:A:136:U:O4'	2.33	0.45
1:A:3656:A:N1	1:A:3657:G:C6	2.84	0.45
32:5:117:LEU:HD11	32:5:124:VAL:HG12	1.97	0.45
21:U:86:VAL:HB	21:U:135:ILE:HG22	1.97	0.45
25:Y:138:ALA:HB1	25:Y:143:ILE:HD13	1.97	0.45
34:7:24:LEU:HD21	34:7:44:ILE:HG13	1.99	0.45
1:A:1216:C:N4	1:A:1217:U:C4	2.85	0.45
35:8:82:MET:SD	35:8:94:VAL:HG11	2.56	0.45
5:E:325:VAL:HG11	5:E:333:ILE:CD1	2.46	0.45
1:A:3658:G:HO2'	1:A:3659:C:H6	1.65	0.45
1:A:2737:C:O5'	1:A:2737:C:C6	2.70	0.45
25:Y:130:LEU:HD11	25:Y:183:VAL:HG21	1.99	0.45
1:A:809:A:OP1	15:O:132:VAL:HG13	2.17	0.45
7:G:100:GLY:HA3	7:G:154:VAL:HG23	1.99	0.45
1:A:2408:G:H4'	20:T:78:GLY:O	2.16	0.45
1:A:3698:U:O3'	5:E:331:ARG:NH2	2.50	0.45
4:D:196:TRP:C	4:D:197:PRO:O	2.55	0.45
1:A:2101:U:H3'	1:A:2102:A:H5'	1.99	0.45
16:P:3:ALA:O	16:P:7:ILE:HG23	2.16	0.45
1:A:3344:C:H2'	1:A:3345:U:O4'	2.17	0.45
1:A:702:U:O2	1:A:702:U:O4'	2.34	0.45
1:A:3632:U:C2'	1:A:3633:U:H5'	2.44	0.45
11:K:10:CYS:HB3	11:K:40:ILE:HG12	1.99	0.45
1:A:3524:G:H2'	1:A:3525:A:O4'	2.16	0.45
33:6:77:ASN:ND2	33:6:91:SER:OG	2.41	0.45
1:A:2163:A:O2'	1:A:3439:G:H4'	2.17	0.45
1:A:10:G:C2'	1:A:11:A:OP1	2.64	0.45
6:F:314:GLN:HE21	6:F:314:GLN:CA	2.28	0.45
10:J:160:VAL:HG11	10:J:186:LEU:HD13	1.98	0.45
13:M:19:LEU:HD21	13:M:25:ILE:HG21	1.99	0.45
9:I:86:VAL:CG1	9:I:96:LEU:HD22	2.46	0.45
3:C:149:C:OP1	16:P:38:ARG:HD3	2.17	0.45
12:L:59:CYS:SG	12:L:69:ARG:HG2	2.57	0.45
1:A:379:G:H4'	1:A:406:A:N1	2.32	0.45
1:A:3629:U:C6	1:A:3629:U:OP2	2.70	0.45
19:S:51:ARG:CB	19:S:82:VAL:HG11	2.44	0.45
28:1:72:ILE:HD12	28:1:111:VAL:HG22	1.99	0.45
20:T:9:LEU:HD22	20:T:37:ARG:HD3	1.99	0.45
1:A:1306:A:N3	1:A:1456:C:O2'	2.45	0.45
32:5:157:LEU:HD21	32:5:201:LEU:HD13	1.98	0.45
17:Q:5:PRO:O	17:Q:6:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:93:LEU:HD12	8:H:178:ILE:HD12	1.99	0.45
19:S:23:ASN:C	19:S:23:ASN:HD22	2.21	0.45
2:B:23:A:C2	2:B:118:A:O2'	2.70	0.45
15:O:73:ILE:HD11	15:O:102:VAL:CG1	2.47	0.44
13:M:31:SER:CB	13:M:104:ILE:HD11	2.46	0.44
9:I:63:LEU:HD12	36:9:40:LEU:HD22	2.00	0.44
1:A:1103:A:C5	1:A:1231:A:C2	3.05	0.44
1:A:594:C:O2	1:A:594:C:C2'	2.65	0.44
28:1:4:LEU:HD22	33:6:65:LEU:HB3	1.98	0.44
1:A:3656:A:C6	1:A:3657:G:C6	3.05	0.44
5:E:249:ILE:CG2	5:E:257:VAL:HG13	2.46	0.44
1:A:812:U:H2'	15:O:139:ALA:HB1	1.99	0.44
13:M:125:ALA:HB2	13:M:138:ILE:CD1	2.44	0.44
9:I:75:THR:OG1	9:I:86:VAL:HG22	2.18	0.44
1:A:433:A:H2'	1:A:434:C:O4'	2.17	0.44
1:A:2208:G:H21	1:A:3754:A:H8	1.65	0.44
1:A:3123:C:O2	12:L:202:ARG:CZ	2.58	0.44
23:W:47:TYR:O	23:W:51:VAL:HG12	2.17	0.44
1:A:3628:C:O3'	1:A:3629:U:H6	2.01	0.44
1:A:3660:A:H4'	1:A:3661:A:OP1	2.17	0.44
1:A:2734:C:OP2	1:A:2734:C:C5	2.70	0.44
1:A:1897:G:H2'	1:A:1898:U:O4'	2.18	0.44
14:N:38:TYR:HH	21:U:5:ILE:N	2.15	0.44
15:O:75:VAL:HB	15:O:116:LEU:HD21	2.00	0.44
22:V:117:ILE:HG13	22:V:129:ILE:HD11	1.99	0.44
1:A:3585:A:H1'	11:K:167:TYR:HB2	2.00	0.44
5:E:235:LEU:HB3	5:E:239:THR:HG21	1.98	0.44
6:F:316:LYS:CB	6:F:324:VAL:HG21	2.48	0.44
1:A:3459:A:H2'	1:A:3460:C:O4'	2.18	0.44
27:0:12:ALA:HB2	27:0:19:ARG:NH1	2.33	0.44
3:C:145:A:H2'	3:C:146:C:C6	2.53	0.44
1:A:1057:C:O2'	1:A:3173:G:O2'	2.34	0.44
1:A:1850:U:O2'	1:A:1969:A:N6	2.50	0.44
1:A:3726:U:H4'	1:A:3727:A:C5'	2.48	0.44
4:D:127:VAL:HG21	4:D:134:ALA:HB2	1.99	0.44
33:6:54:ILE:O	33:6:58:VAL:HG23	2.18	0.44
8:H:45:ILE:HD11	8:H:54:ILE:HD12	1.98	0.44
1:A:975:G:C6	1:A:976:G:N1	2.86	0.44
9:I:212:ASN:O	9:I:213:ASP:CB	2.66	0.44
16:P:201:LEU:O	16:P:202:ARG:CB	2.66	0.44
1:A:1035:G:N1	4:D:207:VAL:HG11	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:A:P	16:P:68:ARG:HH22	2.41	0.44
33:6:44:LEU:HD12	33:6:95:ILE:HD11	1.99	0.44
1:A:1207:U:H2'	1:A:1208:G:O4'	2.18	0.44
1:A:3006:A:H2'	1:A:3007:A:O4'	2.18	0.44
1:A:3008:A:H2'	1:A:3009:G:O4'	2.18	0.44
1:A:2441:U:H2'	1:A:2442:A:C5	2.53	0.44
1:A:3630:U:H6	1:A:3630:U:O5'	2.01	0.43
32:5:115:LEU:HB3	32:5:117:LEU:HD13	2.00	0.43
1:A:1299:G:H2'	1:A:1300:G:O4'	2.18	0.43
1:A:2833:U:O2'	10:J:60:ARG:NH1	2.49	0.43
1:A:3328:A:N7	4:D:215:ASN:ND2	2.65	0.43
1:A:93:C:OP2	1:A:3103:C:O2'	2.29	0.43
1:A:3658:G:N2	1:A:3659:C:C1'	2.80	0.43
1:A:3526:U:O2	1:A:3526:U:O4'	2.34	0.43
1:A:979:G:N3	1:A:979:G:H3'	2.33	0.43
21:U:21:ARG:HB3	21:U:33:VAL:HG12	2.01	0.43
1:A:2550:C:H3'	1:A:2550:C:O2	2.18	0.43
1:A:1910:C:C6	1:A:1910:C:O5'	2.72	0.43
4:D:46:LYS:HG3	4:D:62:ILE:HD12	2.00	0.43
1:A:3667:C:H5"	1:A:3669:U:OP2	2.19	0.43
1:A:715:U:O2'	1:A:716:C:C6	2.71	0.43
1:A:1648:U:H2'	1:A:1649:G:O4'	2.18	0.43
1:A:1578:G:OP2	6:F:109:ARG:NH1	2.52	0.43
1:A:3628:C:H3'	1:A:3629:U:C6	2.50	0.43
6:F:331:ALA:HB3	32:5:57:THR:HG21	2.00	0.43
35:8:85:LEU:HD13	35:8:117:VAL:HG21	2.00	0.43
14:N:59:ALA:HB2	14:N:92:LEU:HD22	2.01	0.43
1:A:1818:C:H5"	20:T:95:ILE:HD13	2.00	0.43
6:F:262:VAL:O	6:F:273:THR:HG22	2.18	0.43
1:A:1121:G:C6	1:A:1122:A:N1	2.86	0.43
1:A:3035:A:H3'	1:A:3036:A:C8	2.53	0.43
1:A:2951:U:H2'	1:A:2952:U:O4'	2.19	0.43
34:7:57:VAL:HG13	34:7:99:THR:HG23	2.00	0.43
3:C:19:G:C6	3:C:20:G:N1	2.87	0.43
1:A:3025:U:H2'	1:A:3026:G:O4'	2.18	0.43
29:2:57:VAL:HG23	29:2:108:LEU:HD22	2.01	0.43
18:R:33:ARG:HG2	18:R:37:ILE:HD12	2.00	0.43
1:A:1435:G:C2	1:A:1436:A:C2	3.07	0.43
1:A:296:A:OP1	16:P:97:ASN:ND2	2.48	0.43
1:A:2144:U:H5"	1:A:2145:A:O4'	2.18	0.43
1:A:493:C:H2'	1:A:494:U:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:G:OP2	18:R:28:THR:HG22	2.19	0.43
11:K:14:LEU:HD12	11:K:14:LEU:HA	1.93	0.43
1:A:2650:A:H2'	1:A:2651:A:C8	2.53	0.43
1:A:195:A:N1	1:A:196:A:N6	2.67	0.43
19:S:8:VAL:O	19:S:8:VAL:HG13	2.19	0.43
19:S:8:VAL:O	19:S:10:ARG:N	2.51	0.43
1:A:3340:U:OP2	5:E:241:ARG:NH1	2.46	0.43
1:A:3572:A:N3	1:A:3572:A:H2'	2.33	0.43
1:A:2551:U:O5'	1:A:2551:U:C6	2.70	0.43
5:E:180:ILE:CD1	5:E:192:VAL:HG22	2.48	0.43
1:A:3752:C:N4	1:A:3753:G:C6	2.86	0.43
2:B:102:C:H2'	2:B:103:A:O4'	2.19	0.43
6:F:37:ILE:HD11	6:F:126:SER:HB2	2.00	0.43
9:I:120:LEU:HB3	9:I:189:LEU:HD11	2.00	0.43
1:A:1222:U:O2'	1:A:1223:U:O5'	2.34	0.43
5:E:280:TYR:CE1	5:E:351:VAL:HG21	2.53	0.43
1:A:84:U:O2'	1:A:101:C:N4	2.51	0.43
1:A:530:U:OP1	32:5:79:ARG:NH2	2.52	0.43
1:A:3615:A:N1	14:N:32:LEU:HD11	2.33	0.43
6:F:164:THR:HG22	6:F:220:ALA:O	2.19	0.43
36:9:71:LYS:HD2	36:9:107:THR:HG21	2.01	0.43
14:N:32:LEU:HB2	14:N:77:LEU:HD21	2.00	0.43
1:A:3669:U:O4	36:9:39:ARG:O	2.37	0.43
1:A:382:A:N3	1:A:385:G:H5'	2.33	0.43
2:B:74:A:N3	21:U:59:LYS:NZ	2.55	0.43
1:A:2733:A:H2'	1:A:2734:C:H6	1.80	0.42
28:1:11:ILE:HD11	28:1:43:VAL:HG11	2.01	0.42
1:A:2667:C:N4	1:A:3300:A:O4'	2.52	0.42
5:E:110:VAL:HG11	5:E:114:PHE:CD1	2.53	0.42
14:N:24:PHE:O	14:N:29:ARG:HG3	2.18	0.42
1:A:643:G:H1'	1:A:684:G:N2	2.34	0.42
21:U:165:THR:HG23	21:U:165:THR:O	2.19	0.42
22:V:117:ILE:CG1	22:V:129:ILE:HD11	2.49	0.42
16:P:201:LEU:HD12	16:P:205:ARG:NH1	2.34	0.42
12:L:73:GLY:HA3	12:L:97:ASP:HB2	2.01	0.42
30:3:24:LEU:HB3	30:3:53:VAL:HG22	2.01	0.42
3:C:126:C:OP1	30:3:64:ARG:NH2	2.52	0.42
10:J:71:TRP:HB3	10:J:75:ILE:HD11	2.00	0.42
3:C:147:U:H2'	3:C:148:C:O4'	2.19	0.42
1:A:2683:A:H2'	1:A:2684:G:O4'	2.19	0.42
1:A:1024:U:O2'	4:D:12:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2813:U:O2'	1:A:2814:U:C6	2.70	0.42
8:H:60:PHE:CE1	14:N:51:ILE:HD11	2.54	0.42
36:9:46:ILE:HD11	36:9:122:ILE:HG12	2.00	0.42
32:5:233:ALA:HB2	32:5:242:TRP:CZ2	2.54	0.42
7:G:12:ILE:HG23	7:G:162:TRP:CD1	2.54	0.42
1:A:1272:U:OP2	35:8:43:ARG:NH2	2.52	0.42
1:A:2026:G:H2'	1:A:2027:A:O4'	2.19	0.42
19:S:100:CYS:HA	19:S:120:LEU:O	2.20	0.42
3:C:78:U:O2	3:C:78:U:O4'	2.37	0.42
1:A:952:U:OP1	20:T:85:ASN:HB2	2.19	0.42
1:A:258:U:H6	1:A:258:U:H5"	1.84	0.42
16:P:201:LEU:HD12	16:P:205:ARG:CZ	2.50	0.42
1:A:3662:U:H3'	1:A:3663:A:H5'	2.01	0.42
6:F:7:VAL:HG12	6:F:21:GLU:HB3	2.01	0.42
1:A:2470:A:H4'	1:A:2473:A:H1'	2.01	0.42
1:A:184:U:C2'	1:A:185:A:OP1	2.68	0.42
1:A:1030:C:O2	1:A:1036:A:N1	2.52	0.42
1:A:3474:C:OP1	5:E:219:LYS:HD2	2.19	0.42
19:S:86:THR:HA	19:S:105:THR:CG2	2.49	0.42
21:U:86:VAL:CB	21:U:135:ILE:HG22	2.50	0.42
13:M:20:PRO:HA	13:M:53:ALA:HA	2.01	0.42
1:A:546:C:N3	21:U:80:ARG:NH2	2.64	0.42
1:A:1575:C:H5"	6:F:42:THR:HG21	2.02	0.42
17:Q:41:ALA:HB3	17:Q:139:ARG:NH2	2.35	0.42
1:A:1537:G:H8	1:A:1537:G:H5"	1.84	0.42
35:8:32:TRP:CZ2	35:8:53:PRO:HD2	2.54	0.42
1:A:1254:G:OP1	17:Q:98:ARG:NH1	2.52	0.42
1:A:2199:A:N6	1:A:2414:G:O4'	2.52	0.42
12:L:89:ALA:HB1	12:L:94:ILE:HG12	2.01	0.42
1:A:256:A:C2	1:A:257:U:C2	3.08	0.42
3:C:27:U:OP1	26:Z:15:ARG:NH1	2.53	0.42
1:A:3585:A:N6	1:A:3593:U:O2'	2.52	0.42
11:K:188:ILE:HD11	14:N:138:LEU:HG	2.00	0.42
34:7:68:TRP:HZ3	34:7:72:VAL:HG13	1.83	0.42
11:K:2:TYR:CZ	36:9:66:LYS:HA	2.54	0.42
1:A:2474:C:OP1	4:D:193:ARG:NH2	2.53	0.42
1:A:595:U:O2	1:A:595:U:O4'	2.38	0.42
15:O:63:LEU:HD12	15:O:65:LYS:HG2	2.02	0.42
1:A:3632:U:H2'	1:A:3633:U:H6	1.85	0.42
5:E:329:LYS:O	5:E:330:LYS:HB2	2.19	0.42
4:D:191:VAL:HG12	4:D:191:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:48:ILE:HD12	14:N:48:ILE:C	2.39	0.42
29:2:37:ASN:ND2	29:2:39:ASN:O	2.53	0.42
1:A:1911:A:H8	1:A:1911:A:O5'	2.02	0.42
1:A:101:C:O4'	1:A:101:C:O2	2.36	0.42
1:A:1560:U:OP1	35:8:105:ARG:NH2	2.52	0.42
1:A:3585:A:H2'	1:A:3586:U:O4'	2.19	0.42
1:A:1121:G:C2	1:A:1122:A:C2	3.07	0.42
1:A:1895:U:H2'	1:A:1896:C:C6	2.55	0.42
36:9:41:TYR:HB3	36:9:134:LEU:HD13	2.01	0.42
21:U:51:TRP:HA	21:U:51:TRP:CE3	2.55	0.42
10:J:97:PHE:CZ	10:J:180:VAL:HG13	2.55	0.42
30:3:121:VAL:O	30:3:121:VAL:HG12	2.20	0.42
3:C:38:G:O2'	3:C:39:C:P	2.78	0.42
32:5:94:PHE:CD2	32:5:253:ILE:HD11	2.55	0.42
21:U:83:ASN:HD21	21:U:152:LEU:HD21	1.84	0.42
16:P:66:VAL:HG21	16:P:102:ALA:HB2	2.02	0.42
12:L:56:ILE:HD11	12:L:110:LYS:HD2	2.02	0.42
1:A:2506:A:H2'	1:A:2507:A:C8	2.54	0.42
1:A:112:U:O2'	1:A:113:C:H5"	2.20	0.42
15:O:3:THR:HA	15:O:6:LYS:HG3	2.01	0.42
21:U:18:ILE:HD11	21:U:46:ALA:HB1	2.02	0.42
1:A:1908:U:C4	1:A:1909:U:O4	2.73	0.41
1:A:257:U:O2'	1:A:258:U:C5'	2.69	0.41
1:A:1098:U:H4'	32:5:168:VAL:HG13	2.01	0.41
1:A:717:G:H4'	1:A:1583:G:C6	2.55	0.41
13:M:138:ILE:HG23	13:M:138:ILE:O	2.20	0.41
14:N:31:CYS:SG	14:N:76:LEU:HD23	2.60	0.41
12:L:185:ALA:HB1	15:O:146:LEU:HD13	2.02	0.41
1:A:950:G:H2'	1:A:951:A:O4'	2.20	0.41
21:U:58:ASN:HD21	22:V:152:ILE:CD1	2.33	0.41
1:A:2210:U:OP2	20:T:73:ARG:NH1	2.54	0.41
1:A:2736:A:N6	1:A:2813:U:N3	2.60	0.41
1:A:2814:U:O2'	1:A:2815:G:C5'	2.68	0.41
36:9:56:GLN:HA	36:9:56:GLN:NE2	2.34	0.41
1:A:123:A:C2'	1:A:123:A:N3	2.83	0.41
1:A:723:A:C8	1:A:727:A:C6	3.09	0.41
1:A:2549:A:H2'	1:A:2549:A:N3	2.35	0.41
5:E:110:VAL:CG1	5:E:114:PHE:CD1	3.03	0.41
3:C:69:A:C2	3:C:99:G:C5	3.07	0.41
6:F:382:ALA:HB1	6:F:386:LYS:NZ	2.35	0.41
17:Q:190:ILE:O	17:Q:190:ILE:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3629:U:C2'	1:A:3630:U:C5'	2.97	0.41
9:I:59:VAL:HG21	9:I:203:TYR:HE2	1.86	0.41
1:A:3776:U:O2	34:7:114:ASN:ND2	2.53	0.41
21:U:85:GLY:CA	21:U:138:ILE:HD11	2.50	0.41
1:A:1186:A:C6	22:V:110:LYS:HG2	2.56	0.41
21:U:36:MET:HE2	21:U:38:ILE:HD11	2.03	0.41
16:P:169:GLY:O	16:P:173:ARG:HG3	2.20	0.41
1:A:2981:A:H2'	1:A:2982:A:C8	2.55	0.41
1:A:2156:A:OP1	5:E:244:ARG:NH1	2.52	0.41
20:T:11:ALA:HA	20:T:21:ILE:HD11	2.01	0.41
3:C:60:G:H2'	3:C:61:C:O4'	2.21	0.41
33:6:33:CYS:SG	33:6:59:ILE:HD12	2.59	0.41
1:A:36:U:O4	1:A:47:A:O2'	2.31	0.41
1:A:2438:A:O4'	1:A:3317:A:H4'	2.19	0.41
1:A:123:A:O2'	1:A:124:U:OP1	2.30	0.41
1:A:889:U:OP2	12:L:191:ARG:NH2	2.53	0.41
15:O:40:HIS:CD2	15:O:41:MET:HG3	2.55	0.41
30:3:68:LEU:HD23	30:3:82:LEU:HD21	2.03	0.41
20:T:97:ARG:O	20:T:101:LEU:HG	2.19	0.41
6:F:209:ILE:N	6:F:209:ILE:HD12	2.36	0.41
18:R:199:LEU:HD12	18:R:236:GLU:HG2	2.01	0.41
17:Q:152:LEU:HA	17:Q:152:LEU:HD23	1.96	0.41
7:G:94:LYS:O	7:G:96:PHE:N	2.53	0.41
1:A:3272:U:H2'	1:A:3273:G:O4'	2.21	0.41
5:E:37:LYS:O	5:E:183:GLY:HA2	2.21	0.41
1:A:3671:A:OP1	36:9:97:ILE:HD11	2.21	0.41
7:G:40:LEU:HD12	7:G:79:ILE:HD12	2.03	0.41
1:A:3443:A:H2'	1:A:3444:G:H5'	2.02	0.41
14:N:42:LEU:HD21	14:N:105:PHE:CE2	2.55	0.41
33:6:37:LEU:HD13	33:6:62:TYR:HB3	2.03	0.41
1:A:3631:U:N3	1:A:3655:U:C2	2.89	0.41
11:K:79:LEU:HD12	11:K:103:VAL:HG11	2.02	0.41
8:H:20:ILE:HD12	8:H:20:ILE:C	2.41	0.41
1:A:3623:A:N7	9:I:211:ARG:HD2	2.36	0.41
21:U:18:ILE:HG23	21:U:67:LEU:HD21	2.01	0.41
36:9:68:VAL:HG11	36:9:77:TYR:CE1	2.56	0.41
1:A:2736:A:N1	1:A:2813:U:C2	2.88	0.41
1:A:2737:C:C4'	1:A:2737:C:C6	3.04	0.41
1:A:63:A:H4'	16:P:186:ARG:O	2.21	0.41
6:F:147:LEU:HD13	6:F:152:LEU:CD1	2.49	0.41
13:M:56:LEU:HD21	13:M:87:TRP:CZ3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2004:U:O4'	1:A:2004:U:O2	2.37	0.41
13:M:104:ILE:HD12	13:M:112:LYS:HD3	2.03	0.41
19:S:6:LYS:O	19:S:8:VAL:N	2.53	0.41
1:A:1540:G:C8	1:A:1565:G:C2	3.09	0.41
1:A:1759:A:H2'	1:A:1760:A:O4'	2.21	0.41
8:H:21:ASN:HA	8:H:21:ASN:HD22	1.70	0.41
19:S:62:LEU:HD23	19:S:140:GLY:HA2	2.02	0.41
24:X:44:LEU:HD22	24:X:132:PHE:CE1	2.55	0.41
1:A:1646:C:H2'	1:A:1647:U:C6	2.56	0.41
28:1:13:ILE:O	28:1:19:ALA:O	2.39	0.41
3:C:107:A:C8	3:C:108:A:C8	3.09	0.41
34:7:27:LEU:HD11	34:7:47:ILE:HD12	2.02	0.41
22:V:41:VAL:HG13	22:V:97:VAL:HG13	2.02	0.41
1:A:1642:G:N7	5:E:5:LYS:NZ	72.45	0.41
1:A:1745:G:H4'	20:T:9:LEU:HD21	2.02	0.41
1:A:2208:G:H2'	1:A:2209:C:O4'	2.20	0.41
1:A:156:U:OP2	10:J:152:GLY:HA2	2.21	0.41
5:E:45:ALA:HB3	5:E:178:VAL:HG13	2.03	0.41
6:F:54:VAL:HG21	6:F:101:MET:SD	2.61	0.41
4:D:229:ALA:HB3	4:D:234:LYS:HG3	2.01	0.41
5:E:56:ILE:HB	5:E:76:CYS:SG	2.61	0.41
9:I:178:LYS:HE2	9:I:182:ILE:HD11	2.02	0.41
1:A:2970:U:OP1	1:A:3096:U:O2'	2.36	0.41
20:T:137:LEU:HD23	20:T:137:LEU:O	2.21	0.41
1:A:3353:A:N7	1:A:3526:U:H5	2.19	0.40
17:Q:38:ARG:CG	17:Q:41:ALA:HB2	2.50	0.40
1:A:716:C:OP1	35:8:21:GLN:NE2	2.54	0.40
1:A:3631:U:C3'	1:A:3631:U:C6	3.04	0.40
1:A:972:G:N2	20:T:128:GLY:O	2.53	0.40
28:1:72:ILE:CD1	28:1:111:VAL:HG22	2.51	0.40
1:A:1008:U:H2'	1:A:1009:C:O4'	2.22	0.40
1:A:2409:G:OP1	1:A:2411:C:N4	2.54	0.40
1:A:3195:C:O5'	1:A:3195:C:O2	2.40	0.40
1:A:3016:G:C2'	1:A:3016:G:N3	2.84	0.40
9:I:71:ARG:O	9:I:92:ASN:ND2	2.54	0.40
16:P:59:PHE:HE1	16:P:149:ILE:HD12	1.86	0.40
1:A:1206:U:H4'	1:A:1207:U:OP1	2.21	0.40
7:G:40:LEU:CD1	7:G:79:ILE:HD12	2.52	0.40
1:A:506:A:H2'	1:A:507:G:C8	2.56	0.40
15:O:99:VAL:HA	15:O:123:VAL:HB	2.03	0.40
1:A:3075:A:H2'	1:A:3076:G:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1244:G:N2	1:A:3176:A:O4'	2.54	0.40
1:A:1965:U:O4'	1:A:1965:U:O2	2.39	0.40
1:A:715:U:H2'	1:A:716:C:C5	2.56	0.40
30:3:68:LEU:HD23	30:3:82:LEU:HD11	2.04	0.40
1:A:824:U:H2'	1:A:825:G:O4'	2.21	0.40
1:A:193:C:H2'	1:A:194:A:O4'	2.21	0.40
1:A:2680:A:H2'	1:A:2681:U:O4'	2.22	0.40
1:A:1020:C:H2'	1:A:1021:G:O4'	2.22	0.40
1:A:3630:U:O2'	1:A:3631:U:H5"	2.22	0.40
12:L:22:ARG:HG3	16:P:198:LEU:HD22	2.04	0.40
5:E:325:VAL:HG11	5:E:333:ILE:HD13	2.03	0.40
1:A:1467:C:H5'	35:8:60:ASN:HA	2.04	0.40
24:X:66:ASP:O	24:X:74:THR:HB	2.22	0.40
8:H:68:CYS:O	8:H:72:VAL:HG23	2.21	0.40
18:R:110:LEU:HA	18:R:110:LEU:HD13	1.97	0.40
1:A:2165:G:H2'	1:A:2166:G:O4'	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
4	D	245/260 (94%)	225 (92%)	15 (6%)	5 (2%)	9 48
5	E	378/386 (98%)	345 (91%)	26 (7%)	7 (2%)	10 50
6	F	388/411 (94%)	359 (92%)	20 (5%)	9 (2%)	8 44
7	G	116/173 (67%)	106 (91%)	7 (6%)	3 (3%)	7 40
8	H	183/190 (96%)	150 (82%)	26 (14%)	7 (4%)	4 28
9	I	203/221 (92%)	179 (88%)	15 (7%)	9 (4%)	3 24
10	J	225/283 (80%)	203 (90%)	16 (7%)	6 (3%)	6 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	199/202 (98%)	185 (93%)	10 (5%)	4 (2%)	9	48
12	L	209/215 (97%)	183 (88%)	17 (8%)	9 (4%)	3	25
13	M	130/139 (94%)	119 (92%)	8 (6%)	3 (2%)	8	44
14	N	144/165 (87%)	135 (94%)	5 (4%)	4 (3%)	6	37
15	O	145/148 (98%)	133 (92%)	12 (8%)	0	100	100
16	P	202/205 (98%)	185 (92%)	11 (5%)	6 (3%)	5	35
17	Q	185/219 (84%)	157 (85%)	22 (12%)	6 (3%)	5	33
18	R	244/294 (83%)	218 (89%)	17 (7%)	9 (4%)	4	29
19	S	184/187 (98%)	167 (91%)	12 (6%)	5 (3%)	6	39
20	T	179/182 (98%)	172 (96%)	4 (2%)	3 (2%)	11	52
21	U	178/184 (97%)	166 (93%)	9 (5%)	3 (2%)	11	52
22	V	153/161 (95%)	134 (88%)	13 (8%)	6 (4%)	4	28
23	W	166/203 (82%)	152 (92%)	13 (8%)	1 (1%)	30	75
24	X	95/139 (68%)	86 (90%)	6 (6%)	3 (3%)	5	33
25	Y	99/190 (52%)	93 (94%)	6 (6%)	0	100	100
26	Z	119/126 (94%)	102 (86%)	14 (12%)	3 (2%)	7	41
27	0	60/162 (37%)	55 (92%)	3 (5%)	2 (3%)	5	32
28	1	136/146 (93%)	125 (92%)	10 (7%)	1 (1%)	26	72
29	2	96/127 (76%)	85 (88%)	9 (9%)	2 (2%)	9	46
30	3	117/124 (94%)	104 (89%)	10 (8%)	3 (3%)	7	40
31	4	64/67 (96%)	56 (88%)	5 (8%)	3 (5%)	3	22
32	5	221/257 (86%)	197 (89%)	20 (9%)	4 (2%)	11	51
33	6	96/108 (89%)	92 (96%)	2 (2%)	2 (2%)	9	46
34	7	92/120 (77%)	88 (96%)	4 (4%)	0	100	100
35	8	123/131 (94%)	109 (89%)	10 (8%)	4 (3%)	5	32
36	9	101/140 (72%)	86 (85%)	12 (12%)	3 (3%)	5	35
37	a	104/150 (69%)	98 (94%)	4 (4%)	2 (2%)	10	50
38	b	91/112 (81%)	86 (94%)	3 (3%)	2 (2%)	8	45
39	c	87/92 (95%)	68 (78%)	15 (17%)	4 (5%)	3	23
40	d	68/87 (78%)	65 (96%)	3 (4%)	0	100	100
41	e	39/51 (76%)	38 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	f	49/128 (38%)	45 (92%)	4 (8%)	0	100	100
43	g	35/39 (90%)	31 (89%)	4 (11%)	0	100	100
44	h	83/96 (86%)	74 (89%)	8 (10%)	1 (1%)	16	60
45	i	93/104 (89%)	82 (88%)	7 (8%)	4 (4%)	3	25
All	All	6124/7124 (86%)	5538 (90%)	438 (7%)	148 (2%)	12	43

All (148) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	197	PRO
5	E	18	PRO
6	F	102	PHE
7	G	130	HIS
7	G	143	ARG
8	H	53	TYR
8	H	110	ARG
9	I	88	PRO
9	I	89	TYR
9	I	213	ASP
10	J	61	PRO
10	J	241	ASP
11	K	108	PRO
11	K	188	ILE
12	L	65	ASN
12	L	131	LYS
12	L	168	LYS
12	L	169	PRO
13	M	12	LYS
13	M	48	LEU
16	P	51	LEU
18	R	58	SER
18	R	90	VAL
18	R	152	ILE
19	S	7	ASN
19	S	8	VAL
20	T	129	ASN
27	0	32	ASP
30	3	4	VAL
30	3	119	LEU
32	5	116	ARG
33	6	71	HIS

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Mol	Chain	Res	Type
35	8	123	LYS
37	a	10	HIS
37	a	75	ALA
39	c	24	ARG
4	D	13	GLY
5	E	183	GLY
5	E	196	LEU
6	F	267	ILE
6	F	321	ASN
8	H	147	GLY
9	I	53	SER
9	I	216	LEU
10	J	242	ASN
12	L	92	ILE
14	N	8	THR
16	P	150	ASN
17	Q	172	GLY
18	R	114	ASN
18	R	151	GLY
18	R	171	GLY
19	S	9	GLY
20	T	15	LYS
21	U	154	ARG
22	V	23	HIS
22	V	45	CYS
22	V	56	ASN
23	W	68	GLY
24	X	76	ASN
24	X	78	LYS
24	X	135	PHE
27	0	14	SER
28	1	42	LEU
30	3	76	LYS
31	4	20	GLY
32	5	204	CYS
38	b	18	ASN
39	c	40	CYS
45	i	68	VAL
45	i	93	GLY
45	i	95	ASP
5	E	62	LYS
5	E	254	PRO

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Mol	Chain	Res	Type
6	F	265	GLY
6	F	295	SER
6	F	314	GLN
7	G	95	ASN
9	I	36	ARG
9	I	159	MET
10	J	75	ILE
11	K	110	PRO
12	L	130	ASN
13	M	136	SER
14	N	31	CYS
16	P	14	LYS
16	P	186	ARG
17	Q	14	ASN
18	R	44	TYR
18	R	229	ASN
19	S	41	ASN
19	S	184	ALA
20	T	4	THR
22	V	82	LYS
22	V	124	ASN
22	V	134	GLU
26	Z	10	SER
26	Z	82	GLU
29	2	38	VAL
29	2	60	LYS
32	5	177	GLN
36	9	54	ARG
45	i	15	LYS
4	D	180	LEU
5	E	68	HIS
6	F	17	ASN
9	I	19	VAL
9	I	49	LYS
14	N	60	PHE
16	P	202	ARG
17	Q	6	ALA
17	Q	24	ARG
18	R	124	LYS
21	U	134	ARG
21	U	183	ARG
32	5	172	ALA

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Mol	Chain	Res	Type
35	8	64	LYS
36	9	66	LYS
36	9	104	VAL
39	c	46	LYS
4	D	144	LYS
5	E	330	LYS
8	H	52	LYS
8	H	137	PRO
10	J	51	ARG
12	L	4	HIS
17	Q	23	CYS
17	Q	60	ILE
35	8	27	ARG
35	8	41	ARG
38	b	86	THR
44	h	18	TYR
6	F	223	ASN
8	H	62	VAL
12	L	50	ILE
31	4	38	ASN
8	H	131	VAL
10	J	101	LEU
4	D	127	VAL
31	4	36	ASP
6	F	19	VAL
12	L	137	GLY
16	P	149	ILE
33	6	103	ILE
14	N	46	VAL
39	c	65	GLY
11	K	190	PRO
26	Z	84	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
4	D	191/202 (95%)	174 (91%)	17 (9%)	12 44
5	E	335/340 (98%)	311 (93%)	24 (7%)	18 57
6	F	336/352 (96%)	306 (91%)	30 (9%)	12 44
7	G	110/155 (71%)	94 (86%)	16 (14%)	4 19
8	H	164/173 (95%)	139 (85%)	25 (15%)	3 17
9	I	189/203 (93%)	169 (89%)	20 (11%)	8 34
10	J	211/260 (81%)	189 (90%)	22 (10%)	9 35
11	K	181/182 (100%)	163 (90%)	18 (10%)	10 38
12	L	190/194 (98%)	168 (88%)	22 (12%)	7 30
13	M	106/110 (96%)	88 (83%)	18 (17%)	2 12
14	N	134/152 (88%)	112 (84%)	22 (16%)	3 13
15	O	121/122 (99%)	114 (94%)	7 (6%)	25 66
16	P	179/180 (99%)	162 (90%)	17 (10%)	11 40
17	Q	165/190 (87%)	156 (94%)	9 (6%)	27 68
18	R	214/254 (84%)	185 (86%)	29 (14%)	5 22
19	S	158/159 (99%)	141 (89%)	17 (11%)	8 33
20	T	161/163 (99%)	144 (89%)	17 (11%)	8 34
21	U	162/166 (98%)	148 (91%)	14 (9%)	13 46
22	V	140/144 (97%)	134 (96%)	6 (4%)	35 75
23	W	128/178 (72%)	113 (88%)	15 (12%)	7 30
24	X	92/131 (70%)	88 (96%)	4 (4%)	35 75
25	Y	90/177 (51%)	84 (93%)	6 (7%)	20 60
26	Z	111/115 (96%)	94 (85%)	17 (15%)	3 17
27	0	53/146 (36%)	47 (89%)	6 (11%)	7 31
28	1	127/132 (96%)	115 (91%)	12 (9%)	11 41
29	2	97/118 (82%)	91 (94%)	6 (6%)	23 64
30	3	110/115 (96%)	94 (86%)	16 (14%)	4 19
31	4	60/61 (98%)	54 (90%)	6 (10%)	9 37
32	5	201/231 (87%)	180 (90%)	21 (10%)	9 35
33	6	83/92 (90%)	69 (83%)	14 (17%)	2 13
34	7	90/112 (80%)	71 (79%)	19 (21%)	1 7
35	8	114/120 (95%)	97 (85%)	17 (15%)	4 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
36	9	90/127 (71%)	73 (81%)	17 (19%)	2 10
37	a	89/128 (70%)	79 (89%)	10 (11%)	7 32
38	b	82/97 (84%)	76 (93%)	6 (7%)	17 57
39	c	73/77 (95%)	65 (89%)	8 (11%)	8 33
40	d	69/83 (83%)	62 (90%)	7 (10%)	9 36
41	e	40/48 (83%)	33 (82%)	7 (18%)	2 12
42	f	45/114 (40%)	40 (89%)	5 (11%)	8 32
43	g	34/35 (97%)	32 (94%)	2 (6%)	24 65
44	h	70/80 (88%)	66 (94%)	4 (6%)	25 67
45	i	87/93 (94%)	80 (92%)	7 (8%)	15 52
All	All	5482/6311 (87%)	4900 (89%)	582 (11%)	13 34

All (582) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	9	ARG
4	D	32	LEU
4	D	40	TYR
4	D	47	ASP
4	D	67	GLU
4	D	102	LEU
4	D	120	THR
4	D	125	THR
4	D	139	GLN
4	D	177	LYS
4	D	193	ARG
4	D	194	ASN
4	D	204	MET
4	D	207	VAL
4	D	227	ARG
4	D	235	VAL
4	D	245	LEU
5	E	10	ARG
5	E	13	SER
5	E	24	ARG
5	E	30	ARG
5	E	53	MET
5	E	56	ILE

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Mol	Chain	Res	Type
5	E	59	GLU
5	E	104	THR
5	E	112	ASP
5	E	113	GLU
5	E	117	ARG
5	E	134	LEU
5	E	196	LEU
5	E	202	VAL
5	E	216	SER
5	E	223	THR
5	E	233	LYS
5	E	241	ARG
5	E	243	LEU
5	E	253	HIS
5	E	260	GLN
5	E	287	ASP
5	E	292	SER
5	E	334	THR
6	F	39	SER
6	F	55	LYS
6	F	73	VAL
6	F	75	ARG
6	F	86	ARG
6	F	92	PHE
6	F	95	MET
6	F	122	TYR
6	F	126	SER
6	F	140	ARG
6	F	144	ILE
6	F	152	LEU
6	F	170	PHE
6	F	182	ARG
6	F	212	GLU
6	F	230	CYS
6	F	232	VAL
6	F	254	GLU
6	F	257	PHE
6	F	312	ARG
6	F	313	LEU
6	F	314	GLN
6	F	316	LYS
6	F	318	SER

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Mol	Chain	Res	Type
6	F	321	ASN
6	F	325	ARG
6	F	333	LYS
6	F	369	GLN
6	F	371	ILE
6	F	376	TYR
7	G	12	ILE
7	G	18	VAL
7	G	23	VAL
7	G	25	GLU
7	G	28	ASP
7	G	40	LEU
7	G	43	GLN
7	G	67	CYS
7	G	77	LEU
7	G	99	THR
7	G	126	ASP
7	G	141	ARG
7	G	144	ARG
7	G	160	MET
7	G	165	THR
7	G	166	LYS
8	H	6	SER
8	H	36	ARG
8	H	41	LEU
8	H	43	ILE
8	H	45	ILE
8	H	46	ARG
8	H	47	LEU
8	H	48	ASN
8	H	55	LYS
8	H	57	VAL
8	H	70	ARG
8	H	73	CYS
8	H	93	LEU
8	H	109	THR
8	H	111	ILE
8	H	119	GLU
8	H	150	ILE
8	H	153	VAL
8	H	155	LEU
8	H	162	GLN

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Mol	Chain	Res	Type
8	H	165	LEU
8	H	166	CYS
8	H	169	LYS
8	H	172	ARG
8	H	184	THR
9	I	33	TYR
9	I	37	LYS
9	I	40	SER
9	I	62	ILE
9	I	73	ILE
9	I	78	LEU
9	I	82	LEU
9	I	83	LEU
9	I	96	LEU
9	I	99	VAL
9	I	102	ARG
9	I	105	VAL
9	I	108	SER
9	I	110	ASN
9	I	111	ILE
9	I	170	ARG
9	I	175	LYS
9	I	185	ASP
9	I	204	LEU
9	I	216	LEU
10	J	44	LEU
10	J	75	ILE
10	J	85	LEU
10	J	96	GLN
10	J	106	THR
10	J	110	LEU
10	J	113	LEU
10	J	129	LEU
10	J	159	LEU
10	J	169	VAL
10	J	179	LEU
10	J	183	LEU
10	J	186	LEU
10	J	200	LYS
10	J	217	LEU
10	J	234	VAL
10	J	235	CYS

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Mol	Chain	Res	Type
10	J	244	ASP
10	J	246	ARG
10	J	259	MET
10	J	261	LEU
10	J	272	GLU
11	K	1	MET
11	K	14	LEU
11	K	15	LEU
11	K	18	LEU
11	K	35	VAL
11	K	38	GLU
11	K	55	GLU
11	K	57	LEU
11	K	59	LEU
11	K	67	LYS
11	K	98	LEU
11	K	121	SER
11	K	124	ARG
11	K	132	ARG
11	K	135	CYS
11	K	137	LEU
11	K	164	LYS
11	K	201	TYR
12	L	18	GLN
12	L	19	ARG
12	L	20	HIS
12	L	38	ARG
12	L	39	GLU
12	L	43	LYS
12	L	48	THR
12	L	50	ILE
12	L	61	THR
12	L	62	GLN
12	L	63	ARG
12	L	84	LEU
12	L	91	THR
12	L	94	ILE
12	L	99	ARG
12	L	122	LEU
12	L	136	ILE
12	L	169	PRO
12	L	170	PHE

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Mol	Chain	Res	Type
12	L	174	ILE
12	L	190	ARG
12	L	201	ARG
13	M	11	ASN
13	M	14	ARG
13	M	30	ASN
13	M	34	LYS
13	M	38	ILE
13	M	48	LEU
13	M	50	ARG
13	M	51	LEU
13	M	55	SER
13	M	56	LEU
13	M	59	MET
13	M	60	VAL
13	M	73	LYS
13	M	85	LYS
13	M	89	ARG
13	M	123	GLU
13	M	130	LYS
13	M	131	LEU
14	N	14	ILE
14	N	29	ARG
14	N	31	CYS
14	N	46	VAL
14	N	48	ILE
14	N	52	THR
14	N	54	VAL
14	N	56	VAL
14	N	62	THR
14	N	64	VAL
14	N	67	MET
14	N	75	LYS
14	N	80	ARG
14	N	92	LEU
14	N	101	VAL
14	N	102	LEU
14	N	118	LYS
14	N	120	ARG
14	N	127	GLU
14	N	138	LEU
14	N	144	THR

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Mol	Chain	Res	Type
14	N	146	LYS
15	O	4	ARG
15	O	5	PHE
15	O	9	ARG
15	O	21	ARG
15	O	22	VAL
15	O	104	ARG
15	O	132	VAL
16	P	7	ILE
16	P	15	GLN
16	P	22	LEU
16	P	46	ASP
16	P	49	ARG
16	P	51	LEU
16	P	76	LYS
16	P	83	LYS
16	P	93	LYS
16	P	98	LEU
16	P	105	LYS
16	P	118	ASN
16	P	133	VAL
16	P	148	LYS
16	P	149	ILE
16	P	188	SER
16	P	203	LYS
17	Q	38	ARG
17	Q	39	LYS
17	Q	87	LEU
17	Q	88	ARG
17	Q	96	VAL
17	Q	98	ARG
17	Q	153	ARG
17	Q	154	ARG
17	Q	187	LYS
18	R	21	ARG
18	R	23	ARG
18	R	38	LEU
18	R	41	LYS
18	R	44	TYR
18	R	56	THR
18	R	69	ILE
18	R	72	ASP

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Mol	Chain	Res	Type
18	R	77	GLU
18	R	82	GLU
18	R	88	ILE
18	R	103	LEU
18	R	104	LEU
18	R	107	ARG
18	R	114	ASN
18	R	153	THR
18	R	159	ASN
18	R	165	LEU
18	R	166	LYS
18	R	169	CYS
18	R	190	ASN
18	R	197	ASN
18	R	209	THR
18	R	223	ASN
18	R	233	ASP
18	R	238	MET
18	R	243	HIS
18	R	273	LEU
18	R	274	ASN
19	S	16	ARG
19	S	17	LYS
19	S	19	LEU
19	S	23	ASN
19	S	28	LEU
19	S	38	ARG
19	S	48	ILE
19	S	74	HIS
19	S	80	VAL
19	S	84	SER
19	S	87	ASP
19	S	94	LEU
19	S	113	GLU
19	S	131	THR
19	S	136	VAL
19	S	177	ARG
19	S	187	LYS
20	T	3	LEU
20	T	20	LYS
20	T	24	ASP
20	T	42	LYS

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Mol	Chain	Res	Type
20	T	59	ARG
20	T	79	LYS
20	T	83	THR
20	T	88	THR
20	T	104	LEU
20	T	141	ILE
20	T	152	LYS
20	T	162	ARG
20	T	166	GLN
20	T	169	ARG
20	T	170	ASN
20	T	176	LYS
20	T	180	VAL
21	U	12	ASN
21	U	35	ARG
21	U	60	LEU
21	U	67	LEU
21	U	91	ASP
21	U	94	THR
21	U	105	ASP
21	U	106	THR
21	U	107	THR
21	U	124	ARG
21	U	144	ARG
21	U	145	ARG
21	U	176	SER
21	U	184	MET
22	V	41	VAL
22	V	42	ASP
22	V	61	LYS
22	V	69	THR
22	V	84	ARG
22	V	153	GLU
23	W	16	LYS
23	W	23	ARG
23	W	34	ARG
23	W	45	LYS
23	W	48	LEU
23	W	50	ASP
23	W	51	VAL
23	W	61	ARG
23	W	69	ARG

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Mol	Chain	Res	Type
23	W	87	SER
23	W	103	GLU
23	W	105	ARG
23	W	107	LEU
23	W	123	ARG
23	W	153	ILE
24	X	60	LEU
24	X	71	ASP
24	X	93	THR
24	X	116	ILE
25	Y	106	ASP
25	Y	127	ILE
25	Y	134	CYS
25	Y	150	LEU
25	Y	167	ASP
25	Y	187	ILE
26	Z	4	ASN
26	Z	13	LYS
26	Z	14	MET
26	Z	20	THR
26	Z	26	ARG
26	Z	27	ARG
26	Z	34	LEU
26	Z	53	ASP
26	Z	59	ARG
26	Z	62	ASN
26	Z	72	ILE
26	Z	82	GLU
26	Z	86	ARG
26	Z	103	VAL
26	Z	105	LEU
26	Z	111	ASP
26	Z	119	ASP
27	0	29	ILE
27	0	37	PHE
27	0	46	LEU
27	0	51	LYS
27	0	60	GLN
27	0	68	LYS
28	1	5	LEU
28	1	9	LYS
28	1	26	VAL

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Mol	Chain	Res	Type
28	1	61	LYS
28	1	63	VAL
28	1	74	CYS
28	1	106	ASN
28	1	108	LYS
28	1	114	LEU
28	1	117	ILE
28	1	123	LEU
28	1	124	GLU
29	2	3	ASN
29	2	23	ASN
29	2	34	ASP
29	2	37	ASN
29	2	86	MET
29	2	96	HIS
30	3	18	LEU
30	3	31	LEU
30	3	42	LYS
30	3	43	ASN
30	3	46	ILE
30	3	52	ASN
30	3	55	ARG
30	3	61	ASN
30	3	67	GLU
30	3	76	LYS
30	3	77	PHE
30	3	87	THR
30	3	97	LYS
30	3	98	GLN
30	3	104	LEU
30	3	119	LEU
31	4	13	ASN
31	4	21	ILE
31	4	28	LYS
31	4	51	GLN
31	4	62	LYS
31	4	63	GLN
32	5	49	LYS
32	5	53	LEU
32	5	54	ARG
32	5	58	LEU
32	5	59	ARG

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Mol	Chain	Res	Type
32	5	115	LEU
32	5	128	VAL
32	5	129	ASN
32	5	134	GLU
32	5	137	LYS
32	5	149	THR
32	5	156	LEU
32	5	160	ARG
32	5	176	ILE
32	5	181	ASP
32	5	182	ILE
32	5	210	LYS
32	5	224	ARG
32	5	231	ARG
32	5	236	GLU
32	5	250	ASN
33	6	19	LEU
33	6	21	MET
33	6	22	LYS
33	6	28	PHE
33	6	33	CYS
33	6	46	ILE
33	6	50	ASN
33	6	54	ILE
33	6	55	GLN
33	6	67	LYS
33	6	77	ASN
33	6	80	LEU
33	6	89	ARG
33	6	101	SER
34	7	21	THR
34	7	25	SER
34	7	32	CYS
34	7	36	LYS
34	7	39	ARG
34	7	57	VAL
34	7	58	ARG
34	7	67	ILE
34	7	72	VAL
34	7	74	ASN
34	7	78	ARG
34	7	80	ARG

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Mol	Chain	Res	Type
34	7	85	ARG
34	7	88	ASN
34	7	99	THR
34	7	101	VAL
34	7	110	LYS
34	7	112	LEU
34	7	114	ASN
35	8	4	LYS
35	8	21	GLN
35	8	26	MET
35	8	33	ARG
35	8	41	ARG
35	8	47	LYS
35	8	49	THR
35	8	63	THR
35	8	67	LEU
35	8	73	LYS
35	8	76	VAL
35	8	87	MET
35	8	90	THR
35	8	103	LYS
35	8	111	ARG
35	8	113	LYS
35	8	125	ARG
36	9	42	GLU
36	9	51	ARG
36	9	53	GLN
36	9	54	ARG
36	9	56	GLN
36	9	57	ASP
36	9	67	ASN
36	9	68	VAL
36	9	69	ASN
36	9	71	LYS
36	9	81	ARG
36	9	100	ILE
36	9	106	ARG
36	9	113	VAL
36	9	125	LYS
36	9	131	VAL
36	9	136	TYR
37	a	4	ARG

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Mol	Chain	Res	Type
37	a	5	VAL
37	a	15	THR
37	a	48	LYS
37	a	66	ARG
37	a	74	ARG
37	a	86	ARG
37	a	90	MET
37	a	94	LEU
37	a	96	GLU
38	b	18	ASN
38	b	38	SER
38	b	50	GLU
38	b	74	LYS
38	b	81	LYS
38	b	93	LYS
39	c	18	THR
39	c	48	ARG
39	c	49	ARG
39	c	51	ASN
39	c	58	ARG
39	c	66	ARG
39	c	70	ILE
39	c	73	LEU
40	d	16	ARG
40	d	25	ILE
40	d	40	LYS
40	d	51	THR
40	d	62	ARG
40	d	65	ASN
40	d	76	TYR
41	e	4	ILE
41	e	5	LYS
41	e	6	ARG
41	e	18	ARG
41	e	38	ASN
41	e	42	ARG
41	e	48	LYS
42	f	9	LEU
42	f	11	GLN
42	f	41	ARG
42	f	46	ARG
42	f	51	LEU

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Mol	Chain	Res	Type
43	g	7	ARG
43	g	35	ARG
44	h	10	LEU
44	h	16	THR
44	h	17	ARG
44	h	47	THR
45	i	8	ARG
45	i	29	LYS
45	i	37	LEU
45	i	41	ARG
45	i	62	LYS
45	i	86	ARG
45	i	87	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	160	HIS
5	E	174	HIS
5	E	179	GLN
6	F	156	ASN
6	F	314	GLN
6	F	321	ASN
7	G	20	ASN
7	G	43	GLN
8	H	21	ASN
8	H	162	GLN
9	I	47	GLN
9	I	146	GLN
11	K	13	HIS
11	K	49	ASN
11	K	54	GLN
11	K	95	GLN
11	K	189	ASN
12	L	10	ASN
12	L	18	GLN
12	L	24	ASN
12	L	54	HIS
12	L	65	ASN
12	L	153	ASN
13	M	11	ASN
13	M	49	ASN

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Mol	Chain	Res	Type
15	O	118	HIS
16	P	15	GLN
16	P	32	GLN
16	P	141	ASN
16	P	145	ASN
16	P	180	HIS
17	Q	95	HIS
17	Q	183	GLN
18	R	47	GLN
18	R	68	HIS
18	R	180	ASN
18	R	190	ASN
18	R	197	ASN
18	R	223	ASN
18	R	249	ASN
18	R	274	ASN
19	S	7	ASN
19	S	23	ASN
19	S	124	GLN
20	T	19	ASN
20	T	57	HIS
20	T	129	ASN
21	U	15	GLN
21	U	45	ASN
21	U	58	ASN
21	U	131	ASN
21	U	162	HIS
22	V	56	ASN
25	Y	185	ASN
27	0	66	ASN
28	1	79	HIS
28	1	106	ASN
29	2	37	ASN
30	3	39	ASN
30	3	43	ASN
30	3	52	ASN
30	3	98	GLN
31	4	6	ASN
31	4	12	GLN
32	5	185	HIS
32	5	250	ASN
33	6	12	ASN

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Mol	Chain	Res	Type
34	7	64	ASN
35	8	78	ASN
36	9	56	GLN
36	9	108	HIS
37	a	6	HIS
37	a	12	HIS
37	a	52	GLN
38	b	18	ASN
38	b	98	GLN
39	c	51	ASN
39	c	79	ASN
40	d	65	ASN
42	f	8	GLN
42	f	14	ASN
42	f	33	ASN
45	i	3	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	3163/3788 (83%)	934 (29%)	167 (5%)
2	B	117/119 (98%)	23 (19%)	1 (0%)
3	C	148/159 (93%)	43 (29%)	8 (5%)
All	All	3428/4066 (84%)	1000 (29%)	176 (5%)

All (1000) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	A
1	A	13	G
1	A	14	U
1	A	16	A
1	A	18	G
1	A	26	A
1	A	32	C
1	A	40	A
1	A	43	A
1	A	44	U
1	A	45	A
1	A	49	U
1	A	55	G

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Mol	Chain	Res	Type
1	A	57	A
1	A	59	G
1	A	60	A
1	A	66	A
1	A	69	U
1	A	73	U
1	A	74	A
1	A	83	U
1	A	87	U
1	A	92	G
1	A	109	A
1	A	110	G
1	A	111	C
1	A	121	U
1	A	122	A
1	A	123	A
1	A	124	U
1	A	130	G
1	A	133	U
1	A	134	G
1	A	135	G
1	A	136	U
1	A	137	G
1	A	139	A
1	A	144	U
1	A	146	U
1	A	147	C
1	A	149	A
1	A	152	G
1	A	155	U
1	A	156	U
1	A	157	G
1	A	158	U
1	A	162	U
1	A	163	G
1	A	165	A
1	A	167	U
1	A	173	A
1	A	174	U
1	A	181	C
1	A	182	U
1	A	183	U

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Mol	Chain	Res	Type
1	A	184	U
1	A	185	A
1	A	186	A
1	A	190	G
1	A	191	A
1	A	192	G
1	A	197	G
1	A	198	U
1	A	199	G
1	A	200	A
1	A	201	G
1	A	204	G
1	A	207	A
1	A	208	U
1	A	211	U
1	A	215	C
1	A	216	C
1	A	218	U
1	A	219	A
1	A	221	A
1	A	226	G
1	A	227	A
1	A	228	A
1	A	229	A
1	A	231	G
1	A	232	C
1	A	235	A
1	A	239	U
1	A	242	U
1	A	246	U
1	A	250	U
1	A	251	U
1	A	257	U
1	A	258	U
1	A	265	U
1	A	268	C
1	A	269	A
1	A	271	G
1	A	276	G
1	A	277	U
1	A	289	A
1	A	290	G

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Mol	Chain	Res	Type
1	A	291	A
1	A	292	U
1	A	293	U
1	A	302	A
1	A	303	A
1	A	304	U
1	A	305	A
1	A	306	C
1	A	307	G
1	A	308	U
1	A	309	G
1	A	310	U
1	A	313	U
1	A	315	C
1	A	324	U
1	A	325	A
1	A	337	A
1	A	338	U
1	A	342	G
1	A	344	A
1	A	345	G
1	A	346	A
1	A	347	C
1	A	362	U
1	A	378	U
1	A	382	A
1	A	384	A
1	A	385	G
1	A	386	U
1	A	392	G
1	A	395	A
1	A	400	C
1	A	401	A
1	A	405	A
1	A	408	U
1	A	409	A
1	A	411	U
1	A	412	A
1	A	413	C
1	A	431	G
1	A	432	A
1	A	439	U

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Mol	Chain	Res	Type
1	A	444	G
1	A	447	A
1	A	448	A
1	A	449	A
1	A	451	C
1	A	458	A
1	A	459	G
1	A	462	G
1	A	463	G
1	A	465	A
1	A	489	U
1	A	494	U
1	A	495	U
1	A	496	C
1	A	497	U
1	A	498	U
1	A	499	U
1	A	500	A
1	A	501	U
1	A	502	U
1	A	503	A
1	A	505	A
1	A	506	A
1	A	520	U
1	A	521	U
1	A	522	A
1	A	523	A
1	A	530	U
1	A	531	U
1	A	532	C
1	A	534	A
1	A	536	A
1	A	538	A
1	A	539	G
1	A	543	U
1	A	545	C
1	A	547	C
1	A	549	G
1	A	552	A
1	A	573	U
1	A	579	C
1	A	580	A

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Mol	Chain	Res	Type
1	A	581	C
1	A	582	U
1	A	585	C
1	A	586	U
1	A	592	C
1	A	593	A
1	A	594	C
1	A	595	U
1	A	599	G
1	A	601	G
1	A	608	A
1	A	609	C
1	A	610	U
1	A	615	U
1	A	617	A
1	A	618	U
1	A	620	U
1	A	621	C
1	A	622	U
1	A	623	U
1	A	624	C
1	A	625	A
1	A	628	U
1	A	631	U
1	A	636	U
1	A	637	U
1	A	641	G
1	A	642	A
1	A	645	A
1	A	646	A
1	A	647	U
1	A	648	U
1	A	649	U
1	A	650	U
1	A	653	A
1	A	659	U
1	A	662	A
1	A	664	U
1	A	665	U
1	A	666	U
1	A	667	U
1	A	668	U

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Mol	Chain	Res	Type
1	A	669	C
1	A	670	U
1	A	674	U
1	A	675	A
1	A	677	A
1	A	678	A
1	A	679	U
1	A	682	A
1	A	683	A
1	A	684	G
1	A	685	U
1	A	694	U
1	A	697	A
1	A	698	G
1	A	699	U
1	A	704	U
1	A	708	A
1	A	714	C
1	A	715	U
1	A	716	C
1	A	727	A
1	A	729	G
1	A	738	A
1	A	755	A
1	A	759	U
1	A	760	A
1	A	761	U
1	A	763	U
1	A	765	A
1	A	767	U
1	A	769	U
1	A	771	U
1	A	773	A
1	A	774	A
1	A	779	U
1	A	794	C
1	A	799	A
1	A	806	G
1	A	809	A
1	A	812	U
1	A	813	G
1	A	825	G

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Mol	Chain	Res	Type
1	A	831	U
1	A	833	G
1	A	834	U
1	A	835	G
1	A	858	C
1	A	859	C
1	A	860	A
1	A	862	U
1	A	866	C
1	A	874	A
1	A	880	A
1	A	885	A
1	A	889	U
1	A	890	G
1	A	891	C
1	A	893	U
1	A	896	U
1	A	899	A
1	A	900	G
1	A	903	C
1	A	904	G
1	A	905	A
1	A	918	G
1	A	925	A
1	A	936	A
1	A	945	G
1	A	951	A
1	A	955	A
1	A	956	A
1	A	965	A
1	A	968	G
1	A	976	G
1	A	980	A
1	A	984	A
1	A	988	G
1	A	993	U
1	A	998	U
1	A	999	G
1	A	1013	U
1	A	1014	C
1	A	1015	A
1	A	1016	A

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Mol	Chain	Res	Type
1	A	1026	G
1	A	1027	G
1	A	1033	A
1	A	1035	G
1	A	1036	A
1	A	1040	A
1	A	1042	C
1	A	1043	G
1	A	1044	A
1	A	1053	U
1	A	1056	G
1	A	1063	A
1	A	1070	A
1	A	1073	G
1	A	1078	C
1	A	1079	U
1	A	1081	A
1	A	1086	C
1	A	1096	G
1	A	1100	A
1	A	1101	A
1	A	1102	U
1	A	1106	A
1	A	1107	U
1	A	1111	A
1	A	1113	C
1	A	1116	G
1	A	1121	G
1	A	1122	A
1	A	1123	U
1	A	1124	A
1	A	1128	A
1	A	1132	G
1	A	1136	A
1	A	1141	G
1	A	1158	G
1	A	1164	U
1	A	1168	C
1	A	1170	A
1	A	1172	C
1	A	1174	C
1	A	1186	A

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Mol	Chain	Res	Type
1	A	1187	A
1	A	1188	A
1	A	1193	G
1	A	1194	A
1	A	1197	U
1	A	1198	A
1	A	1199	A
1	A	1203	A
1	A	1204	A
1	A	1205	U
1	A	1206	U
1	A	1207	U
1	A	1215	A
1	A	1217	U
1	A	1218	C
1	A	1219	A
1	A	1221	A
1	A	1222	U
1	A	1223	U
1	A	1224	A
1	A	1225	A
1	A	1229	A
1	A	1230	A
1	A	1231	A
1	A	1233	A
1	A	1234	A
1	A	1245	G
1	A	1257	A
1	A	1259	G
1	A	1272	U
1	A	1273	G
1	A	1276	G
1	A	1281	C
1	A	1283	C
1	A	1287	A
1	A	1295	A
1	A	1300	G
1	A	1309	U
1	A	1310	A
1	A	1314	G
1	A	1320	G
1	A	1324	U

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Mol	Chain	Res	Type
1	A	1325	C
1	A	1326	C
1	A	1329	U
1	A	1330	A
1	A	1336	U
1	A	1337	G
1	A	1340	G
1	A	1341	G
1	A	1344	C
1	A	1345	A
1	A	1418	A
1	A	1420	C
1	A	1435	G
1	A	1436	A
1	A	1437	U
1	A	1441	G
1	A	1444	A
1	A	1445	A
1	A	1450	G
1	A	1453	U
1	A	1458	A
1	A	1459	U
1	A	1460	A
1	A	1473	A
1	A	1476	A
1	A	1480	G
1	A	1481	A
1	A	1486	A
1	A	1498	U
1	A	1499	U
1	A	1503	A
1	A	1504	A
1	A	1505	U
1	A	1506	C
1	A	1529	G
1	A	1534	U
1	A	1535	G
1	A	1537	G
1	A	1538	U
1	A	1539	U
1	A	1540	G
1	A	1549	U

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Mol	Chain	Res	Type
1	A	1550	A
1	A	1556	G
1	A	1565	G
1	A	1567	A
1	A	1572	U
1	A	1575	C
1	A	1583	G
1	A	1586	C
1	A	1592	G
1	A	1595	A
1	A	1602	A
1	A	1604	U
1	A	1619	U
1	A	1630	A
1	A	1631	A
1	A	1632	G
1	A	1633	U
1	A	1635	G
1	A	1636	A
1	A	1637	G
1	A	1643	U
1	A	1644	U
1	A	1649	G
1	A	1651	C
1	A	1657	U
1	A	1668	G
1	A	1669	A
1	A	1676	C
1	A	1677	G
1	A	1685	G
1	A	1688	A
1	A	1691	G
1	A	1696	A
1	A	1702	U
1	A	1703	U
1	A	1704	U
1	A	1705	A
1	A	1706	A
1	A	1707	A
1	A	1711	G
1	A	1713	G
1	A	1721	C

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Mol	Chain	Res	Type
1	A	1723	C
1	A	1725	U
1	A	1730	A
1	A	1732	A
1	A	1736	A
1	A	1739	C
1	A	1745	G
1	A	1748	A
1	A	1750	U
1	A	1751	C
1	A	1760	A
1	A	1762	A
1	A	1763	G
1	A	1767	U
1	A	1768	A
1	A	1769	U
1	A	1770	G
1	A	1771	A
1	A	1774	U
1	A	1780	G
1	A	1781	A
1	A	1782	U
1	A	1783	G
1	A	1788	C
1	A	1792	U
1	A	1794	U
1	A	1795	A
1	A	1796	U
1	A	1797	A
1	A	1800	U
1	A	1801	G
1	A	1805	U
1	A	1806	C
1	A	1812	C
1	A	1817	G
1	A	1832	U
1	A	1838	U
1	A	1850	U
1	A	1852	C
1	A	1855	U
1	A	1856	U
1	A	1857	A

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Mol	Chain	Res	Type
1	A	1871	A
1	A	1872	A
1	A	1873	U
1	A	1874	C
1	A	1881	C
1	A	1882	U
1	A	1886	A
1	A	1888	A
1	A	1898	U
1	A	1899	U
1	A	1900	G
1	A	1901	A
1	A	1902	A
1	A	1903	C
1	A	1904	U
1	A	1905	C
1	A	1907	A
1	A	1909	U
1	A	1912	A
1	A	1958	U
1	A	1963	U
1	A	1964	G
1	A	1965	U
1	A	1966	A
1	A	1969	A
1	A	1970	A
1	A	1971	U
1	A	1973	G
1	A	1976	A
1	A	1978	U
1	A	1980	G
1	A	1990	A
1	A	1991	U
1	A	1996	C
1	A	1997	G
1	A	1998	A
1	A	1999	A
1	A	2000	G
1	A	2010	C
1	A	2016	U
1	A	2019	A
1	A	2034	G

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Mol	Chain	Res	Type
1	A	2035	G
1	A	2040	G
1	A	2075	U
1	A	2080	C
1	A	2082	C
1	A	2084	U
1	A	2090	U
1	A	2092	G
1	A	2093	U
1	A	2094	A
1	A	2096	G
1	A	2097	A
1	A	2102	A
1	A	2106	A
1	A	2107	C
1	A	2108	A
1	A	2109	A
1	A	2116	C
1	A	2117	A
1	A	2125	A
1	A	2126	A
1	A	2133	C
1	A	2136	C
1	A	2143	U
1	A	2146	A
1	A	2147	A
1	A	2148	U
1	A	2149	A
1	A	2152	A
1	A	2154	A
1	A	2161	G
1	A	2164	A
1	A	2174	G
1	A	2198	A
1	A	2203	G
1	A	2218	C
1	A	2219	A
1	A	2220	U
1	A	2393	A
1	A	2394	C
1	A	2395	U
1	A	2396	C

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Mol	Chain	Res	Type
1	A	2403	G
1	A	2404	A
1	A	2405	A
1	A	2406	A
1	A	2414	G
1	A	2415	G
1	A	2419	A
1	A	2424	A
1	A	2427	G
1	A	2433	U
1	A	2437	A
1	A	2442	A
1	A	2451	A
1	A	2452	A
1	A	2453	A
1	A	2462	C
1	A	2463	U
1	A	2464	G
1	A	2477	U
1	A	2486	U
1	A	2491	A
1	A	2494	G
1	A	2500	A
1	A	2516	A
1	A	2518	U
1	A	2521	A
1	A	2524	C
1	A	2537	A
1	A	2539	G
1	A	2542	G
1	A	2545	A
1	A	2548	A
1	A	2549	A
1	A	2550	C
1	A	2551	U
1	A	2552	A
1	A	2556	C
1	A	2565	G
1	A	2566	G
1	A	2567	U
1	A	2573	A
1	A	2574	A

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Mol	Chain	Res	Type
1	A	2575	U
1	A	2581	G
1	A	2589	A
1	A	2591	U
1	A	2596	A
1	A	2599	C
1	A	2600	G
1	A	2601	C
1	A	2603	U
1	A	2606	A
1	A	2607	U
1	A	2608	G
1	A	2624	C
1	A	2627	U
1	A	2628	G
1	A	2629	U
1	A	2632	C
1	A	2640	U
1	A	2656	A
1	A	2660	A
1	A	2667	C
1	A	2668	G
1	A	2671	C
1	A	2676	C
1	A	2678	A
1	A	2681	U
1	A	2684	G
1	A	2686	G
1	A	2687	G
1	A	2690	A
1	A	2694	A
1	A	2695	A
1	A	2696	G
1	A	2697	A
1	A	2704	U
1	A	2705	G
1	A	2710	U
1	A	2711	U
1	A	2712	A
1	A	2728	G
1	A	2730	G
1	A	2734	C

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Mol	Chain	Res	Type
1	A	2736	A
1	A	2737	C
1	A	2740	A
1	A	2742	G
1	A	2745	G
1	A	2803	A
1	A	2806	U
1	A	2809	A
1	A	2810	A
1	A	2811	A
1	A	2812	G
1	A	2813	U
1	A	2817	U
1	A	2818	U
1	A	2822	U
1	A	2823	U
1	A	2824	A
1	A	2831	U
1	A	2832	A
1	A	2833	U
1	A	2834	A
1	A	2835	G
1	A	2837	G
1	A	2884	G
1	A	2887	U
1	A	2932	A
1	A	2933	C
1	A	2945	G
1	A	2946	G
1	A	2953	G
1	A	2958	G
1	A	2967	A
1	A	2968	U
1	A	2981	A
1	A	2987	G
1	A	2991	U
1	A	2994	A
1	A	2995	A
1	A	2996	A
1	A	3011	G
1	A	3013	A
1	A	3016	G

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Mol	Chain	Res	Type
1	A	3017	A
1	A	3018	A
1	A	3019	A
1	A	3020	U
1	A	3028	A
1	A	3029	G
1	A	3030	A
1	A	3033	A
1	A	3038	G
1	A	3042	A
1	A	3065	C
1	A	3067	G
1	A	3068	A
1	A	3073	G
1	A	3076	G
1	A	3079	A
1	A	3086	A
1	A	3088	G
1	A	3091	U
1	A	3092	G
1	A	3094	C
1	A	3100	G
1	A	3108	A
1	A	3111	U
1	A	3112	U
1	A	3113	U
1	A	3116	A
1	A	3118	A
1	A	3123	C
1	A	3124	G
1	A	3126	A
1	A	3127	A
1	A	3130	U
1	A	3131	A
1	A	3138	A
1	A	3139	C
1	A	3140	U
1	A	3141	G
1	A	3146	U
1	A	3155	G
1	A	3158	U
1	A	3159	G

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Mol	Chain	Res	Type
1	A	3160	A
1	A	3161	A
1	A	3162	A
1	A	3169	C
1	A	3173	G
1	A	3175	G
1	A	3176	A
1	A	3180	C
1	A	3193	G
1	A	3201	C
1	A	3202	U
1	A	3204	C
1	A	3208	C
1	A	3212	G
1	A	3219	U
1	A	3220	U
1	A	3230	G
1	A	3231	A
1	A	3246	A
1	A	3248	C
1	A	3253	G
1	A	3257	G
1	A	3258	C
1	A	3263	G
1	A	3269	A
1	A	3277	G
1	A	3282	U
1	A	3287	C
1	A	3292	A
1	A	3294	U
1	A	3295	A
1	A	3297	G
1	A	3301	C
1	A	3304	G
1	A	3306	G
1	A	3313	U
1	A	3316	G
1	A	3330	A
1	A	3334	U
1	A	3342	C
1	A	3343	C
1	A	3349	G

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Mol	Chain	Res	Type
1	A	3353	A
1	A	3354	A
1	A	3356	U
1	A	3357	U
1	A	3358	U
1	A	3359	A
1	A	3361	U
1	A	3362	A
1	A	3363	U
1	A	3365	U
1	A	3375	A
1	A	3378	C
1	A	3379	A
1	A	3380	U
1	A	3381	A
1	A	3382	U
1	A	3383	A
1	A	3389	G
1	A	3398	A
1	A	3415	A
1	A	3416	G
1	A	3418	A
1	A	3421	A
1	A	3435	A
1	A	3442	C
1	A	3443	A
1	A	3445	C
1	A	3459	A
1	A	3463	G
1	A	3464	U
1	A	3471	A
1	A	3476	A
1	A	3477	A
1	A	3478	G
1	A	3483	U
1	A	3488	U
1	A	3493	G
1	A	3500	G
1	A	3502	C
1	A	3507	A
1	A	3510	C
1	A	3515	A

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Mol	Chain	Res	Type
1	A	3516	A
1	A	3526	U
1	A	3527	U
1	A	3529	A
1	A	3530	A
1	A	3537	U
1	A	3553	G
1	A	3568	G
1	A	3571	A
1	A	3572	A
1	A	3573	U
1	A	3575	U
1	A	3576	A
1	A	3577	A
1	A	3580	G
1	A	3581	A
1	A	3582	G
1	A	3583	A
1	A	3584	A
1	A	3585	A
1	A	3590	A
1	A	3591	U
1	A	3594	G
1	A	3615	A
1	A	3616	U
1	A	3617	A
1	A	3618	A
1	A	3619	U
1	A	3623	A
1	A	3624	U
1	A	3626	A
1	A	3627	C
1	A	3628	C
1	A	3629	U
1	A	3631	U
1	A	3632	U
1	A	3635	G
1	A	3655	U
1	A	3658	G
1	A	3659	C
1	A	3660	A
1	A	3661	A

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Mol	Chain	Res	Type
1	A	3662	U
1	A	3663	A
1	A	3664	G
1	A	3665	U
1	A	3667	C
1	A	3668	U
1	A	3670	U
1	A	3671	A
1	A	3677	A
1	A	3680	A
1	A	3683	G
1	A	3689	C
1	A	3690	A
1	A	3697	G
1	A	3698	U
1	A	3707	U
1	A	3710	U
1	A	3711	U
1	A	3712	G
1	A	3716	C
1	A	3727	A
1	A	3728	A
1	A	3732	U
1	A	3733	G
1	A	3736	A
1	A	3737	G
1	A	3739	A
1	A	3740	A
1	A	3741	A
1	A	3752	C
1	A	3761	G
1	A	3767	U
1	A	3770	C
1	A	3774	A
1	A	3775	G
1	A	3778	G
1	A	3779	U
1	A	3780	A
1	A	3783	G
2	B	3	A
2	B	13	A
2	B	18	A

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Mol	Chain	Res	Type
2	B	22	G
2	B	26	C
2	B	27	A
2	B	31	G
2	B	33	U
2	B	38	U
2	B	51	G
2	B	53	U
2	B	54	A
2	B	55	A
2	B	63	A
2	B	64	A
2	B	71	G
2	B	73	U
2	B	74	A
2	B	76	U
2	B	89	G
2	B	97	G
2	B	100	A
2	B	110	G
3	C	3	G
3	C	5	A
3	C	6	C
3	C	16	G
3	C	17	A
3	C	27	U
3	C	36	C
3	C	37	A
3	C	38	G
3	C	39	C
3	C	43	G
3	C	50	G
3	C	53	G
3	C	63	A
3	C	64	U
3	C	66	C
3	C	67	G
3	C	75	A
3	C	79	G
3	C	85	A
3	C	86	C
3	C	90	G

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Mol	Chain	Res	Type
3	C	92	A
3	C	98	A
3	C	107	A
3	C	108	A
3	C	109	U
3	C	111	U
3	C	112	A
3	C	114	A
3	C	115	C
3	C	116	U
3	C	119	A
3	C	122	A
3	C	123	A
3	C	129	U
3	C	135	G
3	C	137	A
3	C	138	U
3	C	139	A
3	C	140	G
3	C	142	G
3	C	146	C

All (176) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	10	G
1	A	13	G
1	A	25	A
1	A	43	A
1	A	65	A
1	A	123	A
1	A	124	U
1	A	155	U
1	A	162	U
1	A	173	A
1	A	181	C
1	A	184	U
1	A	208	U
1	A	215	C
1	A	218	U
1	A	251	U
1	A	257	U

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Mol	Chain	Res	Type
1	A	270	U
1	A	289	A
1	A	290	G
1	A	306	C
1	A	337	A
1	A	345	G
1	A	416	G
1	A	500	A
1	A	501	U
1	A	504	A
1	A	579	C
1	A	580	A
1	A	581	C
1	A	594	C
1	A	607	A
1	A	608	A
1	A	620	U
1	A	621	C
1	A	641	G
1	A	645	A
1	A	647	U
1	A	648	U
1	A	652	A
1	A	664	U
1	A	666	U
1	A	673	U
1	A	674	U
1	A	683	A
1	A	697	A
1	A	698	G
1	A	703	U
1	A	715	U
1	A	764	G
1	A	771	U
1	A	778	U
1	A	799	A
1	A	859	C
1	A	888	A
1	A	889	U
1	A	899	A
1	A	935	A
1	A	998	U

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Mol	Chain	Res	Type
1	A	1013	U
1	A	1035	G
1	A	1042	C
1	A	1080	C
1	A	1101	A
1	A	1115	G
1	A	1197	U
1	A	1205	U
1	A	1206	U
1	A	1217	U
1	A	1221	A
1	A	1222	U
1	A	1224	A
1	A	1272	U
1	A	1324	U
1	A	1336	U
1	A	1435	G
1	A	1457	G
1	A	1481	A
1	A	1503	A
1	A	1536	U
1	A	1537	G
1	A	1538	U
1	A	1539	U
1	A	1566	A
1	A	1574	C
1	A	1632	G
1	A	1643	U
1	A	1704	U
1	A	1705	A
1	A	1750	U
1	A	1762	A
1	A	1779	A
1	A	1805	U
1	A	1873	U
1	A	1881	C
1	A	1904	U
1	A	1970	A
1	A	1989	A
1	A	1990	A
1	A	1996	C
1	A	1999	A

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Mol	Chain	Res	Type
1	A	2015	C
1	A	2033	C
1	A	2034	G
1	A	2096	G
1	A	2105	A
1	A	2107	C
1	A	2108	A
1	A	2113	C
1	A	2125	A
1	A	2193	U
1	A	2219	A
1	A	2394	C
1	A	2403	G
1	A	2405	A
1	A	2437	A
1	A	2451	A
1	A	2452	A
1	A	2499	G
1	A	2523	U
1	A	2575	U
1	A	2598	G
1	A	2665	A
1	A	2696	G
1	A	2737	C
1	A	2813	U
1	A	2816	U
1	A	2822	U
1	A	2832	A
1	A	2883	U
1	A	2886	A
1	A	2966	C
1	A	3018	A
1	A	3067	G
1	A	3123	C
1	A	3130	U
1	A	3137	U
1	A	3140	U
1	A	3257	G
1	A	3309	G
1	A	3313	U
1	A	3342	C
1	A	3361	U

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Mol	Chain	Res	Type
1	A	3381	A
1	A	3382	U
1	A	3391	G
1	A	3414	G
1	A	3434	A
1	A	3471	A
1	A	3476	A
1	A	3477	A
1	A	3526	U
1	A	3529	A
1	A	3575	U
1	A	3576	A
1	A	3590	A
1	A	3617	A
1	A	3623	A
1	A	3627	C
1	A	3658	G
1	A	3660	A
1	A	3661	A
1	A	3664	G
1	A	3667	C
1	A	3697	G
1	A	3711	U
1	A	3782	A
2	B	63	A
3	C	35	A
3	C	37	A
3	C	64	U
3	C	98	A
3	C	108	A
3	C	134	G
3	C	139	A
3	C	145	A

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 168 ligands modelled in this entry, 168 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.