



## wwPDB EM Map/Model Validation Report ⓘ

Oct 3, 2016 – 10:10 PM EDT

PDB ID : 5GAH  
EMDB ID: : EMD-8004  
Title : RNC in complex with SRP with detached NG domain  
Authors : Jomaa, A.; Boehringer, D.; Leibundgut, M.; Ban, N.  
Deposited on : 2015-11-26  
Resolution : 3.80 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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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) : rb-20027939

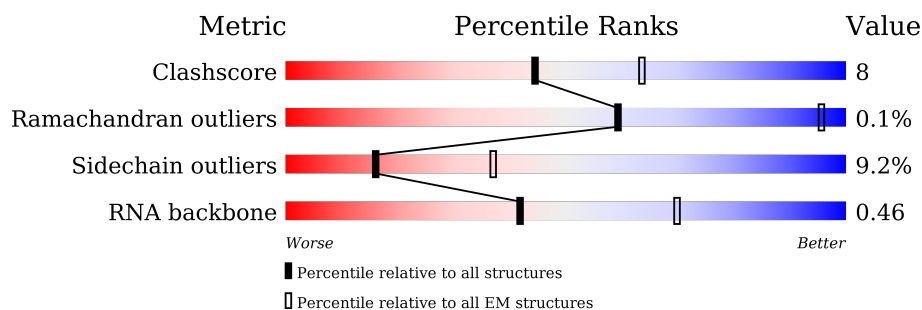
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1	113	17% 18% . 62%
2	2	3	33% 33% 33%
3	A	2903	54% 37% 8% ..
4	B	120	74% 23% .
5	C	273	70% 26% ..
6	D	209	78% 20% .
7	E	201	77% 20% .
8	F	179	60% 35% ..

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Mol	Chain	Length	Quality of chain
9	G	177	
10	H	149	
11	I	165	
12	J	142	
13	K	142	
14	L	123	
15	M	144	
16	N	136	
17	O	127	
18	P	117	
19	Q	115	
20	R	118	
21	S	103	
22	T	110	
23	U	100	
24	V	104	
25	W	94	
26	X	85	
27	Y	78	
28	Z	63	
29	a	59	
30	b	57	
31	c	55	
32	d	46	
33	e	65	

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Mol	Chain	Length	Quality of chain
34	f	38	<div><div></div><div>92%</div><div>8%</div></div>
35	i	453	<div><div></div><div>26%</div><div></div><div>72%</div></div>
36	k	18	<div><div></div><div>89%</div><div>11%</div></div>

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 94027 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 SRP 4.5S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	43	Total	C	N	O	P	0	0
			926	413	174	296	43		

- Molecule 2 is a RNA chain called tRNA CCAend.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	125	Total	C	N	O	S	0	0
			946	599	169	175	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	85	VAL	SER	conflict	UNP P0A7J3
I	86	THR	MET	conflict	UNP P0A7J3

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Signal recognition particle protein Ffh.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	126	Total	C	N	O	S	0	0
			916	575	169	161	11		

- Molecule 36 is a protein called 1A9L SS.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	18	Total	C	N	O	S	0	0
			137	94	20	22	1		

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	P	1	Total	Mg	0
			1	1	
37	D	1	Total	Mg	0
			1	1	
37	E	1	Total	Mg	0
			1	1	
37	B	11	Total	Mg	0
			11	11	
37	b	1	Total	Mg	0
			1	1	
37	C	2	Total	Mg	0
			2	2	
37	A	412	Total	Mg	0
			412	412	
37	2	1	Total	Mg	0
			1	1	
37	R	1	Total	Mg	0
			1	1	

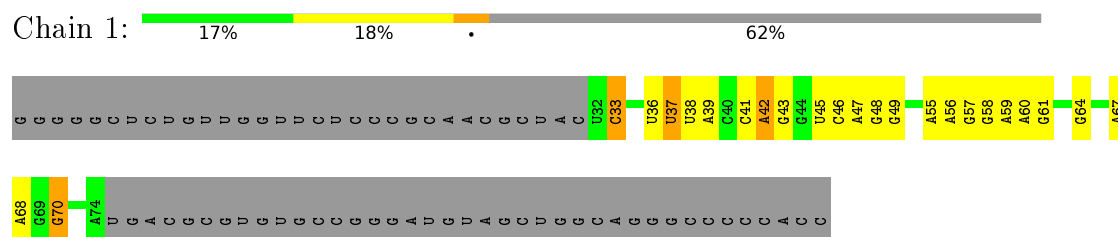
- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

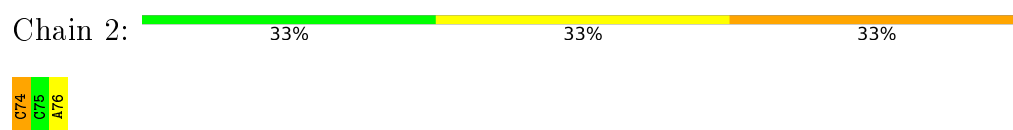
### 3 Residue-property plots

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.

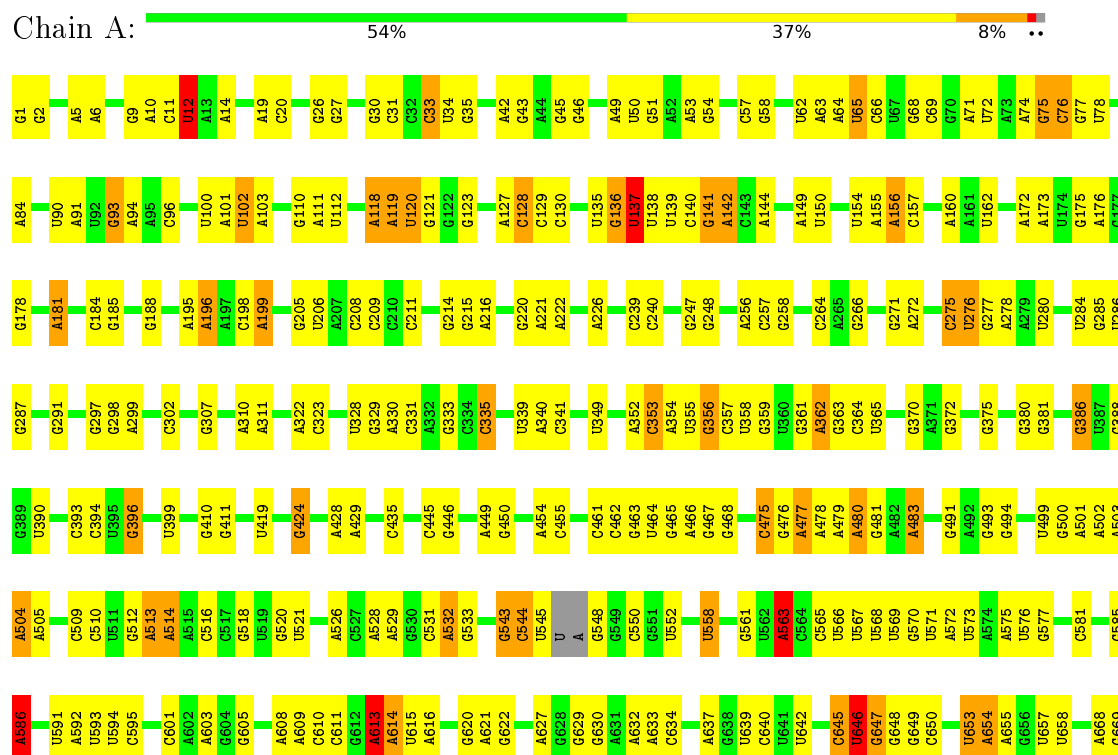
- Molecule 1: SRP 4.5S RNA



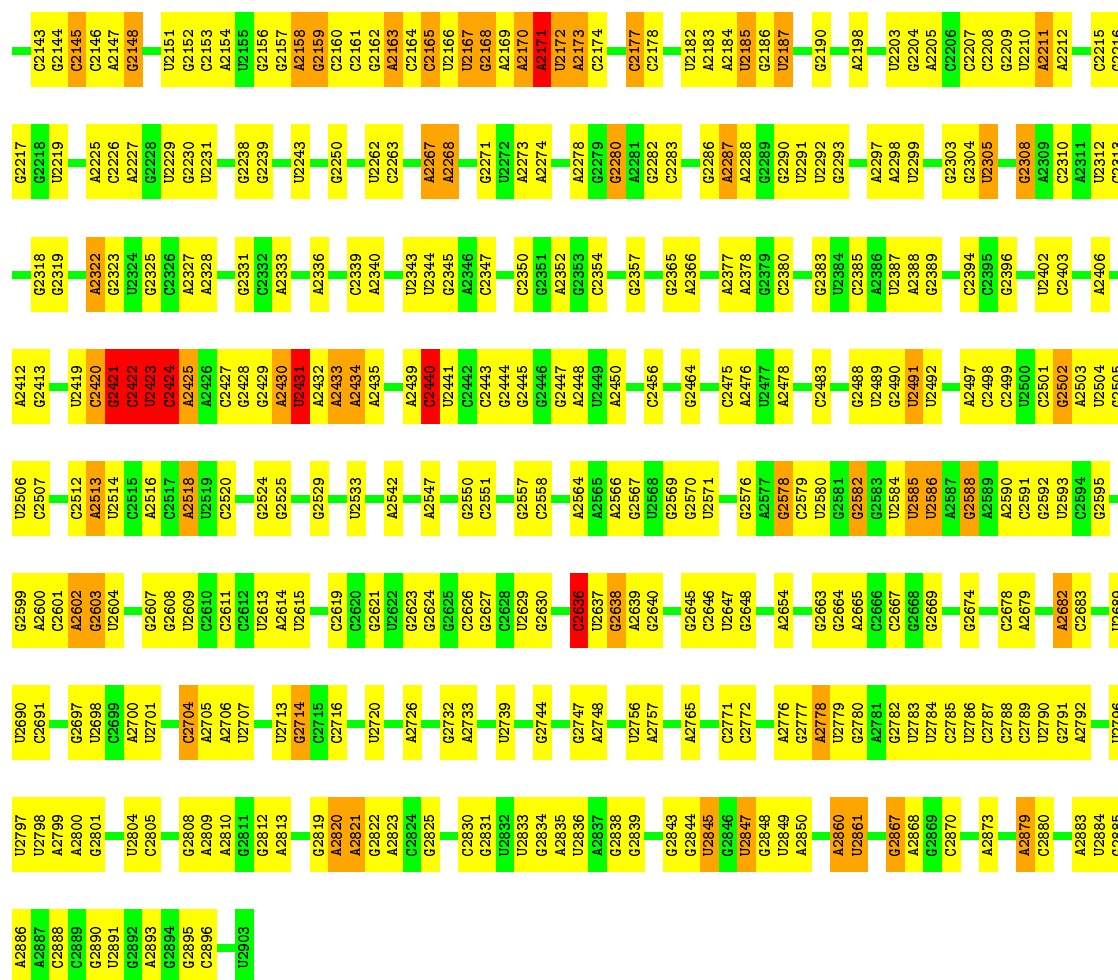
- Molecule 2: tRNA CCAend



- Molecule 3: 23S rRNA

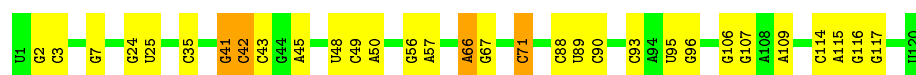


G2066	A1960	C1870	G1774	U1578	G1492	G1440	U199	G1300	U1023	U931	A845	G776	A670
A2060	C1961	A1871	U1775	G1581	C1493	G1414	A1205	U1101	G1024	U932	U846	G777	C671
G2061	U1963	G1873	A1780	C1582	A1494	C1415	G1206	C1102	G1025	A933	U847	G778	C672
A2062	U1966	U1874	U1781	U1583	A1496	G1416	G1210	G1104	A1027	C946	A849	G779	G673
G2069	C1967	G1875	U1782	U1584	U1497	G1417	G1211	U1105	A1028	A947	U850	G780	G674
A2070	A1970	A1876	A1678	C1585	C1498	G1418	G1212	G1106	U1033	C948	U851	A781	A677
A2071	A1977	A1877	G1681	A1590	C1499	A1419	G1218	G1110	G1038	C949	G857	A782	C678
C2072	U1971	U1878	A1786	G1500	A1501	G1420	G1218	A1111	G1039	U953	G858	A783	C679
C2073	G1972	C1879	A1689	G1501	A1502	G1421	U1329	G1112	A1038	U954	U859	G784	C680
U2074	G1973	C1880	C1592	C1592	A1502	G1421	U1329	G1112	A1039	U955	U860	G785	G681
A2077	C1974	C1881	A1597	A1597	U1506	G1422	A1230	G1115	A1040	U956	A861	A788	A685
G2086	A1980	G1888	A1598	A1598	C1507	G1424	U1231	G1116	C1044	U959	A862	A789	U686
G2087	U1981	A1794	A1700	A1700	A1508	G1425	G1236	G1125	A1045	A960	A863	U790	A706
G2088	A1982	C1795	A1603	A1603	A1509	G1426	G1237	G1126	A1046	C961	C864	C791	G707
U2092	U1983	C1604	G1706	C1604	A1510	A1427	G1238	A1126	A1047	A973	A794	A793	A707
A2090	G1983	G1707	G1707	C1605	G1511	A1428	C1243	A1127	A1048	C968	G869	A794	A707
G2093	U1991	C1708	C1708	C1606	A1515	G1432	U1340	G1128	G1056	U970	U870	C795	G711
G2097	G1992	U1709	U1709	C1607	A1516	A1433	A1247	A1129	A1057	A972	U871	C796	G712
A2097	U1993	G1710	A1711	A1608	G1517	A1434	U1249	G1131	A1058	A974	U872	G797	U714
G2101	C1997	A1610	G1715	A1610	A1524	G1436	G1251	A1133	U1060	A975	A877	G798	A717
G2102	G2000	A1614	G1721	A1614	A1525	C1437	G1252	A1134	U1061	A976	A878	A800	A718
C2103	A1912	G1615	A1722	G1615	C1526	U1438	G1253	G1135	G1062	G976	G879	A801	C719
C2104	A	A1616	A1722	A1616	G1527	A1439	A1254	G1136	U1063	A981	G880	A804	U720
U2105	C	C1617	U1725	C1617	A1528	A1440	A1255	G1137	U1064	U982	G881	C806	A722
U2106	U	G1811	U1725	G1811	G1529	U1443	U1256	G1139	U1066	A983	G882	U807	A722
G2107	A	G1816	U1729	G1816	C1530	U1443	C1257	G1140	A1067	U984	G	U808	G729
G2108	A1917	C1837	G1730	C1837	C1531	U1446	U1258	U1141	G1068	A984	U	C809	A730
U2109	A1918	U1818	G1731	U1818	A1532	C1447	U1259	A1142	A1070	C987	C	U810	G733
G2110	A1919	G1819	G1732	G1819	C1533	G1448	A1365	A1143	G1071	U990	U	U811	G733
U2021	C1920	A1819	C1732	A1819	A1534	G1449	A1261	G1149	C1072	C991	U	U813	G738
U2022	G1921	U1820	G1735	U1820	A1535	G1450	A1262	C1150	A1073	C992	C	C814	G738
G2023	G1922	A1821	A1736	A1821	C1536	G1451	A1262	G1154	G1074	G993	G	C815	U741
G2024	U1923	C1822	U1736	C1822	G1537	G1452	U1266	G1155	C1075	C994	A	C816	U742
C2025	C1924	A1637	G1737	C1637	U1542	A1463	U1267	A1156	C1076	C995	C	A743	A743
U2036	U1927	C1638	C1638	C1638	G1543	A1464	U1268	G1168	A1077	A996	U894	A819	U746
G2037	A1928	G1642	G1738	G1642	A1544	G1464	A1269	G1169	U1078	U997	U895	G822	U746
A2030	G1929	U1643	G1743	U1643	A1545	G1465	G1270	C1170	C1079	C998	A896	G823	U747
A2031	A1930	C1644	A1744	C1644	G1546	U1465	G1271	G1171	U1082	C999	C897	U824	A753
G2032	U1931	G1645	U1761	G1645	U1554	U1467	A1272	C1172	U1083	A1000	C898	A825	U754
A2033	C1932	U1646	C1752	U1646	U1555	U1468	A1275	U1173	A1084	U1001	A899	U827	U755
G2038	G1934	U1647	G1752	U1647	G1560	A1470	U1275	U	A1085	G1002	U906	U828	A756
U2039	A1935	G1648	U1756	U1648	U1561	A1471	A1287	A	G1086	G1005	G907	U829	G757
G2040	U1936	U1649	A1757	U1649	C1562	G1473	G1288	U	A1087	C1006	C908	A830	C758
U2041	A1937	A1652	U1758	A1652	G1563	U1474	C1289	G1177	U1088	C1007	A909	G830	G759
A2042	U1938	G1653	A1759	G1653	C1564	U1475	C1290	C1178	A1089	A1008	A910	G831	G763
C2043	U1939	C1761	C1760	C1761	A1565	U1482	U1294	G1179	A1090	A1009	A911	U832	A764
G2129	C1947	A1654	A1762	A1654	U1566	G1483	U1294	U1180	G1093	A1010	A911	A833	C765
U2130	U1946	A1655	G1763	A1655	A1569	U1484	G1300	U1181	U1094	G1011	G914	G834	G765
A2131	A1951	G1660	C1764	G1660	A1570	U1485	G1301	G1182	U1095	U1012	C915	C835	
U2132	U1955	A1664	U1769	A1664	A1571	U1486	A1302	G1187	A1096	C1013	G916		C772
G2133	U1956	A1664	G1770	A1664	A1572	C1489	A1303	U1188	U1097	A1021	U917	U839	U773
A2134	C1957	U1664	G1770	U1664	U1576	A1490	G1303	U1188	A1098	G1022	G930	C840	G774
G2135	U1958	A1667	A1773	A1667	C1577	G1491	A1308	U1198	G1099				G775



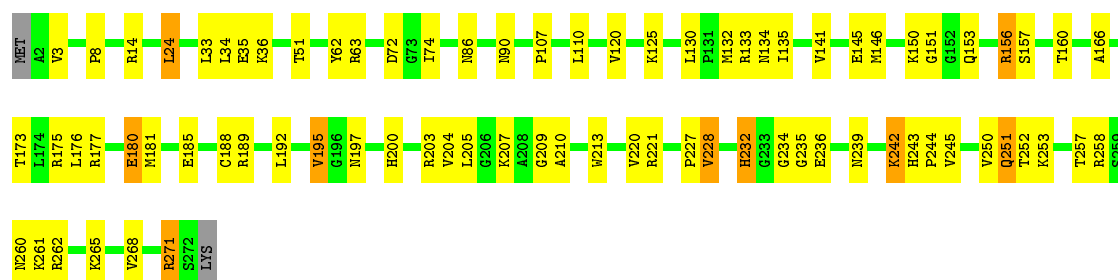
- Molecule 4: 5S rRNA

Chain B: 74% 23%

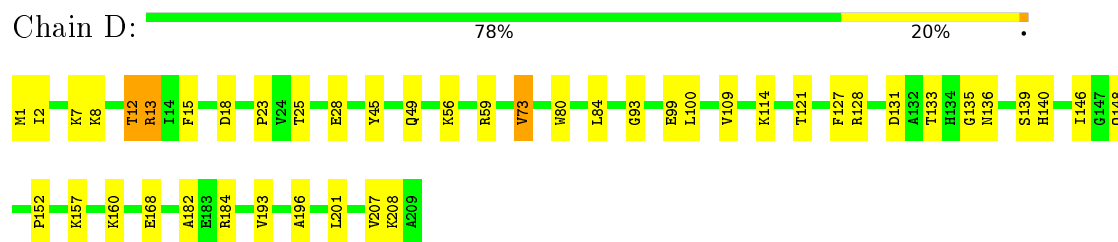


- Molecule 5: 50S ribosomal protein L2

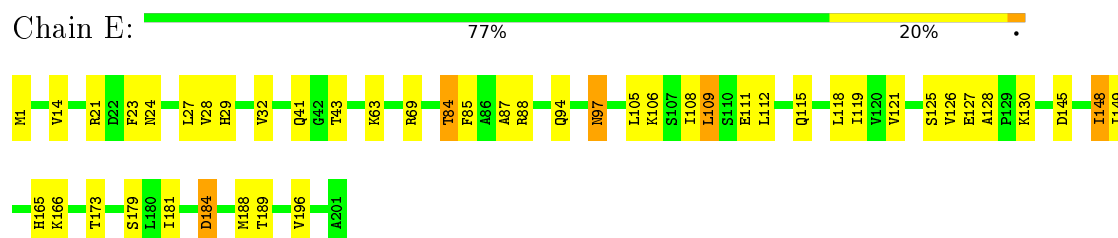
Chain C: 70% 26%



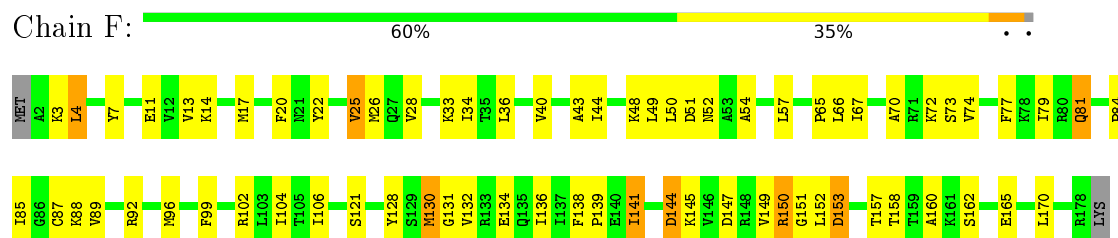
- Molecule 6: 50S ribosomal protein L3



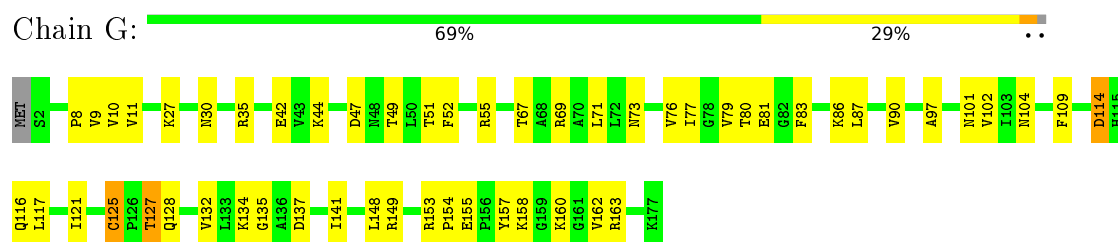
- Molecule 7: 50S ribosomal protein L4



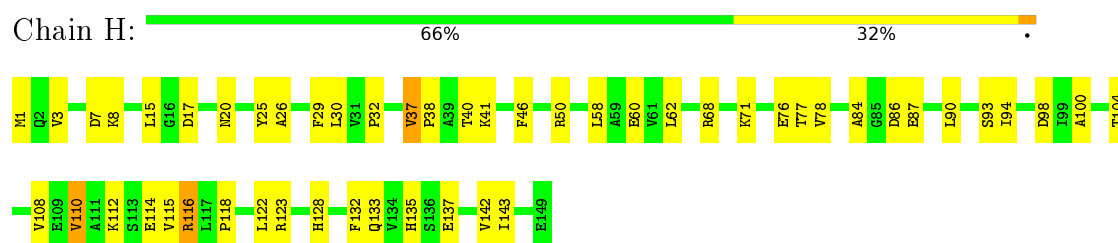
- Molecule 8: 50S ribosomal protein L5



- Molecule 9: 50S ribosomal protein L6

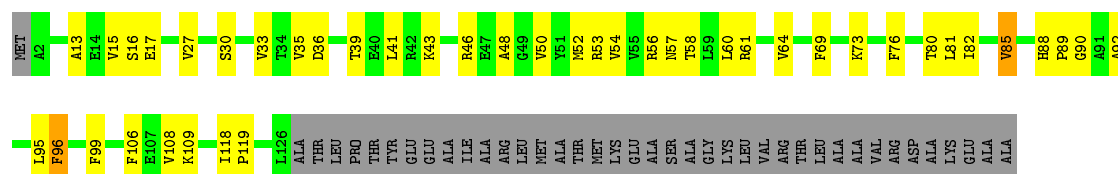


- Molecule 10: 50S ribosomal protein L9



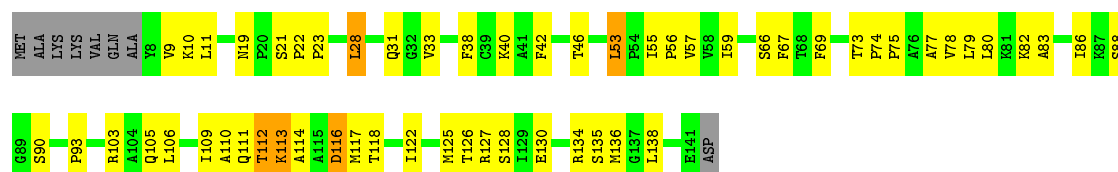
- Molecule 11: 50S ribosomal protein L10





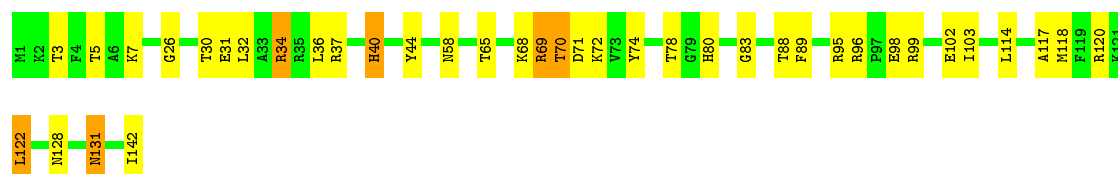
- Molecule 12: 50S ribosomal protein L11

Chain J: 54% 37% 6%



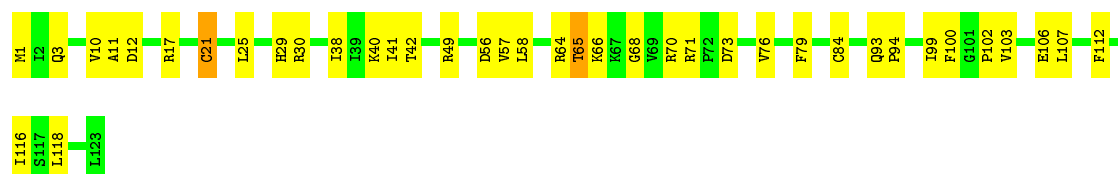
- Molecule 13: 50S ribosomal protein L13

Chain K: 73% 23% 4%



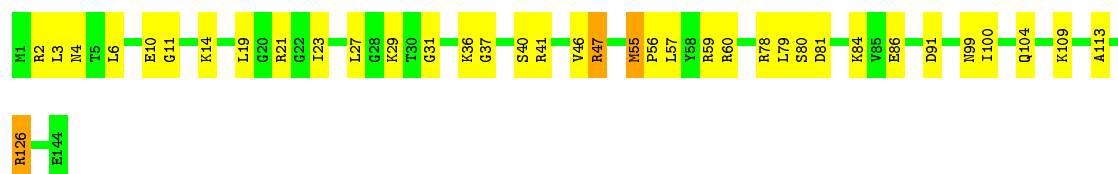
- Molecule 14: 50S ribosomal protein L14

Chain L: 68% 30% 2%



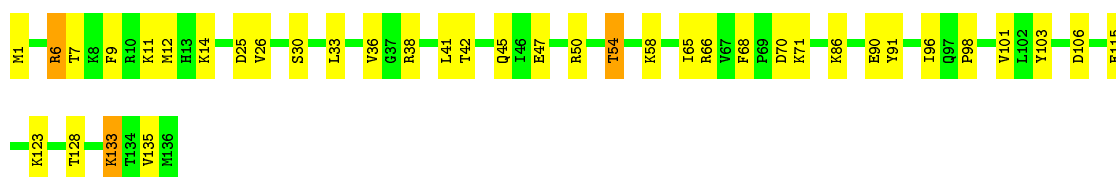
- Molecule 15: 50S ribosomal protein L15

Chain M: 74% 24% 2%



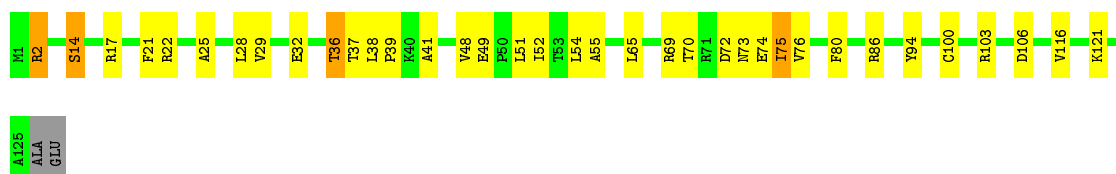
- Molecule 16: 50S ribosomal protein L16

Chain N: 72% 26% 2%



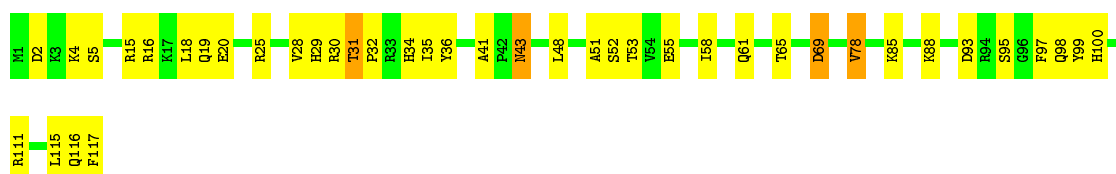
- Molecule 17: 50S ribosomal protein L17

Chain O: 70% 25%



- Molecule 18: 50S ribosomal protein L18

Chain P: 65% 32%



- Molecule 19: 50S ribosomal protein L19

Chain Q: 74% 24%



- Molecule 20: 50S ribosomal protein L20

Chain R: 74% 21%



- Molecule 21: 50S ribosomal protein L21

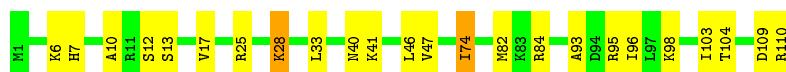
Chain S: 70% 28%



- Molecule 22: 50S ribosomal protein L22

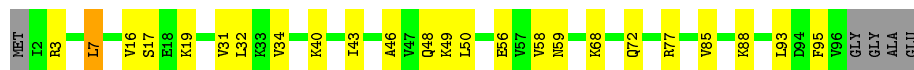
Chain T: 78% 20%





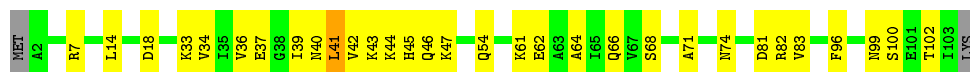
- Molecule 23: 50S ribosomal protein L23

Chain U: 71% 23% 5%



- Molecule 24: 50S ribosomal protein L24

Chain V: 68% 29% 2%



- Molecule 25: 50S ribosomal protein L25

Chain W: 74% 24% 2%



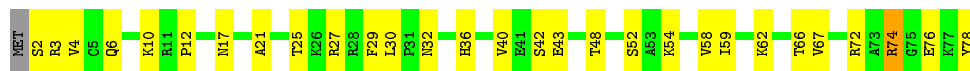
- Molecule 26: 50S ribosomal protein L27

Chain X: 59% 28% 11%



- Molecule 27: 50S ribosomal protein L28

Chain Y: 62% 36% 2%



- Molecule 28: 50S ribosomal protein L29

Chain Z: 67% 27% 5%

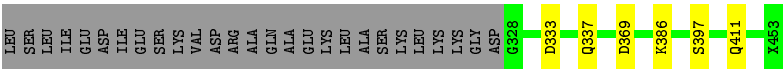


- Molecule 29: 50S ribosomal protein L30

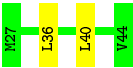
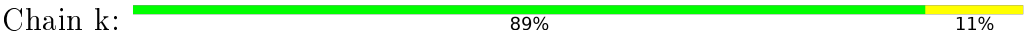
Chain a: 95% 5% 0%







● Molecule 36: 1A9L SS



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	46409	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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	1	0.79	0/1037	1.29	7/1616 (0.4%)
10	H	0.42	0/1121	0.57	0/1515
11	I	0.48	0/958	0.62	1/1292 (0.1%)
12	J	0.58	0/993	0.69	1/1341 (0.1%)
13	K	0.46	0/1152	0.57	0/1551
14	L	0.45	0/955	0.63	0/1279
15	M	0.47	0/1062	0.64	0/1413
16	N	0.48	0/1093	0.59	0/1460
17	O	0.47	0/1006	0.67	0/1345
18	P	0.41	0/910	0.56	0/1219
19	Q	0.48	0/929	0.60	0/1242
2	2	0.57	0/68	1.25	1/103 (1.0%)
20	R	0.56	0/960	0.59	0/1278
21	S	0.46	0/829	0.62	0/1107
22	T	0.52	0/864	0.71	0/1156
23	U	0.45	0/763	0.61	0/1021
24	V	0.38	0/787	0.54	0/1051
25	W	0.40	0/766	0.57	0/1025
26	X	0.50	0/587	0.60	0/776
27	Y	0.48	0/635	0.61	0/848
28	Z	0.41	0/502	0.54	0/667
29	a	0.38	0/453	0.56	0/605
3	A	0.68	14/69329 (0.0%)	1.17	187/108152 (0.2%)
30	b	0.43	0/450	0.62	0/599
31	c	0.44	0/421	0.61	0/561
32	d	0.51	0/380	0.66	0/498
33	e	0.47	0/513	0.62	0/676
34	f	0.49	0/303	0.58	0/397
35	i	0.44	0/672	0.56	0/883
36	k	0.62	0/137	0.85	0/186
4	B	0.51	0/2872	1.04	1/4478 (0.0%)
5	C	0.47	0/2121	0.65	0/2852

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
6	D	0.47	0/1586	0.63	0/2134
7	E	0.44	0/1571	0.61	1/2113 (0.0%)
8	F	0.39	0/1434	0.56	0/1926
9	G	0.39	0/1343	0.58	0/1816
All	All	0.63	14/101562 (0.0%)	1.05	199/152181 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	J	0	1
5	C	0	1
9	G	0	1
All	All	0	3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2542	A	N9-C4	-6.90	1.33	1.37
3	A	1254	A	N9-C4	-6.39	1.34	1.37
3	A	1321	A	N9-C4	6.27	1.41	1.37
3	A	1490	A	N9-C4	6.00	1.41	1.37
3	A	2114	A	N9-C4	5.98	1.41	1.37
3	A	776	G	N9-C4	5.94	1.42	1.38
3	A	563	A	N9-C4	-5.70	1.34	1.37
3	A	1254	A	N3-C4	-5.57	1.31	1.34
3	A	586	A	N3-C4	-5.30	1.31	1.34
3	A	1010	A	N9-C4	-5.29	1.34	1.37
3	A	1678	A	N9-C4	-5.17	1.34	1.37
3	A	960	A	N9-C4	-5.15	1.34	1.37
3	A	514	A	N9-C4	-5.09	1.34	1.37
3	A	1269	A	N9-C4	-5.01	1.34	1.37

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2423	U	C6-N1-C2	-12.25	113.65	121.00
3	A	1838	C	C6-N1-C2	9.39	124.06	120.30
3	A	2422	C	O4'-C1'-N1	9.31	115.65	108.20
3	A	2423	U	C5-C6-N1	8.80	127.10	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1584	U	C2-N1-C1'	8.52	127.92	117.70
3	A	776	G	C8-N9-C4	-8.06	103.17	106.40
3	A	2431	U	N3-C2-O2	-7.90	116.67	122.20
3	A	275	C	C6-N1-C2	-7.75	117.20	120.30
3	A	1760	C	C6-N1-C2	7.62	123.35	120.30
3	A	1584	U	N1-C2-O2	7.29	127.91	122.80
3	A	2422	C	N3-C2-O2	-7.29	116.80	121.90
3	A	2431	U	C5-C4-O4	6.99	130.10	125.90
3	A	1992	G	C4-C5-N7	6.99	113.59	110.80
3	A	2177	C	C6-N1-C2	-6.98	117.51	120.30
3	A	2614	A	C6-N1-C2	-6.84	114.49	118.60
3	A	2424	C	O4'-C1'-N1	6.83	113.66	108.20
3	A	2207	C	C6-N1-C2	-6.82	117.57	120.30
3	A	137	U	C5-C4-O4	-6.82	121.81	125.90
3	A	2636	C	C2-N1-C1'	6.81	126.29	118.80
3	A	214	G	N3-C4-C5	-6.78	125.21	128.60
1	1	42	A	O4'-C1'-N9	6.62	113.49	108.20
3	A	1064	C	C6-N1-C2	-6.61	117.66	120.30
3	A	1027	A	C8-N9-C4	6.60	108.44	105.80
3	A	102	U	C2-N1-C1'	6.60	125.62	117.70
3	A	2422	C	C6-N1-C2	-6.60	117.66	120.30
3	A	776	G	C4-N9-C1'	6.57	135.04	126.50
3	A	1849	G	C8-N9-C4	-6.56	103.78	106.40
3	A	1607	C	C6-N1-C2	-6.56	117.68	120.30
3	A	2542	A	C2-N3-C4	-6.54	107.33	110.60
3	A	2000	C	C6-N1-C2	6.53	122.91	120.30
3	A	784	G	P-O3'-C3'	6.45	127.44	119.70
3	A	2456	C	C6-N1-C2	-6.45	117.72	120.30
3	A	1531	C	C5-C6-N1	6.45	124.22	121.00
3	A	2104	C	C6-N1-C2	-6.41	117.74	120.30
3	A	1313	U	N3-C2-O2	-6.38	117.74	122.20
3	A	906	U	C5-C4-O4	6.37	129.72	125.90
3	A	1849	G	N7-C8-N9	6.36	116.28	113.10
3	A	1652	A	C8-N9-C4	6.34	108.34	105.80
3	A	1128	G	C8-N9-C4	6.33	108.93	106.40
3	A	12	U	N3-C2-O2	-6.26	117.82	122.20
3	A	1695	G	N9-C4-C5	-6.24	102.91	105.40
3	A	1606	C	N3-C2-O2	-6.20	117.56	121.90
3	A	758	C	C6-N1-C2	-6.19	117.82	120.30
3	A	832	U	C5-C6-N1	-6.19	119.60	122.70
3	A	805	G	C8-N9-C4	6.17	108.87	106.40
3	A	483	A	C8-N9-C4	6.17	108.27	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1470	A	C8-N9-C4	-6.14	103.34	105.80
3	A	1848	A	C8-N9-C4	-6.13	103.35	105.80
3	A	611	C	C6-N1-C2	-6.12	117.85	120.30
3	A	733	G	C4-C5-N7	6.11	113.25	110.80
3	A	2499	C	N1-C2-O2	6.09	122.56	118.90
3	A	776	G	N3-C4-C5	-6.08	125.56	128.60
3	A	804	A	C8-N9-C4	6.06	108.23	105.80
3	A	2704	C	C6-N1-C2	-6.06	117.88	120.30
3	A	1072	C	C6-N1-C2	-6.05	117.88	120.30
3	A	1272	A	C8-N9-C4	6.04	108.22	105.80
3	A	2542	A	N3-C4-C5	6.04	131.03	126.80
3	A	1362	C	C6-N1-C2	-6.02	117.89	120.30
3	A	102	U	N1-C2-O2	6.01	127.01	122.80
3	A	2691	C	C6-N1-C2	6.00	122.70	120.30
3	A	2109	U	C6-N1-C2	-5.99	117.40	121.00
3	A	2171	A	O4'-C1'-N9	5.97	112.98	108.20
1	1	42	A	C4-N9-C1'	5.97	137.05	126.30
3	A	130	C	N3-C4-C5	5.97	124.29	121.90
3	A	2077	A	C6-N1-C2	-5.97	115.02	118.60
3	A	1584	U	C5-C6-N1	5.93	125.67	122.70
3	A	2433	A	N1-C2-N3	5.93	132.27	129.30
3	A	774	G	C8-N9-C4	5.93	108.77	106.40
3	A	1261	C	C6-N1-C2	5.90	122.66	120.30
3	A	1531	C	C6-N1-C2	-5.89	117.94	120.30
3	A	832	U	C2-N3-C4	-5.88	123.47	127.00
3	A	2052	A	N1-C6-N6	5.88	122.13	118.60
3	A	1992	G	N9-C4-C5	-5.85	103.06	105.40
3	A	2440	C	C6-N1-C2	5.85	122.64	120.30
3	A	1584	U	N3-C2-O2	-5.84	118.11	122.20
3	A	2153	C	C5-C6-N1	5.84	123.92	121.00
12	J	53	LEU	CA-CB-CG	5.83	128.71	115.30
3	A	790	U	N1-C2-O2	5.82	126.88	122.80
3	A	776	G	O4'-C1'-N9	5.81	112.85	108.20
3	A	2423	U	N3-C4-C5	-5.79	111.12	114.60
3	A	205	G	O4'-C1'-N9	5.79	112.83	108.20
3	A	141	G	N7-C8-N9	5.77	115.98	113.10
3	A	816	C	C6-N1-C2	-5.74	118.00	120.30
3	A	2580	U	C6-N1-C2	-5.73	117.56	121.00
3	A	2582	G	N3-C4-C5	-5.72	125.74	128.60
3	A	2588	G	N3-C4-C5	5.72	131.46	128.60
3	A	1643	G	C8-N9-C4	-5.70	104.12	106.40
3	A	2820	A	C8-N9-C4	5.70	108.08	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	109	LEU	CA-CB-CG	-5.70	102.20	115.30
3	A	987	C	N3-C4-C5	5.68	124.17	121.90
3	A	2845	U	C2-N3-C4	-5.68	123.59	127.00
3	A	783	A	C8-N9-C4	-5.67	103.53	105.80
3	A	1526	C	C6-N1-C2	-5.67	118.03	120.30
3	A	741	U	C5-C6-N1	-5.66	119.87	122.70
3	A	1871	A	C8-N9-C4	-5.64	103.54	105.80
11	I	95	LEU	CA-CB-CG	5.64	128.27	115.30
3	A	793	A	C5-C6-N6	-5.64	119.19	123.70
3	A	1659	G	N3-C4-C5	5.64	131.42	128.60
3	A	2243	U	C5-C6-N1	-5.64	119.88	122.70
3	A	1045	C	C6-N1-C2	5.62	122.55	120.30
3	A	793	A	C2-N3-C4	5.60	113.40	110.60
3	A	1993	U	C5-C6-N1	-5.59	119.90	122.70
3	A	76	C	C5-C6-N1	5.58	123.79	121.00
3	A	410	G	N3-C4-C5	-5.57	125.81	128.60
3	A	2636	C	C6-N1-C1'	-5.57	114.11	120.80
3	A	2145	C	C6-N1-C2	-5.56	118.08	120.30
3	A	776	G	N7-C8-N9	5.54	115.87	113.10
3	A	2498	C	C6-N1-C2	-5.54	118.08	120.30
3	A	972	A	N1-C6-N6	-5.53	115.28	118.60
3	A	1303	G	C8-N9-C4	5.53	108.61	106.40
3	A	1314	C	C6-N1-C2	-5.50	118.10	120.30
3	A	1351	C	C6-N1-C2	5.48	122.49	120.30
3	A	1584	U	C6-N1-C1'	-5.45	113.57	121.20
3	A	2022	U	C6-N1-C2	5.45	124.27	121.00
3	A	1078	U	C5-C6-N1	5.45	125.42	122.70
3	A	2153	C	C6-N1-C2	-5.45	118.12	120.30
3	A	825	A	C6-N1-C2	-5.43	115.34	118.60
3	A	613	A	P-O3'-C3'	5.42	126.20	119.70
3	A	12	U	N1-C2-O2	5.41	126.59	122.80
3	A	1604	C	C5-C6-N1	-5.41	118.29	121.00
3	A	793	A	C5-C6-N1	5.40	120.40	117.70
3	A	206	U	C2-N1-C1'	5.40	124.18	117.70
3	A	280	U	P-O3'-C3'	5.40	126.18	119.70
3	A	2614	A	C5-C6-N1	5.40	120.40	117.70
3	A	1125	G	C8-N9-C4	-5.40	104.24	106.40
3	A	2595	G	C4-N9-C1'	-5.39	119.49	126.50
3	A	2380	C	C6-N1-C2	-5.39	118.14	120.30
3	A	2423	U	N1-C2-N3	5.38	118.13	114.90
3	A	130	C	C6-N1-C2	5.38	122.45	120.30
3	A	1642	G	N3-C4-C5	5.37	131.29	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	755	U	C5-C6-N1	-5.37	120.02	122.70
3	A	642	U	O4'-C1'-N1	5.35	112.48	108.20
3	A	1172	C	C6-N1-C2	-5.35	118.16	120.30
3	A	946	C	N3-C2-O2	-5.34	118.17	121.90
3	A	790	U	C2-N1-C1'	5.33	124.10	117.70
3	A	1072	C	C5-C6-N1	5.33	123.66	121.00
3	A	1970	A	N1-C2-N3	5.32	131.96	129.30
1	1	33	C	C5-C6-N1	5.31	123.65	121.00
3	A	2645	G	N3-C4-C5	-5.30	125.95	128.60
3	A	2645	G	C4-N9-C1'	5.30	133.39	126.50
1	1	42	A	N7-C8-N9	5.30	116.45	113.80
3	A	128	C	C6-N1-C2	5.29	122.42	120.30
3	A	1848	A	N7-C8-N9	5.29	116.44	113.80
3	A	2000	C	C5-C6-N1	-5.29	118.35	121.00
3	A	906	U	O4'-C1'-N1	5.29	112.43	108.20
3	A	135	U	C5-C6-N1	5.29	125.34	122.70
3	A	264	C	N3-C2-O2	-5.29	118.20	121.90
3	A	1494	A	P-O3'-C3'	5.28	126.04	119.70
3	A	809	G	N3-C4-C5	-5.28	125.96	128.60
3	A	569	U	C5-C6-N1	-5.27	120.06	122.70
3	A	1606	C	N1-C2-O2	5.26	122.06	118.90
3	A	1664	A	C8-N9-C4	-5.25	103.70	105.80
4	B	42	C	C6-N1-C2	-5.25	118.20	120.30
1	1	42	A	C6-C5-N7	-5.25	128.62	132.30
3	A	375	G	N3-C4-N9	5.24	129.15	126.00
3	A	1848	A	O4'-C1'-N9	5.24	112.39	108.20
3	A	2022	U	C5-C6-N1	-5.24	120.08	122.70
1	1	42	A	C8-N9-C1'	-5.23	118.28	127.70
3	A	972	A	N9-C4-C5	5.23	107.89	105.80
3	A	672	C	N3-C2-O2	-5.22	118.25	121.90
3	A	2090	A	C8-N9-C4	5.22	107.89	105.80
2	2	74	C	C5-C6-N1	5.20	123.60	121.00
3	A	828	U	C5-C6-N1	-5.20	120.10	122.70
3	A	2542	A	C8-N9-C4	5.18	107.87	105.80
3	A	906	U	C2-N1-C1'	-5.18	111.49	117.70
1	1	70	G	N3-C4-N9	5.17	129.10	126.00
3	A	2074	U	C2-N1-C1'	5.17	123.90	117.70
3	A	375	G	N3-C4-C5	-5.17	126.02	128.60
3	A	2114	A	C8-N9-C4	-5.16	103.74	105.80
3	A	1769	U	C5-C6-N1	-5.15	120.12	122.70
3	A	981	A	C8-N9-C4	5.12	107.85	105.80
3	A	30	G	C8-N9-C4	5.10	108.44	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2115	G	N3-C4-C5	-5.10	126.05	128.60
3	A	2074	U	N3-C2-O2	-5.09	118.63	122.20
3	A	211	C	C6-N1-C2	5.09	122.33	120.30
3	A	2847	U	C5-C6-N1	-5.08	120.16	122.70
3	A	2267	A	C8-N9-C4	-5.08	103.77	105.80
3	A	646	U	C6-N1-C2	-5.07	117.96	121.00
3	A	271	G	C8-N9-C4	5.07	108.43	106.40
3	A	2516	A	C8-N9-C4	5.07	107.83	105.80
3	A	1617	C	C5-C6-N1	-5.06	118.47	121.00
3	A	1958	C	C6-N1-C2	-5.06	118.28	120.30
3	A	1652	A	N7-C8-N9	-5.05	111.28	113.80
3	A	906	U	C6-N1-C1'	5.04	128.26	121.20
3	A	66	C	N3-C2-O2	-5.04	118.38	121.90
3	A	1102	C	C6-N1-C2	-5.04	118.29	120.30
3	A	2580	U	N3-C2-O2	-5.03	118.68	122.20
3	A	2421	G	C4-C5-N7	5.03	112.81	110.80
3	A	878	A	C8-N9-C4	-5.03	103.79	105.80
3	A	2424	C	C5'-C4'-O4'	5.02	115.13	109.10
3	A	2614	A	C8-N9-C4	-5.02	103.79	105.80
3	A	783	A	N1-C6-N6	-5.02	115.59	118.60
3	A	102	U	C6-N1-C1'	-5.01	114.18	121.20
3	A	2013	A	C6-N1-C2	-5.01	115.59	118.60
3	A	1570	A	C8-N9-C4	5.01	107.80	105.80
3	A	804	A	C2-N3-C4	-5.01	108.10	110.60
3	A	1617	C	C2-N3-C4	-5.00	117.40	119.90
3	A	1314	C	C2-N1-C1'	5.00	124.31	118.80
3	A	516	C	C6-N1-C2	5.00	122.30	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	C	232	HIS	Peptide
9	G	47	ASP	Peptide
12	J	19	ASN	Peptide

## 5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	926	0	467	10	0
2	2	62	0	34	1	0
3	A	61902	0	31133	683	0
4	B	2569	0	1301	19	0
5	C	2082	0	2154	51	0
6	D	1565	0	1616	32	0
7	E	1552	0	1619	27	0
8	F	1410	0	1444	42	0
9	G	1323	0	1371	35	0
10	H	1110	0	1148	23	0
11	I	946	0	978	31	0
12	J	979	0	1028	39	0
13	K	1129	0	1162	24	0
14	L	946	0	1023	21	0
15	M	1053	0	1129	26	0
16	N	1074	0	1157	23	0
17	O	993	0	1034	25	0
18	P	900	0	935	23	0
19	Q	917	0	962	19	0
20	R	947	0	1019	24	0
21	S	816	0	839	20	0
22	T	857	0	922	14	0
23	U	756	0	817	14	0
24	V	779	0	831	18	0
25	W	753	0	780	14	0
26	X	580	0	594	16	0
27	Y	625	0	652	17	0
28	Z	501	0	531	13	0
29	a	449	0	488	0	0
30	b	444	0	458	0	0
31	c	414	0	442	0	0
32	d	377	0	418	0	0
33	e	504	0	572	0	0
34	f	302	0	340	0	0
35	i	916	0	944	0	0
36	k	137	0	168	0	0
37	2	1	0	0	0	0
37	A	412	0	0	0	0
37	B	11	0	0	0	0
37	C	2	0	0	0	0
37	D	1	0	0	0	0
37	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	P	1	0	0	0	0
37	R	1	0	0	0	0
37	b	1	0	0	0	0
38	f	1	0	0	0	0
All	All	94027	0	62510	1167	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1167) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1818:U:OP2	5:C:156:ARG:NH1	2.00	0.95
3:A:1168:G:H1	3:A:1181:U:H3	1.20	0.90
3:A:276:U:O2	3:A:278:A:N6	2.08	0.87
3:A:1827:U:OP2	5:C:221:ARG:NH1	2.08	0.86
10:H:3:VAL:HG12	10:H:38:PRO:HA	1.57	0.86
3:A:2135:A:N6	3:A:2156:G:O2'	2.10	0.84
3:A:287:G:O6	3:A:352:A:N6	2.10	0.84
3:A:2107:G:H1	3:A:2182:U:H3	1.22	0.83
5:C:107:PRO:HD2	5:C:110:LEU:HD22	1.59	0.82
3:A:807:U:OP2	15:M:41:ARG:NH1	2.14	0.81
15:M:109:LYS:HG2	15:M:126:ARG:HB2	1.64	0.80
3:A:2128:G:N3	3:A:2173:A:O2'	2.14	0.79
3:A:994:C:O2	21:S:10:LYS:NZ	2.16	0.79
18:P:15:ARG:NH2	18:P:95:SER:OG	2.18	0.77
11:I:41:LEU:HD21	11:I:96:PHE:HE1	1.50	0.77
5:C:245:VAL:HG12	5:C:251:GLN:HA	1.67	0.76
3:A:614:A:O2'	3:A:616:A:N7	2.18	0.76
3:A:2135:A:HO2'	3:A:2159:G:HO2'	1.32	0.76
3:A:2599:G:N7	5:C:236:GLU:HB2	2.02	0.74
3:A:545:U:O2	3:A:548:G:N1	2.19	0.74
3:A:2848:G:O2'	3:A:2867:G:N2	2.19	0.73
5:C:181:MET:HB2	5:C:268:VAL:HB	1.69	0.73
3:A:720:U:H2'	3:A:721:A:C8	2.24	0.72
13:K:131:ASN:N	13:K:131:ASN:OD1	2.22	0.72
3:A:2119:A:N6	3:A:2167:U:O2	2.22	0.72
3:A:331:C:H41	3:A:1210:G:H22	1.37	0.72
7:E:1:MET:HG3	7:E:14:VAL:HG23	1.71	0.71
13:K:70:THR:OG1	13:K:71:ASP:OD1	2.08	0.71
3:A:331:C:H41	3:A:1210:G:N2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2423:U:H2'	3:A:2424:C:O4'	1.89	0.71
14:L:70:ARG:HD3	14:L:76:VAL:HG22	1.72	0.70
3:A:1801:A:OP2	5:C:150:LYS:NZ	2.18	0.70
3:A:2310:C:H2'	8:F:77:PHE:HE2	1.54	0.70
3:A:2163:A:OP1	3:A:2170:A:O2'	2.08	0.70
11:I:50:VAL:HG22	11:I:85:VAL:HG13	1.74	0.70
3:A:1069:A:H4'	3:A:1070:A:H5''	1.71	0.70
3:A:971:G:H2'	3:A:972:A:O4'	1.92	0.70
3:A:258:G:H1'	15:M:104:GLN:HE22	1.56	0.69
3:A:513:A:O2'	20:R:11:ARG:NH1	2.26	0.69
9:G:35:ARG:HD3	9:G:71:LEU:HD13	1.74	0.69
11:I:43:LYS:HG2	11:I:46:ARG:HH22	1.56	0.68
14:L:79:PHE:HD1	19:Q:70:VAL:HG22	1.58	0.68
3:A:1536:C:H4'	3:A:1537:G:H5''	1.75	0.68
3:A:2830:C:H5''	6:D:56:LYS:HE3	1.75	0.68
3:A:362:A:H3'	3:A:363:G:H8	1.59	0.68
3:A:2135:A:O2'	3:A:2159:G:O2'	2.06	0.68
12:J:79:LEU:HB3	12:J:109:ILE:HG12	1.76	0.68
14:L:21:CYS:HA	14:L:41:ILE:HG22	1.76	0.68
3:A:878:A:H3'	3:A:879:G:H8	1.60	0.67
3:A:358:U:H2'	3:A:359:G:H8	1.60	0.67
18:P:31:THR:HG22	18:P:34:HIS:H	1.59	0.67
3:A:1340:U:OP1	23:U:19:LYS:NZ	2.26	0.67
3:A:286:U:H2'	3:A:287:G:H8	1.60	0.67
3:A:2103:C:O2	3:A:2186:G:N1	2.27	0.67
3:A:2122:U:OP1	3:A:2168:G:N2	2.26	0.67
3:A:1105:U:H2'	3:A:1106:G:C8	2.29	0.66
3:A:196:A:OP2	15:M:47:ARG:NH1	2.28	0.66
3:A:286:U:H2'	3:A:287:G:C8	2.31	0.66
27:Y:32:ASN:O	27:Y:52:SER:HA	1.95	0.66
3:A:2209:G:H1	3:A:2215:C:H42	1.44	0.66
3:A:2590:A:H2'	3:A:2591:C:H6	1.61	0.66
13:K:31:GLU:HG3	13:K:142:ILE:HG13	1.77	0.66
3:A:2713:U:H3'	3:A:2714:G:H5''	1.77	0.66
3:A:2305:U:C2	8:F:151:GLY:HA3	2.31	0.66
10:H:84:ALA:HA	10:H:90:LEU:HA	1.78	0.66
4:B:43:C:O2	8:F:92:ARG:NH2	2.28	0.66
3:A:2216:G:H2'	3:A:2217:G:H8	1.60	0.66
3:A:572:A:OP2	21:S:80:ARG:NH2	2.27	0.66
3:A:2303:G:O2'	8:F:121:SER:O	2.13	0.65
28:Z:10:SER:N	28:Z:13:GLU:OE1	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1344:U:O2'	3:A:1345:C:OP1	2.14	0.65
3:A:1597:A:H5''	3:A:1598:A:H5'	1.78	0.65
9:G:9:VAL:HG22	9:G:69:ARG:HE	1.61	0.65
3:A:860:U:H1'	3:A:2268:A:H5'	1.78	0.65
7:E:87:ALA:O	7:E:88:ARG:NH2	2.30	0.65
1:1:49:G:H1	1:1:60:A:H61	1.43	0.65
8:F:158:THR:HG22	8:F:160:ALA:H	1.62	0.65
3:A:370:G:O2'	3:A:424:G:OP1	2.11	0.65
3:A:1794:A:H2'	3:A:1795:C:H6	1.61	0.65
16:N:50:ARG:O	16:N:54:THR:OG1	2.13	0.64
3:A:1869:G:N2	3:A:1871:A:O2'	2.30	0.64
3:A:1007:C:OP1	13:K:37:ARG:NH2	2.29	0.64
3:A:1342:A:O2'	3:A:1344:U:OP2	2.16	0.64
3:A:2674:G:H4'	14:L:30:ARG:HG3	1.78	0.64
3:A:1510:G:H2'	3:A:1511:G:C8	2.32	0.64
3:A:2788:C:O2'	3:A:2809:A:N3	2.28	0.64
26:X:65:GLY:HA2	26:X:85:GLU:HG2	1.78	0.64
3:A:2424:C:H5''	3:A:2425:A:H5'	1.79	0.64
3:A:968:C:H2'	3:A:969:G:H8	1.62	0.64
3:A:1105:U:H2'	3:A:1106:G:H8	1.63	0.64
3:A:2102:G:N2	3:A:2187:U:O2	2.31	0.63
3:A:322:A:H5'	3:A:340:A:H1'	1.78	0.63
20:R:74:ILE:HD11	20:R:78:LYS:HB3	1.80	0.63
3:A:1094:U:N3	3:A:1097:U:OP2	2.30	0.63
3:A:1614:A:N1	22:T:93:ALA:HB2	2.13	0.63
8:F:144:ASP:OD1	8:F:144:ASP:N	2.30	0.63
8:F:74:VAL:HG22	8:F:79:ILE:HD11	1.79	0.63
16:N:14:LYS:O	16:N:71:LYS:NZ	2.32	0.63
3:A:1980:G:O2'	3:A:1982:U:OP2	2.16	0.63
21:S:41:ILE:HB	21:S:48:LYS:HD2	1.79	0.63
22:T:82:MET:HB3	22:T:84:ARG:HH22	1.63	0.63
3:A:284:U:H3	3:A:356:G:H1	1.44	0.63
3:A:2151:U:H2'	3:A:2152:G:C8	2.34	0.63
19:Q:91:ALA:HB2	19:Q:113:ARG:HA	1.80	0.63
3:A:1187:G:OP1	21:S:85:LYS:NZ	2.31	0.62
3:A:2116:G:N7	3:A:2165:C:N4	2.44	0.62
25:W:21:ARG:NH2	25:W:87:GLN:O	2.28	0.62
3:A:1433:A:N1	3:A:1434:A:N6	2.47	0.62
13:K:117:ALA:HA	13:K:120:ARG:HH21	1.64	0.62
3:A:514:A:N3	3:A:581:C:O2'	2.32	0.62
17:O:49:GLU:HA	17:O:52:ILE:HD12	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:58:ARG:HA	20:R:61:TRP:CE3	2.34	0.62
3:A:784:G:C6	5:C:228:VAL:HG11	2.35	0.62
19:Q:4:ILE:H	19:Q:4:ILE:HD12	1.65	0.62
3:A:2809:A:H2'	3:A:2810:A:C8	2.34	0.62
3:A:825:A:H2'	3:A:826:U:O4'	1.98	0.62
3:A:2590:A:H2'	3:A:2591:C:C6	2.35	0.62
10:H:68:ARG:HA	10:H:71:LYS:HD2	1.81	0.62
3:A:2822:G:O6	17:O:2:ARG:NH1	2.32	0.61
12:J:53:LEU:HD11	12:J:82:LYS:HD2	1.83	0.61
11:I:57:ASN:ND2	11:I:76:PHE:O	2.33	0.61
3:A:1079:C:O2'	12:J:134:ARG:NH1	2.33	0.61
15:M:57:LEU:HD13	15:M:60:ARG:HH11	1.65	0.61
3:A:2636:C:HO2'	6:D:45:TYR:HH	1.47	0.61
3:A:2639:A:H2'	3:A:2640:G:O4'	2.01	0.61
3:A:2310:C:H2'	8:F:77:PHE:CE2	2.35	0.61
17:O:54:LEU:HD21	17:O:65:LEU:HD23	1.82	0.61
3:A:1001:A:H2'	3:A:1002:G:O4'	2.01	0.61
5:C:235:GLY:HA3	5:C:239:ASN:HB2	1.83	0.61
11:I:41:LEU:HD21	11:I:96:PHE:CE1	2.34	0.61
3:A:585:G:N7	20:R:6:ARG:NH1	2.48	0.60
3:A:503:A:H4'	3:A:504:A:H5'	1.83	0.60
6:D:12:THR:OG1	6:D:13:ARG:N	2.34	0.60
3:A:2060:A:H3'	7:E:63:LYS:HZ1	1.65	0.60
22:T:6:LYS:HG2	22:T:104:THR:HG23	1.82	0.60
3:A:570:G:H2'	3:A:2030:A:N7	2.16	0.60
9:G:137:ASP:O	9:G:141:ILE:HG22	2.01	0.60
26:X:56:ASP:N	26:X:56:ASP:OD1	2.28	0.60
3:A:1076:C:H2'	3:A:1077:A:C8	2.37	0.60
3:A:1363:C:O2'	3:A:1809:A:N3	2.33	0.60
3:A:1794:A:H2'	3:A:1795:C:C6	2.37	0.60
6:D:2:ILE:HG13	6:D:100:LEU:HD21	1.83	0.60
11:I:27:VAL:HG22	11:I:82:ILE:HG22	1.83	0.60
7:E:97:ASN:OD1	7:E:97:ASN:N	2.34	0.60
15:M:81:ASP:HA	15:M:84:LYS:HD2	1.82	0.60
3:A:2831:G:OP1	6:D:56:LYS:NZ	2.35	0.60
3:A:776:G:O2'	3:A:777:G:OP1	2.19	0.60
3:A:355:U:H2'	3:A:356:G:C8	2.37	0.59
8:F:44:ILE:HG21	8:F:79:ILE:HG22	1.83	0.59
3:A:1796:U:H2'	3:A:1797:G:H8	1.67	0.59
3:A:2584:U:H3'	3:A:2585:U:H5''	1.84	0.59
3:A:2819:G:H2'	3:A:2821:A:N7	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:36:LEU:HD11	13:K:122:LEU:HB2	1.83	0.59
9:G:27:LYS:NZ	9:G:27:LYS:HB3	2.17	0.59
18:P:99:TYR:OH	18:P:111:ARG:NH1	2.36	0.59
3:A:2205:A:H61	3:A:2219:U:H3	1.50	0.59
3:A:878:A:H3'	3:A:879:G:C8	2.38	0.59
11:I:64:VAL:HG22	11:I:69:PHE:HB2	1.84	0.59
24:V:81:ASP:OD1	24:V:82:ARG:N	2.35	0.59
4:B:7:G:OP1	18:P:4:LYS:NZ	2.27	0.59
3:A:1170:C:O2	3:A:1179:G:N2	2.33	0.58
3:A:2021:C:OP1	20:R:25:TYR:OH	2.21	0.58
3:A:2127:G:O2'	3:A:2128:G:O5'	2.19	0.58
3:A:1808:A:H3'	3:A:1809:A:C8	2.38	0.58
3:A:1130:U:O2'	3:A:1131:G:H8	1.87	0.58
3:A:833:A:H2'	3:A:834:G:C8	2.38	0.58
3:A:396:G:OP2	27:Y:10:LYS:NZ	2.36	0.58
3:A:2127:G:O2'	3:A:2128:G:O4'	2.20	0.58
17:O:73:ASN:HA	17:O:76:VAL:HG22	1.86	0.58
21:S:37:GLU:HB3	21:S:53:PHE:CE1	2.39	0.58
25:W:76:ASP:OD1	25:W:77:VAL:N	2.37	0.58
12:J:106:LEU:HB3	12:J:126:THR:HG23	1.85	0.58
18:P:41:ALA:HB2	18:P:48:LEU:HD21	1.86	0.58
6:D:148:GLN:HB2	6:D:152:PRO:HD2	1.85	0.58
3:A:1715:G:O2'	3:A:1743:G:O6	2.17	0.57
3:A:2412:A:H2'	3:A:2413:G:O4'	2.04	0.57
7:E:21:ARG:HD3	7:E:106:LYS:HB3	1.85	0.57
3:A:2291:U:H2'	3:A:2292:U:C6	2.38	0.57
3:A:2602:A:H4'	3:A:2603:G:O5'	2.04	0.57
5:C:227:PRO:HG3	5:C:234:GLY:H	1.69	0.57
12:J:59:ILE:HD13	12:J:69:PHE:HB3	1.86	0.57
3:A:849:A:H2'	3:A:850:U:C6	2.39	0.57
6:D:157:LYS:HD2	13:K:80:HIS:CE1	2.40	0.57
17:O:94:TYR:O	17:O:116:VAL:HG23	2.05	0.57
3:A:1645:G:H5''	3:A:1646:C:H5'	1.86	0.57
3:A:2447:G:N2	3:A:2450:A:OP2	2.37	0.57
10:H:37:VAL:HG22	10:H:38:PRO:HD2	1.85	0.57
3:A:340:A:H2'	3:A:341:C:O4'	2.05	0.57
3:A:839:U:H2'	3:A:840:C:C6	2.40	0.57
6:D:13:ARG:HD2	6:D:15:PHE:CZ	2.38	0.57
7:E:112:LEU:HB3	7:E:118:LEU:HB2	1.87	0.57
3:A:876:C:H2'	3:A:877:A:O4'	2.05	0.57
6:D:1:MET:HG2	6:D:2:ILE:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2216:G:H2'	3:A:2217:G:C8	2.40	0.56
8:F:33:LYS:HG2	8:F:157:THR:HB	1.87	0.56
24:V:18:ASP:OD2	24:V:40:ASN:N	2.38	0.56
3:A:1905:C:H2'	3:A:1930:G:C8	2.40	0.56
3:A:299:A:N1	3:A:322:A:O2'	2.27	0.56
3:A:1063:G:H5'	12:J:77:ALA:HB1	1.87	0.56
3:A:1796:U:H2'	3:A:1797:G:C8	2.40	0.56
3:A:721:A:H2'	3:A:722:A:C8	2.41	0.56
3:A:26:G:C6	3:A:27:G:N1	2.73	0.56
11:I:60:LEU:O	11:I:64:VAL:HB	2.06	0.56
3:A:1800:C:H5'	5:C:146:MET:HE1	1.87	0.56
3:A:480:A:OP2	24:V:44:LYS:NZ	2.23	0.56
5:C:166:ALA:HB3	5:C:173:THR:HB	1.86	0.56
3:A:2162:G:H5''	3:A:2171:A:H2'	1.86	0.56
3:A:1790:C:H3'	3:A:1828:G:N2	2.21	0.56
3:A:388:G:N7	3:A:390:U:H2'	2.21	0.56
9:G:30:ASN:HB3	9:G:79:VAL:HA	1.88	0.56
3:A:1076:C:H2'	3:A:1077:A:H8	1.69	0.56
3:A:2491:U:H5''	3:A:2570:G:H5''	1.88	0.56
4:B:42:C:C5	8:F:66:LEU:HD22	2.41	0.56
3:A:2133:G:H2'	3:A:2157:G:H1	1.70	0.56
3:A:2430:A:N3	3:A:2430:A:H2'	2.21	0.56
3:A:2584:U:H3'	3:A:2585:U:C5'	2.36	0.56
12:J:73:THR:HB	12:J:112:THR:HG22	1.87	0.56
3:A:1251:C:OP2	20:R:6:ARG:NH2	2.35	0.56
3:A:2298:A:H2'	3:A:2299:U:O4'	2.05	0.56
12:J:53:LEU:HD22	12:J:78:VAL:HG13	1.87	0.56
13:K:72:LYS:HE3	13:K:74:TYR:CE1	2.39	0.56
3:A:812:C:H4'	20:R:13:ARG:NH1	2.21	0.56
3:A:1442:U:H2'	3:A:1443:U:C6	2.41	0.55
17:O:2:ARG:HB3	17:O:2:ARG:NH1	2.21	0.55
25:W:62:THR:HG22	25:W:71:LYS:HG2	1.88	0.55
12:J:127:ARG:HA	12:J:130:GLU:HB2	1.89	0.55
18:P:16:ARG:HA	18:P:16:ARG:HH21	1.71	0.55
3:A:19:A:H2'	3:A:20:C:C6	2.41	0.55
3:A:2171:A:H3'	3:A:2173:A:C8	2.41	0.55
3:A:849:A:H2'	3:A:850:U:H6	1.70	0.55
3:A:2783:U:H2'	3:A:2784:U:C6	2.42	0.55
10:H:7:ASP:OD1	10:H:8:LYS:N	2.40	0.55
24:V:33:LYS:HB3	24:V:64:ALA:HB1	1.87	0.55
3:A:184:C:H2'	3:A:185:G:C8	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:591:U:H2'	3:A:592:A:H8	1.72	0.55
3:A:882:G:H1	3:A:894:U:H3	1.54	0.55
5:C:160:THR:HG22	5:C:177:ARG:HG2	1.89	0.55
3:A:2591:C:H2'	3:A:2592:G:C8	2.41	0.55
3:A:639:U:H2'	3:A:640:C:C6	2.42	0.55
17:O:48:VAL:O	17:O:51:LEU:HB2	2.05	0.55
3:A:2070:A:H2'	3:A:2071:A:C8	2.42	0.55
6:D:8:LYS:HB2	6:D:201:LEU:HD11	1.88	0.55
8:F:132:VAL:HG22	8:F:152:LEU:HB3	1.88	0.55
18:P:69:ASP:N	18:P:69:ASP:OD1	2.40	0.55
3:A:2262:U:H2'	3:A:2263:C:H6	1.72	0.54
8:F:134:GLU:HB3	8:F:136:ILE:HG12	1.89	0.54
3:A:833:A:H2'	3:A:834:G:H8	1.72	0.54
6:D:184:ARG:NH1	19:Q:7:GLN:OE1	2.40	0.54
7:E:88:ARG:HH21	7:E:88:ARG:HA	1.72	0.54
13:K:34:ARG:HH22	13:K:40:HIS:HB3	1.71	0.54
3:A:1837:C:H2'	3:A:1899:A:H61	1.73	0.54
3:A:586:A:H5'	7:E:84:THR:HG21	1.90	0.54
3:A:609:A:H2'	3:A:610:C:O4'	2.08	0.54
3:A:2619:C:H5''	6:D:157:LYS:HG3	1.89	0.54
3:A:2424:C:H5''	3:A:2425:A:C5'	2.37	0.54
12:J:79:LEU:HA	12:J:82:LYS:HG2	1.88	0.54
3:A:996:A:OP2	21:S:10:LYS:HD3	2.07	0.54
3:A:1923:U:H2'	3:A:1924:C:C6	2.43	0.54
3:A:2267:A:H5''	3:A:2268:A:H5''	1.89	0.54
12:J:56:PRO:HD3	12:J:75:PRO:HD3	1.90	0.54
3:A:172:A:H2'	3:A:173:A:C8	2.43	0.54
21:S:48:LYS:HE3	21:S:103:ALA:HB1	1.90	0.54
23:U:68:LYS:HG3	23:U:77:ARG:NH2	2.23	0.54
23:U:56:GLU:HA	23:U:88:LYS:HE3	1.89	0.54
3:A:2845:U:H5''	19:Q:52:ASN:O	2.08	0.54
3:A:2579:C:O2'	6:D:136:ASN:ND2	2.41	0.54
9:G:104:ASN:ND2	9:G:114:ASP:OD1	2.41	0.54
3:A:2834:G:O6	3:A:2879:A:H2'	2.08	0.54
21:S:20:VAL:HG13	21:S:96:VAL:HG23	1.89	0.53
3:A:2443:C:H2'	3:A:2444:G:C8	2.43	0.53
3:A:2808:G:O2'	3:A:2890:G:O6	2.21	0.53
5:C:145:GLU:HB2	5:C:188:CYS:HB3	1.89	0.53
3:A:284:U:O2	3:A:356:G:N2	2.37	0.53
3:A:608:A:H2'	3:A:609:A:C8	2.44	0.53
14:L:38:ILE:HD11	14:L:112:PHE:HZ	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2547:A:H4'	14:L:29:HIS:CD2	2.44	0.53
14:L:40:LYS:HE3	14:L:57:VAL:HG12	1.91	0.53
3:A:1056:G:H5''	3:A:1057:A:H5'	1.90	0.53
3:A:720:U:H2'	3:A:721:A:H8	1.72	0.53
3:A:9:G:O2'	3:A:2800:A:N6	2.42	0.53
11:I:88:HIS:ND1	11:I:89:PRO:O	2.42	0.53
17:O:36:THR:OG1	17:O:37:THR:N	2.42	0.53
3:A:1069:A:C2	3:A:1096:A:H5''	2.44	0.53
3:A:788:A:OP1	3:A:791:C:N4	2.41	0.53
11:I:54:VAL:HG22	11:I:81:LEU:HD13	1.90	0.53
3:A:2171:A:H3'	3:A:2173:A:H8	1.74	0.53
3:A:1056:G:O2'	3:A:1103:A:N6	2.40	0.52
3:A:1873:G:H2'	3:A:1874:C:H6	1.74	0.52
10:H:116:ARG:HH21	10:H:133:GLN:HB3	1.74	0.52
17:O:36:THR:HG23	17:O:41:ALA:HB2	1.90	0.52
3:A:2086:U:H2'	3:A:2087:G:C8	2.44	0.52
3:A:2210:U:H4'	3:A:2211:A:H5'	1.91	0.52
3:A:2280:G:O2'	3:A:2388:A:N1	2.37	0.52
5:C:62:TYR:HA	5:C:86:ASN:HD21	1.73	0.52
3:A:1425:G:H2'	3:A:1426:G:O4'	2.09	0.52
3:A:1428:C:C5	3:A:1569:A:H5''	2.45	0.52
3:A:1993:U:H4'	6:D:133:THR:OG1	2.10	0.52
3:A:653:U:H1'	3:A:654:A:H5''	1.91	0.52
3:A:679:C:H2'	3:A:680:C:C6	2.44	0.52
3:A:68:G:H2'	3:A:69:C:O4'	2.10	0.52
25:W:55:GLU:CD	25:W:55:GLU:H	2.12	0.52
1:1:60:A:H2'	1:1:61:G:O4'	2.09	0.52
3:A:1410:G:H1	3:A:1592:C:H42	1.57	0.52
3:A:671:C:H2'	3:A:672:C:H6	1.74	0.52
8:F:99:PHE:HD1	8:F:102:ARG:HH22	1.57	0.52
13:K:3:THR:HB	20:R:57:PHE:HE1	1.75	0.52
3:A:1421:G:C2	3:A:1422:G:C8	2.98	0.52
1:1:47:A:OP2	1:1:61:G:N1	2.42	0.52
1:1:48:G:H3'	1:1:49:G:H8	1.75	0.52
3:A:1791:A:N6	3:A:1828:G:O2'	2.42	0.52
3:A:2127:G:H2'	3:A:2128:G:C8	2.45	0.52
3:A:845:A:H61	3:A:932:U:H3	1.58	0.52
6:D:114:LYS:HD3	6:D:196:ALA:HB2	1.92	0.52
3:A:898:C:H2'	3:A:899:A:O4'	2.10	0.52
21:S:52:PRO:HG2	21:S:53:PHE:CD2	2.45	0.52
3:A:1289:C:H2'	3:A:1290:C:C6	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1798:U:H5''	5:C:258:ARG:HB2	1.92	0.52
3:A:2637:U:C2'	3:A:2638:G:H5'	2.39	0.52
4:B:93:C:OP2	25:W:18:ARG:NH1	2.42	0.52
7:E:28:VAL:O	7:E:32:VAL:HG13	2.09	0.52
23:U:93:LEU:HD13	23:U:95:PHE:CZ	2.44	0.52
3:A:1451:C:H1'	3:A:1452:G:C2	2.45	0.52
3:A:1681:G:H21	3:A:1762:A:H3'	1.75	0.52
3:A:90:U:H3'	3:A:91:A:H8	1.74	0.52
3:A:120:U:H4'	3:A:121:G:H5''	1.89	0.52
3:A:2133:G:H21	3:A:2158:A:H62	1.58	0.52
24:V:74:ASN:HD21	24:V:99:ASN:HD21	1.58	0.52
3:A:1437:C:H2'	3:A:1438:U:C6	2.45	0.51
12:J:73:THR:OG1	12:J:113:LYS:NZ	2.40	0.51
3:A:2439:A:H4'	3:A:2440:C:H5''	1.91	0.51
3:A:256:A:H2'	3:A:257:C:H6	1.74	0.51
3:A:2850:A:N7	3:A:2868:A:O2'	2.39	0.51
28:Z:2:LYS:HG3	28:Z:5:GLU:OE1	2.10	0.51
3:A:1790:C:H2'	3:A:1791:A:C5	2.45	0.51
8:F:128:TYR:HE2	8:F:130:MET:HG2	1.76	0.51
3:A:1000:A:OP2	3:A:1154:G:N1	2.32	0.51
3:A:1115:G:O2'	3:A:1116:G:H5''	2.10	0.51
3:A:1414:C:H2'	3:A:1415:U:O4'	2.11	0.51
3:A:968:C:H2'	3:A:969:G:C8	2.42	0.51
7:E:24:ASN:ND2	7:E:27:LEU:HB2	2.25	0.51
3:A:2647:U:H2'	3:A:2648:G:H8	1.76	0.51
3:A:948:C:H2'	3:A:949:G:C8	2.45	0.51
17:O:55:ALA:HA	17:O:80:PHE:CE2	2.45	0.51
3:A:2720:U:OP1	19:Q:53:ARG:NH2	2.41	0.51
3:A:141:G:H2'	3:A:142:A:O4'	2.11	0.51
3:A:499:U:H2'	3:A:500:G:O4'	2.10	0.51
7:E:145:ASP:HA	7:E:166:LYS:HB3	1.92	0.51
20:R:24:TYR:N	20:R:24:TYR:CD1	2.78	0.51
3:A:364:C:H2'	3:A:365:U:C6	2.45	0.51
3:A:576:U:H2'	3:A:577:G:C8	2.46	0.51
7:E:41:GLN:HG2	7:E:43:THR:HG23	1.92	0.51
15:M:36:LYS:O	15:M:40:SER:HB3	2.11	0.51
3:A:621:A:OP2	15:M:99:ASN:ND2	2.40	0.51
19:Q:16:ASP:N	19:Q:16:ASP:OD1	2.33	0.51
21:S:28:ALA:HB3	21:S:31:GLU:HG3	1.93	0.51
3:A:2502:G:H5''	3:A:2503:A:H5''	1.93	0.51
3:A:645:C:O2'	3:A:646:U:OP1	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2271:G:H5''	26:X:18:ALA:HB1	1.93	0.51
3:A:1405:U:H2'	3:A:1406:U:C6	2.46	0.51
3:A:2333:A:P	26:X:77:ARG:HH22	2.34	0.51
12:J:113:LYS:HE3	12:J:116:ASP:HB3	1.92	0.50
16:N:1:MET:HA	16:N:47:GLU:HG3	1.94	0.50
3:A:1394:U:H4'	3:A:1603:A:H4'	1.92	0.50
13:K:32:LEU:O	13:K:36:LEU:HB2	2.12	0.50
3:A:1132:U:H2'	3:A:1133:A:C8	2.46	0.50
3:A:1927:A:H2'	3:A:1928:A:C8	2.46	0.50
3:A:357:C:H2'	3:A:358:U:C6	2.47	0.50
8:F:40:VAL:HG11	8:F:43:ALA:HB2	1.92	0.50
16:N:30:SER:H	16:N:106:ASP:HB3	1.75	0.50
22:T:40:ASN:O	22:T:41:LYS:HG2	2.10	0.50
3:A:1342:A:OP1	23:U:40:LYS:NZ	2.33	0.50
3:A:2024:G:H2'	3:A:2025:C:H6	1.76	0.50
3:A:2282:G:C6	3:A:2425:A:C2	3.00	0.50
3:A:256:A:H2'	3:A:257:C:C6	2.46	0.50
14:L:64:ARG:NH1	14:L:102:PRO:O	2.44	0.50
15:M:23:ILE:HG12	21:S:82:HIS:CD2	2.47	0.50
3:A:128:C:H2'	3:A:129:C:C6	2.46	0.50
23:U:7:LEU:HD13	23:U:46:ALA:HA	1.92	0.50
20:R:65:ILE:HD11	20:R:95:LEU:HB2	1.93	0.50
24:V:46:GLN:OE1	24:V:54:GLN:NE2	2.44	0.50
3:A:2183:A:H2'	3:A:2184:A:C8	2.46	0.50
3:A:90:U:C2	3:A:91:A:N7	2.80	0.50
10:H:94:ILE:HB	10:H:122:LEU:HB2	1.94	0.50
28:Z:39:GLN:HB3	28:Z:41:HIS:CE1	2.47	0.50
3:A:2308:G:H3'	3:A:2310:C:OP2	2.11	0.50
3:A:738:G:H1'	3:A:759:G:N2	2.27	0.50
4:B:2:G:H2'	4:B:3:C:C6	2.47	0.50
5:C:132:MET:HG2	5:C:135:ILE:HD12	1.94	0.50
9:G:127:THR:HG22	9:G:128:GLN:H	1.77	0.50
20:R:76:TYR:CZ	20:R:80:ILE:HG13	2.46	0.50
8:F:17:MET:SD	8:F:22:TYR:HB2	2.52	0.50
9:G:83:PHE:O	9:G:134:LYS:HA	2.12	0.50
12:J:83:ALA:O	12:J:105:GLN:NE2	2.45	0.50
3:A:1021:A:N3	3:A:1021:A:H3'	2.27	0.49
3:A:1638:C:H1'	3:A:2698:U:O2'	2.12	0.49
3:A:1327:A:N6	3:A:1647:U:O2	2.45	0.49
3:A:878:A:N6	3:A:899:A:O2'	2.45	0.49
17:O:14:SER:HA	17:O:17:ARG:NH1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:75:GLN:HB2	25:W:92:VAL:HG12	1.94	0.49
3:A:1187:G:HO2'	3:A:1188:U:H6	1.60	0.49
3:A:2171:A:H5'	3:A:2173:A:N7	2.26	0.49
3:A:613:A:O2'	3:A:614:A:O5'	2.30	0.49
9:G:8:PRO:HB3	9:G:51:THR:HG22	1.94	0.49
19:Q:23:GLY:O	19:Q:90:GLY:HA3	2.11	0.49
3:A:1506:U:H2'	3:A:1507:C:C6	2.48	0.49
3:A:2809:A:H2'	3:A:2810:A:H8	1.75	0.49
8:F:50:LEU:O	8:F:54:ALA:N	2.38	0.49
3:A:2747:G:O2'	9:G:67:THR:HG23	2.12	0.49
18:P:30:ARG:HG3	18:P:35:ILE:HD12	1.94	0.49
26:X:34:GLY:N	26:X:61:ALA:O	2.37	0.49
3:A:1088:A:N6	12:J:135:SER:HB3	2.26	0.49
3:A:2576:G:O2'	3:A:2579:C:OP2	2.23	0.49
3:A:2626:C:H2'	3:A:2627:G:O4'	2.12	0.49
7:E:184:ASP:N	7:E:184:ASP:OD1	2.43	0.49
9:G:101:ASN:ND2	9:G:116:GLN:OE1	2.46	0.49
15:M:4:ASN:N	15:M:4:ASN:OD1	2.39	0.49
3:A:1939:U:OP1	3:A:2604:U:O2'	2.28	0.49
3:A:2073:C:H2'	3:A:2074:U:H6	1.77	0.49
3:A:27:G:N2	3:A:512:G:H1'	2.28	0.49
3:A:671:C:H2'	3:A:672:C:C6	2.47	0.49
3:A:1243:C:H1'	15:M:4:ASN:O	2.13	0.49
3:A:563:A:C4	3:A:2018:G:C2	3.01	0.49
11:I:33:VAL:HG21	11:I:106:PHE:CE2	2.47	0.49
15:M:19:LEU:HD23	15:M:27:LEU:HD13	1.95	0.49
3:A:1606:C:H5'	3:A:1607:C:OP1	2.13	0.49
21:S:65:ALA:HB3	21:S:95:ASP:HB2	1.94	0.49
3:A:1005:C:H2'	3:A:1006:C:C6	2.47	0.49
3:A:1903:G:C2	3:A:1904:G:C8	3.00	0.49
3:A:2564:A:OP1	3:A:2648:G:O2'	2.19	0.49
7:E:23:PHE:CD1	7:E:111:GLU:HG3	2.48	0.49
10:H:110:VAL:HG12	10:H:114:GLU:HB2	1.94	0.49
14:L:10:VAL:HG12	14:L:12:ASP:H	1.78	0.49
3:A:1093:G:C2'	3:A:1098:A:H61	2.26	0.48
3:A:184:C:H2'	3:A:185:G:H8	1.77	0.48
3:A:2151:U:H2'	3:A:2152:G:H8	1.77	0.48
3:A:2483:C:N3	16:N:123:LYS:NZ	2.60	0.48
3:A:1819:A:H5''	5:C:160:THR:HG21	1.94	0.48
3:A:784:G:H5'	3:A:785:G:OP1	2.13	0.48
12:J:113:LYS:O	12:J:117:MET:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1654:A:H2'	3:A:1655:A:H8	1.78	0.48
3:A:1790:C:H3'	3:A:1828:G:H22	1.77	0.48
3:A:2290:G:H2'	3:A:2291:U:O4'	2.12	0.48
4:B:116:G:H2'	4:B:117:G:C8	2.49	0.48
27:Y:17:ASN:HB2	27:Y:25:THR:OG1	2.13	0.48
27:Y:6:GLN:NE2	27:Y:76:GLU:OE2	2.39	0.48
3:A:719:C:H2'	3:A:720:U:H6	1.78	0.48
3:A:140:C:H4'	3:A:141:G:OP1	2.13	0.48
3:A:2116:G:C5	3:A:2165:C:N4	2.82	0.48
3:A:813:U:H2'	3:A:814:C:C6	2.49	0.48
9:G:86:LYS:HG2	9:G:132:VAL:HG22	1.96	0.48
27:Y:17:ASN:OD1	27:Y:27:ARG:HD2	2.13	0.48
3:A:1179:G:H2'	3:A:1180:U:C6	2.48	0.48
3:A:136:G:H2'	3:A:137:U:O4'	2.13	0.48
3:A:1773:A:N7	3:A:1829:A:H1'	2.28	0.48
3:A:2158:A:H4'	3:A:2159:G:O5'	2.14	0.48
3:A:467:G:H2'	3:A:468:G:O4'	2.13	0.48
5:C:145:GLU:HG2	5:C:151:GLY:C	2.34	0.48
9:G:80:THR:OG1	9:G:81:GLU:N	2.46	0.48
18:P:51:ALA:HB3	18:P:78:VAL:HG13	1.95	0.48
23:U:68:LYS:HG3	23:U:77:ARG:HH21	1.79	0.48
26:X:40:GLN:NE2	26:X:43:THR:HA	2.29	0.48
1:1:49:G:H1	1:1:60:A:N6	2.10	0.48
3:A:2209:G:H1	3:A:2215:C:N4	2.11	0.48
17:O:38:LEU:HB3	17:O:39:PRO:HD3	1.95	0.48
3:A:175:G:N2	3:A:176:A:N3	2.62	0.48
3:A:2428:G:H21	15:M:60:ARG:NH2	2.12	0.48
3:A:428:A:H2'	3:A:429:A:C8	2.49	0.48
3:A:914:G:H5'	3:A:915:C:OP2	2.13	0.48
13:K:72:LYS:HE3	13:K:74:TYR:CZ	2.49	0.48
28:Z:14:LEU:HB3	28:Z:57:LEU:HD21	1.96	0.48
3:A:1132:U:H3'	3:A:1133:A:H5''	1.95	0.48
3:A:160:A:N3	3:A:2208:C:O2'	2.43	0.48
5:C:175:ARG:HG3	5:C:181:MET:HE1	1.96	0.48
3:A:782:A:N7	5:C:220:VAL:HG21	2.29	0.48
6:D:25:THR:HG21	6:D:193:VAL:HG22	1.95	0.48
8:F:7:TYR:CD1	8:F:11:GLU:HG3	2.48	0.48
10:H:115:VAL:HG22	10:H:132:PHE:CE2	2.48	0.48
16:N:11:LYS:HD3	16:N:86:LYS:HD3	1.96	0.48
23:U:58:VAL:HG22	23:U:85:VAL:HG22	1.96	0.48
3:A:2433:A:H2	27:Y:21:ALA:HB1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1268:A:H2'	3:A:1269:A:O4'	2.13	0.48
3:A:1386:C:H2'	3:A:1387:A:C8	2.49	0.48
3:A:1527:G:N1	3:A:1544:A:OP2	2.32	0.48
3:A:1846:G:H5''	3:A:1847:A:OP2	2.14	0.48
3:A:2570:G:H2'	3:A:2571:U:O4'	2.14	0.48
3:A:2834:G:H2'	3:A:2879:A:N6	2.29	0.48
5:C:260:ASN:OD1	5:C:262:ARG:N	2.37	0.48
3:A:2305:U:H5''	8:F:131:GLY:HA3	1.96	0.48
13:K:58:ASN:ND2	13:K:128:ASN:OD1	2.42	0.48
16:N:41:LEU:HG	16:N:96:ILE:HG13	1.95	0.48
3:A:156:A:H2'	3:A:157:C:O4'	2.13	0.47
3:A:2226:C:H2'	3:A:2227:A:O4'	2.13	0.47
9:G:155:GLU:OE1	9:G:157:TYR:N	2.45	0.47
10:H:142:VAL:HG12	10:H:143:ILE:H	1.79	0.47
3:A:483:A:O4'	24:V:45:HIS:HB3	2.14	0.47
3:A:2060:A:H3'	7:E:63:LYS:NZ	2.29	0.47
3:A:208:C:H2'	3:A:209:C:H6	1.78	0.47
3:A:2444:G:OP2	7:E:63:LYS:HD2	2.14	0.47
3:A:477:A:H2'	3:A:478:A:C8	2.49	0.47
3:A:910:A:H2'	3:A:911:A:C8	2.48	0.47
13:K:32:LEU:O	13:K:36:LEU:HG	3.31	0.47
13:K:78:THR:HG23	13:K:83:GLY:O	2.13	0.47
6:D:56:LYS:HB2	6:D:59:ARG:HB2	1.95	0.47
9:G:35:ARG:CD	9:G:71:LEU:HD13	2.44	0.47
10:H:93:SER:HB3	10:H:123:ARG:HG2	1.95	0.47
12:J:10:LYS:O	12:J:11:LEU:HD12	2.15	0.47
12:J:42:PHE:O	12:J:46:THR:OG1	2.32	0.47
22:T:96:ILE:HA	22:T:96:ILE:HD13	1.74	0.47
3:A:1027:A:C6	3:A:1126:A:C4	3.02	0.47
3:A:112:U:H5'	28:Z:58:ASN:HD21	1.80	0.47
3:A:1438:U:H2'	3:A:1439:A:H8	1.79	0.47
3:A:795:C:H2'	3:A:796:C:C6	2.49	0.47
3:A:957:C:C5	3:A:959:A:C5	3.01	0.47
3:A:995:C:OP2	20:R:54:LYS:NZ	2.44	0.47
13:K:114:LEU:O	13:K:118:MET:HG3	2.14	0.47
3:A:1446:C:H2'	3:A:1447:C:C6	2.49	0.47
3:A:1873:G:H2'	3:A:1874:C:C6	2.49	0.47
11:I:85:VAL:HG22	11:I:92:ALA:HB2	1.96	0.47
12:J:40:LYS:N	12:J:40:LYS:HD2	2.30	0.47
15:M:55:MET:SD	15:M:56:PRO:HD2	2.55	0.47
24:V:14:LEU:HD11	24:V:71:ALA:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1007:C:H5''	13:K:37:ARG:NH2	2.28	0.47
3:A:127:A:H5''	3:A:128:C:O4'	2.14	0.47
3:A:2592:G:C6	3:A:2593:U:N3	2.83	0.47
18:P:31:THR:HG23	18:P:32:PRO:HD2	1.96	0.47
18:P:43:ASN:ND2	18:P:43:ASN:H	2.13	0.47
18:P:30:ARG:HB3	18:P:97:PHE:CE1	2.50	0.47
25:W:2:PHE:HB3	25:W:50:MET:CE	2.45	0.47
3:A:1672:A:C6	3:A:1673:G:C6	3.03	0.47
3:A:911:A:H2'	16:N:9:PHE:HZ	1.78	0.47
7:E:125:SER:OG	7:E:126:VAL:N	2.46	0.47
3:A:911:A:H2'	16:N:9:PHE:CZ	2.50	0.47
27:Y:62:LYS:HE3	27:Y:66:THR:HG21	1.96	0.47
1:1:45:U:H3	1:1:64:G:H1	1.63	0.47
3:A:2431:U:H5	3:A:2433:A:H5''	1.79	0.47
3:A:2557:G:H2'	3:A:2558:C:C6	2.49	0.47
6:D:121:THR:HB	6:D:127:PHE:CD2	2.50	0.47
7:E:149:ILE:HB	7:E:188:MET:HG2	1.96	0.47
9:G:102:VAL:HG22	9:G:116:GLN:HE22	1.78	0.47
10:H:29:PHE:O	10:H:32:PRO:HD2	2.15	0.47
3:A:1085:A:H61	11:I:35:VAL:HG22	1.78	0.47
3:A:323:C:C4	3:A:333:G:C8	3.03	0.47
8:F:25:VAL:O	8:F:28:VAL:HG12	2.14	0.47
22:T:7:HIS:CE1	22:T:10:ALA:HB2	2.49	0.47
3:A:1799:G:C5	5:C:176:LEU:HD13	2.50	0.47
3:A:2419:U:O2'	3:A:2420:C:H5'	2.15	0.47
3:A:713:G:H2'	3:A:714:U:C6	2.50	0.47
3:A:825:A:C2	3:A:833:A:C2	3.03	0.47
3:A:975:A:H1'	3:A:990:A:C2	2.50	0.47
3:A:998:C:H2'	3:A:999:U:O4'	2.14	0.47
12:J:28:LEU:HD11	12:J:33:VAL:HG11	1.97	0.47
12:J:75:PRO:HD2	12:J:78:VAL:HB	1.96	0.47
17:O:25:ALA:O	17:O:29:VAL:HG23	2.15	0.47
19:Q:100:LEU:HD23	19:Q:100:LEU:HA	1.67	0.47
27:Y:40:VAL:HG12	27:Y:43:GLU:H	1.80	0.47
1:1:37:U:O4	1:1:68:A:N6	2.49	0.47
3:A:1060:U:C2	3:A:1062:G:H5'	2.50	0.47
3:A:1689:A:C6	3:A:1700:A:C2	3.03	0.47
3:A:2339:C:H2'	3:A:2340:A:H8	1.80	0.47
3:A:861:A:C6	3:A:917:A:C8	3.03	0.47
8:F:73:SER:OG	8:F:81:GLN:N	2.33	0.47
24:V:41:LEU:HD22	24:V:62:GLU:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2039:U:H2'	3:A:2040:G:C8	2.51	0.46
3:A:857:G:H2'	3:A:858:G:O4'	2.16	0.46
5:C:252:THR:OG1	5:C:253:LYS:N	2.48	0.46
9:G:42:GLU:CG	9:G:55:ARG:HH21	2.29	0.46
11:I:39:THR:HG22	11:I:43:LYS:HE3	1.98	0.46
19:Q:88:ARG:NH2	19:Q:112:GLU:HB2	2.31	0.46
3:A:1038:G:H2'	3:A:1039:A:C8	2.50	0.46
3:A:1097:U:H2'	3:A:1098:A:O4'	2.15	0.46
3:A:144:A:H1'	23:U:3:ARG:HH22	1.80	0.46
3:A:1808:A:H3'	3:A:1809:A:H8	1.79	0.46
3:A:1946:U:H2'	3:A:1947:C:C6	2.51	0.46
10:H:40:THR:HG22	10:H:41:LYS:H	1.79	0.46
21:S:38:VAL:O	21:S:54:VAL:HG23	2.15	0.46
3:A:2230:G:H2'	3:A:2231:U:C6	2.51	0.46
3:A:796:C:H2'	3:A:797:G:C8	2.51	0.46
3:A:861:A:H2'	3:A:862:G:O4'	2.15	0.46
3:A:871:U:H2'	3:A:872:U:C6	2.50	0.46
9:G:121:ILE:HD13	9:G:135:GLY:HA3	1.98	0.46
11:I:27:VAL:HG13	11:I:80:THR:HG23	1.97	0.46
18:P:53:THR:HB	18:P:65:THR:HB	1.98	0.46
20:R:49:ASP:HA	20:R:52:GLN:HB2	1.96	0.46
3:A:75:G:H4'	28:Z:48:ARG:CZ	2.45	0.46
1:1:59:A:H2'	1:1:60:A:C8	2.50	0.46
3:A:1028:A:N6	3:A:1125:G:H2'	2.30	0.46
3:A:1420:A:N7	3:A:2211:A:N6	2.62	0.46
3:A:2047:C:O2'	3:A:2823:A:N1	2.42	0.46
3:A:247:G:H4'	3:A:386:G:C5	2.50	0.46
4:B:116:G:H2'	4:B:117:G:H8	1.80	0.46
13:K:98:GLU:OE1	13:K:98:GLU:N	2.41	0.46
20:R:18:LEU:HD11	20:R:32:TYR:HA	1.97	0.46
3:A:1510:G:H2'	3:A:1511:G:H8	1.78	0.46
3:A:2788:C:H2'	3:A:2789:C:C6	2.50	0.46
5:C:176:LEU:HA	5:C:176:LEU:HD23	1.80	0.46
5:C:232:HIS:NE2	5:C:244:PRO:HA	2.30	0.46
3:A:1062:G:N2	12:J:93:PRO:HG2	2.30	0.46
15:M:21:ARG:HD3	15:M:21:ARG:HA	1.66	0.46
3:A:483:A:H5''	24:V:47:LYS:HG2	1.97	0.46
3:A:2821:A:H2'	3:A:2822:G:C8	2.51	0.46
14:L:73:ASP:OD1	14:L:73:ASP:N	2.39	0.46
3:A:2126:A:H61	3:A:2163:A:H5'	1.80	0.46
3:A:358:U:H2'	3:A:359:G:C8	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:125:LYS:HB2	5:C:125:LYS:HE2	1.77	0.46
13:K:95:ARG:HG2	13:K:96:ARG:N	2.30	0.46
16:N:66:ARG:HB2	16:N:101:VAL:O	2.16	0.46
3:A:1342:A:C6	3:A:1397:U:C5	3.04	0.46
3:A:1709:U:H2'	3:A:1710:G:H8	1.80	0.46
3:A:2786:U:H2'	3:A:2787:C:H6	1.79	0.46
3:A:878:A:H5'	3:A:879:G:OP2	2.16	0.46
5:C:33:LEU:HA	5:C:33:LEU:HD23	1.58	0.46
14:L:25:LEU:HD23	14:L:25:LEU:HA	1.67	0.46
22:T:25:ARG:NH2	22:T:74:ILE:O	2.49	0.46
3:A:1387:A:H5'	3:A:1469:A:H1'	1.97	0.46
3:A:2069:G:N2	3:A:2443:C:C2	2.83	0.46
3:A:532:A:H2'	3:A:532:A:N3	2.31	0.46
3:A:880:G:N2	3:A:898:C:C2	2.84	0.46
4:B:95:U:H2'	4:B:96:G:H8	1.81	0.46
9:G:155:GLU:OE2	9:G:158:LYS:N	2.48	0.46
11:I:30:SER:HB3	11:I:81:LEU:HB2	1.98	0.46
19:Q:106:LYS:O	19:Q:109:ARG:NH2	2.45	0.46
3:A:1785:A:O2'	3:A:1786:A:H2'	2.16	0.46
3:A:1869:G:N2	3:A:1873:G:C5	2.83	0.46
3:A:2229:U:H2'	3:A:2230:G:C8	2.51	0.46
6:D:99:GLU:OE2	6:D:182:ALA:HB2	2.15	0.46
17:O:28:LEU:O	17:O:32:GLU:N	2.45	0.46
3:A:1563:U:H2'	3:A:1564:C:C6	2.51	0.45
12:J:80:LEU:HB3	12:J:138:LEU:CD1	2.46	0.45
24:V:81:ASP:OD2	24:V:96:PHE:HB3	2.16	0.45
3:A:1570:A:H5'	5:C:36:LYS:HB2	1.98	0.45
3:A:208:C:H2'	3:A:209:C:C6	2.52	0.45
6:D:184:ARG:HH11	19:Q:7:GLN:CD	2.20	0.45
22:T:13:SER:O	22:T:17:VAL:HG23	2.17	0.45
3:A:1706:C:O2'	3:A:1757:A:H5'	2.17	0.45
3:A:1848:A:H3'	3:A:1849:G:H8	1.80	0.45
3:A:772:C:H2'	3:A:773:U:C6	2.52	0.45
5:C:160:THR:O	5:C:195:VAL:HG23	2.17	0.45
14:L:17:ARG:HD3	14:L:17:ARG:HA	1.77	0.45
15:M:27:LEU:O	15:M:31:GLY:HA2	2.16	0.45
14:L:79:PHE:CD1	19:Q:70:VAL:HG22	2.46	0.45
3:A:1086:A:H4'	3:A:1103:A:C2	2.52	0.45
3:A:1149:G:H2'	3:A:1150:C:C6	2.50	0.45
8:F:20:PHE:CZ	8:F:165:GLU:HA	2.51	0.45
24:V:37:GLU:O	24:V:39:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1466:U:H5''	3:A:1467:U:H5'	1.98	0.45
3:A:2052:A:OP1	6:D:146:ILE:HG12	2.17	0.45
6:D:207:VAL:HG13	6:D:208:LYS:HG3	1.98	0.45
10:H:62:LEU:HD23	10:H:135:HIS:CD2	2.52	0.45
11:I:53:ARG:O	11:I:81:LEU:HD12	2.16	0.45
14:L:66:LYS:HB3	14:L:66:LYS:HE2	1.64	0.45
3:A:1653:G:H3'	17:O:2:ARG:HG3	1.98	0.45
18:P:88:LYS:HG2	18:P:116:GLN:HB2	1.98	0.45
25:W:25:LYS:HB3	25:W:25:LYS:HE2	1.71	0.45
3:A:111:A:H2'	3:A:112:U:O4'	2.16	0.45
3:A:1545:A:H2'	3:A:1546:G:O4'	2.17	0.45
3:A:172:A:H2'	3:A:173:A:H8	1.81	0.45
3:A:1848:A:N3	3:A:1849:G:C8	2.85	0.45
3:A:257:C:H2'	3:A:258:G:O4'	2.15	0.45
3:A:831:G:H5''	15:M:37:GLY:HA2	1.97	0.45
6:D:49:GLN:HA	6:D:80:TRP:O	2.16	0.45
3:A:2667:C:H1'	9:G:109:PHE:CD1	2.52	0.45
3:A:908:C:O2'	16:N:70:ASP:OD2	2.30	0.45
23:U:34:VAL:HG21	23:U:43:ILE:HD11	1.99	0.45
25:W:83:LYS:HB3	25:W:85:LYS:HG3	1.98	0.45
26:X:23:VAL:HG22	26:X:38:VAL:HB	1.99	0.45
3:A:1416:G:N2	3:A:1582:C:O2	2.33	0.45
3:A:1313:U:H2'	3:A:1610:A:C2	2.51	0.45
3:A:1631:G:N2	3:A:1634:A:OP2	2.32	0.45
3:A:2165:C:H2'	3:A:2166:U:O4'	2.16	0.45
3:A:2433:A:H5'	3:A:2434:A:P	2.57	0.45
14:L:99:ILE:HG12	14:L:118:LEU:HB2	1.98	0.45
3:A:499:U:H5''	24:V:43:LYS:HE3	1.99	0.45
3:A:1022:G:O2'	3:A:1024:G:O6	2.27	0.45
3:A:1287:A:H3'	3:A:1288:G:N2	2.32	0.45
3:A:1972:G:H2'	3:A:1973:G:H8	1.81	0.45
3:A:2134:A:H1'	3:A:2159:G:H21	1.82	0.45
3:A:2396:G:N3	3:A:2421:G:N2	2.64	0.45
3:A:239:C:H2'	3:A:240:C:O4'	2.16	0.45
3:A:629:G:H5''	3:A:650:C:O2'	2.16	0.45
3:A:657:U:H2'	3:A:658:U:C6	2.52	0.45
3:A:706:A:C2	3:A:707:G:H1'	2.52	0.45
3:A:2667:C:H1'	9:G:109:PHE:HD1	1.82	0.45
10:H:100:ALA:O	10:H:104:THR:HG23	2.17	0.45
18:P:18:LEU:HD23	18:P:18:LEU:HA	1.71	0.45
3:A:2327:A:H2'	3:A:2328:A:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2524:G:H2'	3:A:2525:G:O4'	2.16	0.45
3:A:593:U:H2'	3:A:594:U:C6	2.52	0.45
3:A:718:A:H2'	3:A:719:C:O4'	2.16	0.45
3:A:764:A:H5'	5:C:209:GLY:HA2	1.98	0.45
3:A:948:C:H1'	3:A:984:A:C8	2.52	0.45
12:J:117:MET:HB2	12:J:125:MET:HG2	1.99	0.45
17:O:17:ARG:HG2	17:O:21:PHE:HE2	1.82	0.45
17:O:2:ARG:CZ	17:O:2:ARG:HB3	2.47	0.45
3:A:1177:G:H2'	3:A:1178:C:C6	2.51	0.45
3:A:1918:A:O2'	3:A:1920:C:N4	2.50	0.45
5:C:243:HIS:HA	5:C:244:PRO:HD3	1.79	0.45
8:F:136:ILE:HG22	8:F:141:ILE:HG21	1.98	0.45
9:G:148:LEU:HD23	9:G:148:LEU:HA	1.71	0.45
11:I:41:LEU:HB2	11:I:99:PHE:CE1	2.52	0.45
13:K:69:ARG:O	13:K:89:PHE:HB3	2.17	0.45
16:N:65:ILE:HG12	16:N:103:TYR:CD2	2.51	0.45
21:S:4:VAL:HA	21:S:12:HIS:O	2.16	0.45
3:A:154:U:H2'	3:A:155:A:C8	2.53	0.44
3:A:2273:A:H2'	3:A:2274:A:C8	2.52	0.44
3:A:2313:C:H5''	8:F:88:LYS:HD3	1.98	0.44
3:A:2683:C:H4'	6:D:13:ARG:HH12	1.81	0.44
6:D:7:LYS:HB3	6:D:7:LYS:HE2	1.78	0.44
12:J:130:GLU:HB3	12:J:134:ARG:NH2	2.32	0.44
12:J:86:ILE:CD1	12:J:138:LEU:HD21	2.46	0.44
19:Q:89:ARG:HB3	19:Q:113:ARG:NH1	2.32	0.44
3:A:1450:G:C6	3:A:1451:C:N4	2.86	0.44
3:A:1667:G:N2	3:A:1992:G:OP2	2.44	0.44
3:A:2396:G:C2	3:A:2421:G:C2	3.05	0.44
3:A:594:U:H2'	3:A:595:C:C6	2.51	0.44
3:A:620:G:H4'	3:A:621:A:O5'	2.17	0.44
7:E:121:VAL:O	7:E:189:THR:HA	2.18	0.44
11:I:52:MET:HE3	11:I:81:LEU:HD11	1.99	0.44
13:K:65:THR:O	13:K:68:LYS:HB2	2.16	0.44
16:N:90:GLU:HB3	16:N:91:TYR:CD1	2.53	0.44
26:X:55:ARG:HE	26:X:55:ARG:HB2	1.45	0.44
3:A:2230:G:H1'	27:Y:32:ASN:HB2	1.99	0.44
3:A:198:C:O2'	3:A:199:A:H5'	2.17	0.44
3:A:2489:U:C4	3:A:2490:G:C6	3.06	0.44
3:A:2569:G:C2	3:A:2570:G:C8	3.05	0.44
3:A:2776:A:C8	3:A:2782:G:C5	3.05	0.44
9:G:117:LEU:HD13	9:G:121:ILE:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:10:GLU:OE2	15:M:11:GLY:N	2.50	0.44
21:S:27:ILE:HG22	21:S:28:ALA:O	2.18	0.44
3:A:1198:U:H2'	3:A:1199:U:C6	2.52	0.44
3:A:2704:C:H2'	3:A:2705:A:O4'	2.17	0.44
3:A:77:G:H2'	3:A:78:U:O4'	2.16	0.44
19:Q:62:ARG:NH2	19:Q:101:ARG:HG2	2.32	0.44
25:W:21:ARG:HE	25:W:87:GLN:HA	1.83	0.44
3:A:2387:U:H1'	26:X:41:ARG:NH1	2.32	0.44
26:X:36:ILE:HG23	26:X:58:THR:HG23	2.00	0.44
28:Z:56:LEU:HA	28:Z:56:LEU:HD22	1.82	0.44
3:A:141:G:H3'	3:A:141:G:C8	2.51	0.44
3:A:1508:A:O2'	3:A:1509:A:O4'	2.19	0.44
3:A:1420:A:N7	3:A:2211:A:C6	2.85	0.44
3:A:2318:G:C6	3:A:2319:G:N1	2.86	0.44
12:J:122:ILE:O	12:J:126:THR:OG1	2.22	0.44
14:L:3:GLN:HE21	14:L:3:GLN:HB3	1.66	0.44
3:A:149:A:C2	3:A:150:U:C2	3.06	0.44
3:A:1591:A:H2'	3:A:1592:C:C6	2.53	0.44
3:A:2377:A:H2'	3:A:2378:A:C8	2.53	0.44
3:A:356:G:H2'	3:A:357:C:O4'	2.18	0.44
3:A:57:C:H2'	3:A:58:G:O4'	2.18	0.44
3:A:870:U:OP1	16:N:6:ARG:NH1	2.51	0.44
8:F:147:ASP:OD1	8:F:150:ARG:NH2	2.51	0.44
8:F:67:ILE:HD12	8:F:84:PRO:HB3	2.00	0.44
3:A:1082:U:O2'	11:I:39:THR:HG23	2.18	0.44
3:A:1301:A:H2'	3:A:1301:A:N3	2.33	0.44
3:A:181:A:H1'	3:A:435:C:O4'	2.17	0.44
3:A:630:G:N2	3:A:633:A:OP2	2.43	0.44
3:A:2683:C:H4'	6:D:13:ARG:NH1	2.33	0.44
3:A:997:G:H5''	20:R:92:ARG:NH1	2.33	0.44
3:A:1056:G:H1'	3:A:1103:A:N6	2.33	0.44
3:A:1082:U:H4'	11:I:46:ARG:NH1	2.32	0.44
3:A:1093:G:H1'	3:A:1099:G:N1	2.32	0.44
3:A:2024:G:H2'	3:A:2025:C:C6	2.53	0.44
3:A:746:U:HO2'	3:A:2611:C:HO2'	1.66	0.44
3:A:2678:C:H2'	3:A:2679:A:O4'	2.18	0.44
10:H:26:ALA:HA	10:H:30:LEU:HB2	1.99	0.44
18:P:52:SER:O	18:P:58:ILE:HD12	2.18	0.44
19:Q:53:ARG:HB2	19:Q:56:HIS:HB2	1.99	0.44
27:Y:59:ILE:HG12	27:Y:67:VAL:HG21	1.99	0.44
3:A:1230:A:H2'	3:A:1231:U:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1614:A:C2	22:T:93:ALA:HB2	2.52	0.44
3:A:2443:C:H2'	3:A:2444:G:H8	1.82	0.44
3:A:277:G:H4'	3:A:278:A:N7	2.33	0.44
3:A:33:C:N4	3:A:446:G:O2'	2.45	0.44
5:C:141:VAL:HG12	5:C:192:LEU:HA	1.98	0.44
3:A:1205:A:H2'	7:E:165:HIS:HE1	1.83	0.44
8:F:128:TYR:CE2	8:F:130:MET:HG2	2.53	0.44
9:G:42:GLU:HG3	9:G:55:ARG:HH21	1.83	0.44
18:P:85:LYS:HB3	18:P:85:LYS:HE2	1.79	0.44
19:Q:25:THR:HB	19:Q:88:ARG:HG2	1.99	0.44
3:A:1287:A:H5'	17:O:103:ARG:HD2	1.98	0.43
3:A:1710:G:H2'	3:A:1711:A:C8	2.53	0.43
3:A:1853:A:N6	3:A:1888:G:O2'	2.51	0.43
3:A:1266:G:N2	3:A:2012:G:H2'	2.33	0.43
3:A:1266:G:O2'	3:A:2012:G:O6	2.34	0.43
3:A:2292:U:H2'	3:A:2293:G:C8	2.52	0.43
4:B:114:C:H2'	4:B:115:A:H8	1.83	0.43
12:J:110:ALA:O	12:J:114:ALA:HB2	2.18	0.43
23:U:31:VAL:O	23:U:32:LEU:HD23	2.18	0.43
3:A:1962:C:H4'	3:A:1963:U:C5	2.52	0.43
3:A:2654:A:OP1	3:A:2654:A:H8	2.01	0.43
3:A:475:C:N4	3:A:476:G:C6	2.86	0.43
3:A:677:A:O2'	3:A:2071:A:H5'	2.17	0.43
12:J:90:SER:HB2	12:J:136:MET:O	2.18	0.43
3:A:1048:A:N1	3:A:1112:G:O2'	2.36	0.43
3:A:1351:C:H4'	3:A:1572:A:O4'	2.18	0.43
3:A:2172:U:H4'	3:A:2173:A:H5'	2.00	0.43
3:A:380:G:H2'	3:A:381:G:O4'	2.18	0.43
3:A:969:G:H2'	3:A:970:U:C6	2.53	0.43
8:F:145:LYS:HA	8:F:145:LYS:HD3	1.89	0.43
15:M:80:SER:O	15:M:84:LYS:HE3	2.19	0.43
21:S:91:GLN:NE2	21:S:92:TRP:H	2.16	0.43
3:A:1735:A:H2'	3:A:1736:U:O4'	2.18	0.43
3:A:2647:U:H2'	3:A:2648:G:C8	2.54	0.43
3:A:776:G:HO2'	3:A:777:G:P	2.39	0.43
3:A:973:A:OP2	21:S:81:LYS:HE3	2.18	0.43
22:T:47:VAL:HG22	22:T:103:ILE:HD13	2.00	0.43
3:A:1044:C:O2'	3:A:1111:A:N1	2.45	0.43
3:A:1354:A:H2'	3:A:1355:G:O4'	2.19	0.43
3:A:1515:A:H3'	3:A:1516:G:H8	1.84	0.43
3:A:1627:G:C2	3:A:1628:G:C8	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2292:U:H2'	3:A:2293:G:H8	1.84	0.43
3:A:93:G:H2'	3:A:94:A:H8	1.84	0.43
4:B:49:C:H2'	4:B:50:A:C8	2.54	0.43
10:H:46:PHE:HD1	10:H:50:ARG:NH2	2.16	0.43
17:O:86:ARG:HD3	17:O:121:LYS:HG3	1.98	0.43
20:R:24:TYR:O	20:R:29:SER:HB3	2.19	0.43
3:A:112:U:H5'	28:Z:58:ASN:ND2	2.34	0.43
3:A:976:G:HO2'	3:A:1155:A:HO2'	1.60	0.43
3:A:11:C:H2'	3:A:12:U:H5'	2.00	0.43
3:A:1434:A:C2	3:A:1435:G:C5	3.07	0.43
3:A:2786:U:H2'	3:A:2787:C:C6	2.53	0.43
3:A:463:G:N1	3:A:467:G:C6	2.86	0.43
3:A:834:G:C2	3:A:835:C:C2	3.06	0.43
5:C:153:GLN:O	5:C:156:ARG:HG3	2.18	0.43
6:D:131:ASP:O	6:D:140:HIS:HD2	2.01	0.43
7:E:108:ILE:O	7:E:112:LEU:HG	2.18	0.43
8:F:138:PHE:HA	8:F:139:PRO:HD3	1.90	0.43
1:1:55:A:H2'	1:1:56:A:C8	2.53	0.43
3:A:14:A:C6	3:A:526:A:C2	3.07	0.43
3:A:2138:G:C6	3:A:2154:A:C2	3.06	0.43
3:A:2847:U:H2'	3:A:2848:G:O4'	2.18	0.43
3:A:76:C:H6	3:A:76:C:O5'	2.02	0.43
5:C:90:ASN:ND2	5:C:197:ASN:HB2	2.34	0.43
10:H:62:LEU:HD22	10:H:137:GLU:OE1	2.19	0.43
15:M:6:LEU:HA	15:M:6:LEU:HD23	1.82	0.43
20:R:74:ILE:HG12	20:R:75:SER:N	2.34	0.43
22:T:46:LEU:HA	22:T:46:LEU:HD23	1.82	0.43
3:A:1542:U:H2'	3:A:1543:G:O4'	2.18	0.43
3:A:1597:A:C5'	3:A:1598:A:H5'	2.47	0.43
3:A:1858:A:H2'	3:A:1859:U:O4'	2.17	0.43
3:A:2114:A:C2	3:A:2166:U:H2'	2.53	0.43
3:A:2130:U:O2'	3:A:2133:G:O2'	2.32	0.43
3:A:239:C:HO2'	3:A:622:G:HO2'	1.62	0.43
3:A:2512:C:H5''	3:A:2513:A:OP2	2.17	0.43
3:A:2588:G:O6	3:A:2607:G:C6	2.72	0.43
3:A:591:U:H2'	3:A:592:A:C8	2.54	0.43
3:A:783:A:C5	3:A:785:G:H1'	2.53	0.43
7:E:128:ALA:O	7:E:130:LYS:N	2.51	0.43
11:I:118:ILE:HA	11:I:119:PRO:HD2	1.84	0.43
3:A:566:U:H5''	15:M:29:LYS:HE3	1.99	0.43
16:N:26:VAL:HB	16:N:133:LYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:9:ILE:HD12	20:R:9:ILE:H	1.84	0.43
21:S:4:VAL:HG12	21:S:39:LEU:HB2	2.00	0.43
3:A:1473:G:H2'	3:A:1474:U:O4'	2.19	0.43
3:A:1517:G:C2	3:A:1732:C:N3	2.86	0.43
3:A:493:G:H2'	3:A:494:G:O4'	2.19	0.43
5:C:8:PRO:HB3	5:C:14:ARG:HG3	1.99	0.43
6:D:148:GLN:N	6:D:148:GLN:OE1	2.51	0.43
6:D:109:VAL:HG12	6:D:201:LEU:HD22	2.01	0.43
10:H:104:THR:HA	10:H:108:VAL:O	2.19	0.43
13:K:26:GLY:O	13:K:30:THR:HG23	2.18	0.43
16:N:33:LEU:HD11	16:N:128:THR:HB	2.00	0.43
20:R:17:ILE:HD13	20:R:17:ILE:HA	1.63	0.43
25:W:29:ILE:O	25:W:91:PHE:HB2	2.19	0.43
26:X:47:ALA:HB1	26:X:51:VAL:O	2.19	0.43
3:A:1141:U:H4'	3:A:1142:A:O4'	2.19	0.43
3:A:1341:G:O2'	23:U:59:ASN:ND2	2.47	0.43
3:A:1501:G:H2'	3:A:1502:A:H8	1.84	0.43
3:A:2038:G:H2'	3:A:2039:U:O4'	2.17	0.43
3:A:2843:G:H2'	3:A:2844:G:C8	2.54	0.43
8:F:170:LEU:HD23	8:F:170:LEU:HA	1.75	0.43
9:G:44:LYS:HB2	9:G:44:LYS:HE3	1.80	0.43
12:J:33:VAL:HG13	12:J:67:PHE:CD2	2.54	0.43
17:O:72:ASP:OD1	17:O:73:ASN:N	2.51	0.43
23:U:34:VAL:HG11	23:U:43:ILE:HD13	2.01	0.43
3:A:141:G:C8	3:A:142:A:O4'	2.72	0.42
3:A:1494:A:H2'	3:A:1495:A:H8	1.83	0.42
3:A:1759:A:H2'	3:A:1760:C:C6	2.54	0.42
3:A:2144:G:N2	3:A:2148:G:O6	2.52	0.42
3:A:2771:C:H2'	3:A:2772:C:C6	2.54	0.42
3:A:5:A:H2'	3:A:6:A:C8	2.54	0.42
5:C:245:VAL:HA	5:C:252:THR:HG22	2.01	0.42
3:A:195:A:H5''	15:M:47:ARG:HH22	1.84	0.42
3:A:1614:A:H8	3:A:1614:A:O5'	2.02	0.42
3:A:2533:U:OP1	3:A:2665:A:O2'	2.34	0.42
3:A:2646:C:OP2	3:A:2732:G:O2'	2.35	0.42
3:A:461:C:H2'	3:A:462:C:H6	1.84	0.42
3:A:464:U:C2	3:A:788:A:C6	3.07	0.42
5:C:200:HIS:C	5:C:200:HIS:CD2	2.92	0.42
5:C:210:ALA:HA	5:C:213:TRP:CE3	2.53	0.42
3:A:1088:A:H61	12:J:135:SER:HB3	1.82	0.42
3:A:1064:C:H5''	12:J:88:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1524:G:H2'	3:A:1525:A:O4'	2.20	0.42
3:A:1590:A:H2'	3:A:1591:A:C8	2.54	0.42
3:A:1736:U:H2'	3:A:1737:G:O4'	2.18	0.42
3:A:1922:G:H2'	3:A:1923:U:O4'	2.18	0.42
3:A:2184:A:H2'	3:A:2185:U:C6	2.53	0.42
3:A:2700:A:H2'	3:A:2701:U:C6	2.54	0.42
3:A:2790:U:H5'	3:A:2893:A:N7	2.34	0.42
3:A:674:G:H2'	3:A:804:A:H61	1.83	0.42
4:B:106:G:H2'	4:B:107:G:O4'	2.19	0.42
4:B:66:A:H61	4:B:107:G:H2'	1.84	0.42
5:C:133:ARG:HD2	10:H:123:ARG:NH1	2.35	0.42
7:E:29:HIS:O	7:E:32:VAL:HG22	2.19	0.42
8:F:79:ILE:HG21	8:F:85:ILE:HD11	2.01	0.42
9:G:149:ARG:HG3	9:G:162:VAL:O	2.20	0.42
14:L:65:THR:HB	14:L:68:GLY:H	1.84	0.42
1:1:48:G:H3'	1:1:49:G:C8	2.54	0.42
3:A:1387:A:H2'	3:A:1388:G:O4'	2.18	0.42
3:A:1637:A:H2'	3:A:1638:C:C6	2.54	0.42
3:A:543:G:H5'	3:A:544:C:OP2	2.18	0.42
5:C:24:LEU:HD12	5:C:24:LEU:HA	1.66	0.42
12:J:113:LYS:HA	12:J:116:ASP:HB2	2.01	0.42
12:J:38:PHE:CD1	12:J:59:ILE:HD11	2.54	0.42
20:R:24:TYR:HD1	20:R:24:TYR:N	2.17	0.42
3:A:571:U:H3'	21:S:80:ARG:NH2	2.34	0.42
24:V:61:LYS:HG2	24:V:62:GLU:H	1.85	0.42
16:N:36:VAL:HG13	25:W:82:TYR:CD2	2.55	0.42
3:A:1039:A:H2'	3:A:1040:A:O4'	2.20	0.42
3:A:123:G:N2	3:A:129:C:C2	2.87	0.42
3:A:1751:U:H2'	3:A:1752:C:C6	2.54	0.42
3:A:1759:A:C2	3:A:2697:G:H1'	2.54	0.42
3:A:729:G:H2'	3:A:1775:U:H1'	2.01	0.42
3:A:2518:A:N3	3:A:2518:A:H2'	2.34	0.42
3:A:653:U:C1'	3:A:654:A:H5"	2.49	0.42
3:A:729:G:C5	5:C:207:LYS:HB2	2.55	0.42
8:F:48:LYS:HE2	8:F:48:LYS:HB2	1.85	0.42
12:J:103:ARG:H	12:J:103:ARG:HD2	1.83	0.42
3:A:1798:U:OP2	5:C:271:ARG:NH2	2.52	0.42
3:A:2304:G:H22	3:A:2312:U:H3	1.67	0.42
3:A:2322:A:C4	3:A:2323:G:C8	3.07	0.42
3:A:307:G:N1	3:A:310:A:OP2	2.52	0.42
3:A:794:A:H2'	3:A:795:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:812:C:C2	3:A:1250:G:N1	2.87	0.42
3:A:877:A:C6	3:A:899:A:C6	3.08	0.42
3:A:1902:C:H4'	5:C:242:LYS:O	2.19	0.42
10:H:94:ILE:HG23	10:H:98:ASP:HB2	2.01	0.42
11:I:15:VAL:HG11	11:I:60:LEU:CD2	2.50	0.42
12:J:22:PRO:HB2	12:J:23:PRO:HD3	2.02	0.42
12:J:74:PRO:HA	12:J:75:PRO:HD3	1.89	0.42
19:Q:106:LYS:O	19:Q:109:ARG:HD3	2.20	0.42
20:R:117:LEU:HD23	20:R:117:LEU:HA	1.77	0.42
25:W:2:PHE:HE1	25:W:53:LYS:HD2	1.84	0.42
3:A:1110:G:HO2'	3:A:1111:A:P	2.43	0.42
3:A:1327:A:H2'	3:A:1328:A:O4'	2.19	0.42
3:A:1400:U:H2'	3:A:1401:G:O4'	2.19	0.42
3:A:819:A:H2'	3:A:819:A:N3	2.34	0.42
4:B:57:A:C4	8:F:26:MET:HB3	2.54	0.42
10:H:1:MET:O	10:H:20:ASN:HA	2.20	0.42
11:I:85:VAL:HG21	11:I:90:GLY:O	2.20	0.42
17:O:75:ILE:HD12	17:O:75:ILE:HA	1.82	0.42
3:A:1047:G:OP1	11:I:56:ARG:NH1	2.52	0.42
3:A:1463:C:H2'	3:A:1464:G:H8	1.85	0.42
3:A:2796:U:HO2'	3:A:2797:U:H6	1.63	0.42
3:A:647:G:H2'	3:A:648:G:C8	2.55	0.42
17:O:103:ARG:HB3	17:O:106:ASP:OD1	2.20	0.42
3:A:1065:U:H2'	3:A:1066:U:O4'	2.19	0.42
3:A:1068:G:N2	3:A:1095:A:O3'	2.44	0.42
3:A:1324:G:C4	3:A:1328:A:N6	2.88	0.42
3:A:1509:A:O2'	3:A:1510:G:H8	2.03	0.42
3:A:2119:A:H62	3:A:2167:U:H1'	1.85	0.42
3:A:2433:A:H5'	3:A:2434:A:OP2	2.19	0.42
3:A:2776:A:C2	3:A:2778:A:C4	3.07	0.42
3:A:669:G:N2	3:A:670:A:C2	2.88	0.42
3:A:910:A:C6	3:A:911:A:C6	3.08	0.42
8:F:34:ILE:HB	8:F:96:MET:HG3	2.02	0.42
11:I:43:LYS:HE2	12:J:118:THR:HA	2.01	0.42
14:L:11:ALA:O	14:L:100:PHE:N	2.46	0.42
16:N:42:THR:N	16:N:45:GLN:OE1	2.47	0.42
20:R:31:VAL:HG12	20:R:34:VAL:H	1.85	0.42
3:A:1499:C:H2'	3:A:1500:G:H8	1.85	0.42
3:A:1880:U:H2'	3:A:1881:C:C6	2.55	0.42
3:A:565:C:H4'	3:A:1253:A:C6	2.55	0.42
8:F:4:LEU:HA	8:F:4:LEU:HD23	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:97:ALA:HB3	9:G:104:ASN:HB2	2.01	0.42
22:T:28:LYS:HE2	22:T:28:LYS:HB2	1.41	0.42
3:A:1417:C:H2'	3:A:1418:G:C8	2.55	0.41
3:A:1463:C:H2'	3:A:1464:G:C8	2.55	0.41
3:A:648:G:C2	3:A:649:G:C5	3.08	0.41
5:C:205:LEU:HD23	5:C:205:LEU:HA	1.68	0.41
7:E:109:LEU:HA	7:E:109:LEU:HD23	1.79	0.41
8:F:79:ILE:O	8:F:79:ILE:HD12	2.20	0.41
8:F:57:LEU:HD12	8:F:87:CYS:SG	2.60	0.41
3:A:1056:G:H5'	11:I:35:VAL:HG21	2.02	0.41
3:A:1449:G:N2	3:A:1463:C:C2	2.88	0.41
3:A:1825:U:O2	5:C:253:LYS:NZ	2.31	0.41
3:A:1877:A:H2'	3:A:1878:G:O4'	2.20	0.41
3:A:1770:G:C6	3:A:1983:G:C6	3.07	0.41
3:A:2706:A:C2	3:A:2707:U:C2	3.08	0.41
3:A:449:A:C4	3:A:450:G:C8	3.08	0.41
9:G:73:ASN:O	9:G:77:ILE:HG13	2.20	0.41
3:A:1005:C:H2'	3:A:1006:C:H6	1.84	0.41
3:A:118:A:N3	3:A:178:G:H1'	2.36	0.41
3:A:1484:U:H2'	3:A:1485:U:C6	2.55	0.41
3:A:1780:A:H3'	3:A:1781:U:H2'	2.01	0.41
3:A:1946:U:H2'	3:A:1947:C:H6	1.84	0.41
3:A:2209:G:C2	3:A:2216:G:C2	3.08	0.41
3:A:2339:C:O3'	4:B:41:G:N2	2.52	0.41
3:A:2838:G:H2'	3:A:2839:G:O4'	2.20	0.41
3:A:393:C:H2'	3:A:394:C:H6	1.85	0.41
3:A:53:A:H2'	3:A:54:G:O4'	2.20	0.41
3:A:981:A:N1	3:A:2027:G:O2'	2.42	0.41
5:C:176:LEU:HB2	5:C:180:GLU:O	2.20	0.41
7:E:181:ILE:H	7:E:181:ILE:HG13	1.70	0.41
8:F:70:ALA:HB3	8:F:81:GLN:HA	2.02	0.41
9:G:76:VAL:O	9:G:80:THR:HG23	2.20	0.41
14:L:93:GLN:HA	14:L:94:PRO:HD3	1.88	0.41
3:A:1432:G:H2'	3:A:1433:A:C8	2.55	0.41
3:A:1482:G:H2'	3:A:1483:G:H8	1.84	0.41
3:A:2860:A:H5''	3:A:2861:U:OP2	2.21	0.41
3:A:2895:G:H2'	3:A:2896:C:C6	2.56	0.41
3:A:335:C:H5''	24:V:82:ARG:HD2	2.02	0.41
3:A:848:C:H42	3:A:930:G:H1	1.68	0.41
6:D:73:VAL:HG11	6:D:93:GLY:HA2	2.02	0.41
9:G:83:PHE:HB2	9:G:135:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:133:LYS:HE3	16:N:133:LYS:HB3	1.42	0.41
3:A:1078:U:O2	3:A:1088:A:H3'	2.21	0.41
3:A:1972:G:H2'	3:A:1973:G:C8	2.55	0.41
3:A:2267:A:H5''	3:A:2268:A:C5'	2.49	0.41
3:A:297:G:H2'	3:A:298:G:O4'	2.20	0.41
4:B:48:U:H4'	18:P:100:HIS:HD2	1.84	0.41
4:B:71:C:C2	4:B:106:G:C2	3.08	0.41
8:F:13:VAL:O	8:F:17:MET:HB2	2.21	0.41
14:L:71:ARG:HD3	14:L:71:ARG:HA	1.81	0.41
3:A:2102:G:C2	3:A:2187:U:O2	2.73	0.41
3:A:2812:G:H2'	3:A:2813:A:O4'	2.20	0.41
3:A:528:A:C8	3:A:2042:A:C2	3.09	0.41
3:A:558:U:OP1	13:K:114:LEU:N	2.47	0.41
3:A:75:G:H4'	28:Z:48:ARG:NH2	2.35	0.41
3:A:807:U:H2'	3:A:808:G:H8	1.84	0.41
3:A:2352:A:N1	26:X:34:GLY:HA3	2.35	0.41
3:A:2365:G:H4'	26:X:60:PHE:CE2	2.55	0.41
27:Y:3:ARG:NE	27:Y:30:LEU:HD13	2.35	0.41
28:Z:21:LEU:HD23	28:Z:21:LEU:HA	1.82	0.41
2:2:74:C:O5'	2:2:74:C:H6	2.04	0.41
3:A:1073:A:H2'	3:A:1074:G:O4'	2.21	0.41
3:A:1709:U:H2'	3:A:1710:G:C8	2.55	0.41
3:A:1821:A:H2'	3:A:1822:C:C6	2.55	0.41
3:A:2286:G:C8	3:A:2287:A:N6	2.88	0.41
3:A:2550:G:C6	3:A:2551:C:C4	3.09	0.41
3:A:2682:A:C2	6:D:23:PRO:HB3	2.56	0.41
3:A:31:C:O3'	3:A:1238:G:H5'	2.21	0.41
3:A:678:C:H2'	3:A:679:C:H6	1.84	0.41
4:B:95:U:H2'	4:B:96:G:C8	2.56	0.41
15:M:78:ARG:HG2	15:M:113:ALA:HB3	2.03	0.41
22:T:33:LEU:HD23	22:T:33:LEU:HA	1.66	0.41
3:A:1057:A:N7	3:A:1086:A:H2'	2.35	0.41
3:A:1275:A:OP2	3:A:1646:C:N4	2.52	0.41
3:A:1366:A:H2'	3:A:1367:A:O4'	2.21	0.41
3:A:1789:A:H2'	3:A:1790:C:O4'	2.21	0.41
3:A:2343:U:H2'	3:A:2344:U:C6	2.55	0.41
3:A:2785:C:H2'	3:A:2786:U:H6	1.85	0.41
3:A:561:G:H4'	20:R:48:ARG:HH22	1.86	0.41
3:A:799:G:C6	3:A:800:A:C6	3.08	0.41
8:F:36:LEU:HA	8:F:153:ASP:O	2.21	0.41
9:G:154:PRO:HA	9:G:160:LYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:71:LEU:HD23	9:G:71:LEU:HA	1.83	0.41
27:Y:54:LYS:O	27:Y:58:VAL:HG23	2.19	0.41
3:A:1341:G:C2	3:A:1398:C:H4'	2.56	0.41
3:A:1869:G:C2	3:A:1873:G:C6	3.09	0.41
3:A:396:G:H1'	27:Y:29:PHE:HB3	2.02	0.41
3:A:465:G:C6	3:A:466:A:N6	2.89	0.41
3:A:520:G:H2'	3:A:521:U:C6	2.56	0.41
3:A:681:G:C2	3:A:797:G:C2	3.09	0.41
3:A:779:U:H2'	3:A:780:G:C8	2.56	0.41
3:A:997:G:OP1	20:R:92:ARG:HD2	2.21	0.41
4:B:7:G:H5''	18:P:29:HIS:CE1	2.56	0.41
11:I:48:ALA:HB3	11:I:50:VAL:HG23	2.03	0.41
3:A:328:U:H4'	24:V:66:GLN:HE21	1.86	0.41
25:W:2:PHE:HB3	25:W:50:MET:HE3	2.03	0.41
26:X:41:ARG:HA	26:X:41:ARG:HD3	1.53	0.41
3:A:1374:G:H8	3:A:1374:G:OP2	2.04	0.41
3:A:1423:G:N2	3:A:1576:U:O2	2.54	0.41
3:A:2061:G:H2'	3:A:2501:C:O2'	2.21	0.41
3:A:601:C:O2'	3:A:605:G:H5''	2.21	0.41
3:A:64:A:C6	3:A:65:U:C4	3.09	0.41
3:A:743:A:OP1	6:D:135:GLY:HA2	2.21	0.41
14:L:103:VAL:HB	14:L:107:LEU:HD12	2.02	0.41
15:M:81:ASP:HB3	15:M:100:ILE:HD13	2.02	0.41
16:N:6:ARG:HB2	16:N:6:ARG:CZ	2.50	0.41
18:P:115:LEU:HD23	18:P:117:PHE:CE2	2.56	0.41
27:Y:74:ARG:HB3	27:Y:74:ARG:HE	1.45	0.41
27:Y:72:ARG:HG3	27:Y:78:TYR:HE2	1.86	0.41
28:Z:37:LEU:HD12	28:Z:37:LEU:HA	1.82	0.41
3:A:141:G:C8	3:A:141:G:C3'	3.04	0.41
3:A:199:A:N6	3:A:2434:A:C5	2.89	0.41
3:A:2578:G:OP2	3:A:2578:G:H4'	2.20	0.41
3:A:948:C:H2'	3:A:949:G:H8	1.85	0.41
10:H:128:HIS:O	10:H:143:ILE:HA	2.20	0.41
11:I:61:ARG:HG2	11:I:73:LYS:HG2	2.02	0.41
16:N:38:ARG:HB2	16:N:98:PRO:HD3	2.03	0.41
21:S:85:LYS:HE2	21:S:85:LYS:HB3	1.80	0.41
28:Z:38:GLN:HG3	28:Z:39:GLN:H	1.85	0.41
3:A:1045:C:OP1	3:A:1046:A:O2'	2.37	0.40
3:A:811:U:C2	3:A:1251:C:C5	3.09	0.40
3:A:1818:U:C5	5:C:156:ARG:NH2	2.90	0.40
3:A:2229:U:H2'	3:A:2230:G:H8	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2663:G:H2'	3:A:2664:G:O4'	2.21	0.40
3:A:2804:U:H2'	3:A:2805:C:C6	2.56	0.40
3:A:778:G:H5''	3:A:779:U:OP2	2.21	0.40
16:N:65:ILE:HG12	16:N:103:TYR:HD2	1.86	0.40
17:O:72:ASP:O	17:O:76:VAL:HG13	2.21	0.40
19:Q:40:LEU:HD23	19:Q:40:LEU:HA	1.75	0.40
27:Y:3:ARG:O	27:Y:12:PRO:HD3	2.21	0.40
3:A:1024:G:C6	3:A:1025:G:C6	3.09	0.40
3:A:1071:G:O2'	3:A:1089:A:OP2	2.36	0.40
3:A:118:A:C8	3:A:119:A:C8	3.09	0.40
3:A:2143:C:H2'	3:A:2144:G:O4'	2.21	0.40
3:A:2388:A:H5'	3:A:2389:G:OP2	2.21	0.40
3:A:2431:U:O2	3:A:2431:U:O4'	2.39	0.40
3:A:2603:G:C6	3:A:2604:U:C4	3.09	0.40
3:A:277:G:H4'	3:A:278:A:C5	2.57	0.40
3:A:2847:U:C5	3:A:2848:G:C5	3.09	0.40
3:A:42:A:C6	3:A:43:G:C5	3.10	0.40
3:A:501:A:H2'	3:A:502:A:C8	2.56	0.40
5:C:34:LEU:HD21	5:C:63:ARG:HG3	2.03	0.40
9:G:9:VAL:HG23	9:G:52:PHE:HE1	1.86	0.40
12:J:42:PHE:CE1	12:J:57:VAL:HB	2.56	0.40
22:T:109:ASP:OD1	22:T:110:ARG:N	2.54	0.40
26:X:70:GLU:HG3	26:X:72:LYS:HE2	2.04	0.40
3:A:1127:A:N7	3:A:2488:G:O2'	2.55	0.40
3:A:1807:G:N2	3:A:1811:G:C5	2.89	0.40
3:A:1838:C:H4'	3:A:1839:G:H8	1.85	0.40
3:A:2421:G:H4'	3:A:2421:G:OP1	2.21	0.40
3:A:2600:A:H2'	3:A:2601:C:C6	2.56	0.40
3:A:2627:G:H1'	3:A:2777:G:N2	2.36	0.40
3:A:719:C:H2'	3:A:720:U:C6	2.57	0.40
3:A:863:A:H2'	3:A:864:G:C8	2.57	0.40
3:A:863:A:H2'	3:A:864:G:H8	1.86	0.40
11:I:99:PHE:HD2	11:I:106:PHE:HZ	1.69	0.40
17:O:22:ARG:HG3	17:O:70:THR:HA	2.03	0.40
18:P:115:LEU:HD23	18:P:117:PHE:HE2	1.86	0.40
24:V:96:PHE:O	24:V:100:SER:HA	2.21	0.40
26:X:45:PHE:CD1	26:X:80:ILE:HD11	2.56	0.40
3:A:987:C:O2'	3:A:1000:A:N3	2.44	0.40
3:A:1672:A:N6	3:A:1673:G:C6	2.89	0.40
3:A:1:G:H2'	3:A:2:G:C8	2.57	0.40
3:A:2423:U:H2'	3:A:2424:C:C1'	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:445:C:H2'	3:A:446:G:O4'	2.22	0.40
3:A:822:G:H2'	3:A:823:C:C6	2.57	0.40
3:A:871:U:H4'	16:N:68:PHE:CD2	2.56	0.40
4:B:49:C:H2'	4:B:50:A:H8	1.87	0.40
5:C:157:SER:O	5:C:160:THR:OG1	2.38	0.40
7:E:148:ILE:HG12	7:E:148:ILE:H	1.64	0.40
8:F:65:PRO:HA	8:F:89:VAL:HG22	2.01	0.40
9:G:125:CYS:HB2	9:G:127:THR:O	2.22	0.40
9:G:90:VAL:HG21	9:G:163:ARG:NH1	2.37	0.40
11:I:13:ALA:O	11:I:17:GLU:HB2	2.22	0.40
13:K:99:ARG:HD2	13:K:102:GLU:OE1	2.22	0.40
15:M:79:LEU:HB2	15:M:113:ALA:O	2.21	0.40
18:P:28:VAL:HG12	18:P:93:ASP:O	2.21	0.40
28:Z:46:VAL:O	28:Z:50:VAL:HG23	2.21	0.40
3:A:1139:G:OP2	3:A:1139:G:H8	2.05	0.40
3:A:1258:U:C2	3:A:1259:G:C8	3.09	0.40
3:A:1707:G:C5	3:A:1756:G:C6	3.10	0.40
3:A:2394:C:H42	3:A:2422:C:N4	2.19	0.40
3:A:2586:U:OP2	3:A:2608:G:N1	2.48	0.40
3:A:339:U:H6	3:A:339:U:O5'	2.05	0.40
3:A:353:C:H2'	3:A:354:A:O4'	2.22	0.40
3:A:717:C:C5	3:A:718:A:C8	3.10	0.40
3:A:729:G:C6	5:C:207:LYS:HB2	2.56	0.40
3:A:991:C:H2'	3:A:992:C:H6	1.85	0.40
7:E:69:ARG:HG2	7:E:69:ARG:H	1.76	0.40
15:M:3:LEU:HA	15:M:3:LEU:HD23	1.77	0.40
17:O:65:LEU:HD12	17:O:65:LEU:HA	1.85	0.40
18:P:25:ARG:O	18:P:25:ARG:HG3	2.22	0.40
23:U:49:LYS:HG3	23:U:50:LEU:HD23	2.03	0.40
24:V:36:VAL:HB	24:V:39:ILE:HB	2.03	0.40
27:Y:36:HIS:O	27:Y:48:THR:HA	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	C	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
6	D	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
7	E	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
8	F	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
9	G	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
10	H	147/149 (99%)	138 (94%)	8 (5%)	1 (1%)	26	72
11	I	123/165 (74%)	113 (92%)	9 (7%)	1 (1%)	24	70
12	J	132/142 (93%)	126 (96%)	6 (4%)	0	100	100
13	K	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
14	L	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
15	M	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
16	N	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
17	O	123/127 (97%)	118 (96%)	5 (4%)	0	100	100
18	P	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
19	Q	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
20	R	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
21	S	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
22	T	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
23	U	93/100 (93%)	90 (97%)	3 (3%)	0	100	100
24	V	100/104 (96%)	99 (99%)	1 (1%)	0	100	100
25	W	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
26	X	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
27	Y	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
28	Z	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
29	a	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
30	b	54/57 (95%)	50 (93%)	4 (7%)	0	100	100
31	c	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
32	d	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
33	e	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
34	f	36/38 (95%)	36 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	i	84/453 (18%)	84 (100%)	0	0	100	100
36	k	16/18 (89%)	12 (75%)	4 (25%)	0	100	100
All	All	3532/4045 (87%)	3415 (97%)	115 (3%)	2 (0%)	59	90

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	H	118	PRO
11	I	108	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	C	216/218 (99%)	192 (89%)	24 (11%)	8	39
6	D	164/164 (100%)	154 (94%)	10 (6%)	23	65
7	E	165/165 (100%)	152 (92%)	13 (8%)	15	55
8	F	148/150 (99%)	130 (88%)	18 (12%)	6	34
9	G	137/138 (99%)	129 (94%)	8 (6%)	25	66
10	H	114/114 (100%)	100 (88%)	14 (12%)	6	34
11	I	95/123 (77%)	89 (94%)	6 (6%)	22	63
12	J	104/110 (94%)	93 (89%)	11 (11%)	8	41
13	K	116/116 (100%)	105 (90%)	11 (10%)	11	46
14	L	104/104 (100%)	94 (90%)	10 (10%)	10	46
15	M	103/103 (100%)	94 (91%)	9 (9%)	13	50
16	N	109/109 (100%)	100 (92%)	9 (8%)	14	52
17	O	102/103 (99%)	95 (93%)	7 (7%)	19	60
18	P	87/87 (100%)	75 (86%)	12 (14%)	4	30
19	Q	99/100 (99%)	90 (91%)	9 (9%)	12	48
20	R	89/90 (99%)	82 (92%)	7 (8%)	15	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	S	84/84 (100%)	76 (90%)	8 (10%)	11	46
22	T	93/93 (100%)	88 (95%)	5 (5%)	27	68
23	U	82/84 (98%)	77 (94%)	5 (6%)	23	65
24	V	83/85 (98%)	76 (92%)	7 (8%)	14	52
25	W	78/78 (100%)	72 (92%)	6 (8%)	16	56
26	X	57/63 (90%)	51 (90%)	6 (10%)	8	41
27	Y	67/68 (98%)	63 (94%)	4 (6%)	24	65
28	Z	54/55 (98%)	47 (87%)	7 (13%)	5	32
29	a	48/49 (98%)	46 (96%)	2 (4%)	36	74
30	b	47/48 (98%)	35 (74%)	12 (26%)	1	6
31	c	45/49 (92%)	40 (89%)	5 (11%)	8	39
32	d	38/38 (100%)	32 (84%)	6 (16%)	3	23
33	e	51/52 (98%)	47 (92%)	4 (8%)	16	55
34	f	34/34 (100%)	31 (91%)	3 (9%)	12	50
35	i	71/341 (21%)	65 (92%)	6 (8%)	13	52
36	k	17/17 (100%)	15 (88%)	2 (12%)	6	35
All	All	2901/3232 (90%)	2635 (91%)	266 (9%)	16	48

All (266) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	C	3	VAL
5	C	24	LEU
5	C	35	GLU
5	C	51	THR
5	C	72	ASP
5	C	74	ILE
5	C	120	VAL
5	C	130	LEU
5	C	134	ASN
5	C	156	ARG
5	C	180	GLU
5	C	185	GLU
5	C	189	ARG
5	C	195	VAL
5	C	203	ARG

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Mol	Chain	Res	Type
5	C	204	VAL
5	C	228	VAL
5	C	242	LYS
5	C	250	VAL
5	C	251	GLN
5	C	257	THR
5	C	261	LYS
5	C	265	LYS
5	C	271	ARG
6	D	12	THR
6	D	13	ARG
6	D	18	ASP
6	D	28	GLU
6	D	73	VAL
6	D	84	LEU
6	D	128	ARG
6	D	139	SER
6	D	160	LYS
6	D	168	GLU
7	E	84	THR
7	E	85	PHE
7	E	94	GLN
7	E	97	ASN
7	E	105	LEU
7	E	115	GLN
7	E	119	ILE
7	E	127	GLU
7	E	148	ILE
7	E	173	THR
7	E	179	SER
7	E	184	ASP
7	E	196	VAL
8	F	3	LYS
8	F	4	LEU
8	F	14	LYS
8	F	25	VAL
8	F	49	LEU
8	F	51	ASP
8	F	52	ASN
8	F	72	LYS
8	F	81	GLN
8	F	104	ILE

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Mol	Chain	Res	Type
8	F	106	ILE
8	F	130	MET
8	F	141	ILE
8	F	144	ASP
8	F	149	VAL
8	F	150	ARG
8	F	153	ASP
8	F	162	SER
9	G	10	VAL
9	G	11	VAL
9	G	49	THR
9	G	87	LEU
9	G	114	ASP
9	G	125	CYS
9	G	127	THR
9	G	153	ARG
10	H	15	LEU
10	H	17	ASP
10	H	25	TYR
10	H	37	VAL
10	H	58	LEU
10	H	60	GLU
10	H	76	GLU
10	H	77	THR
10	H	78	VAL
10	H	86	ASP
10	H	87	GLU
10	H	110	VAL
10	H	112	LYS
10	H	116	ARG
11	I	16	SER
11	I	36	ASP
11	I	58	THR
11	I	85	VAL
11	I	96	PHE
11	I	109	LYS
12	J	9	VAL
12	J	21	SER
12	J	28	LEU
12	J	31	GLN
12	J	55	ILE
12	J	66	SER

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Mol	Chain	Res	Type
12	J	111	GLN
12	J	112	THR
12	J	113	LYS
12	J	116	ASP
12	J	128	SER
13	K	5	THR
13	K	7	LYS
13	K	34	ARG
13	K	40	HIS
13	K	44	TYR
13	K	69	ARG
13	K	70	THR
13	K	88	THR
13	K	103	ILE
13	K	122	LEU
13	K	131	ASN
14	L	1	MET
14	L	21	CYS
14	L	42	THR
14	L	49	ARG
14	L	56	ASP
14	L	58	LEU
14	L	65	THR
14	L	84	CYS
14	L	106	GLU
14	L	116	ILE
15	M	2	ARG
15	M	14	LYS
15	M	46	VAL
15	M	47	ARG
15	M	55	MET
15	M	59	ARG
15	M	86	GLU
15	M	91	ASP
15	M	126	ARG
16	N	6	ARG
16	N	7	THR
16	N	12	MET
16	N	25	ASP
16	N	54	THR
16	N	58	LYS
16	N	115	GLU

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Mol	Chain	Res	Type
16	N	133	LYS
16	N	135	VAL
17	O	2	ARG
17	O	14	SER
17	O	36	THR
17	O	69	ARG
17	O	74	GLU
17	O	75	ILE
17	O	100	CYS
18	P	2	ASP
18	P	5	SER
18	P	19	GLN
18	P	20	GLU
18	P	31	THR
18	P	36	TYR
18	P	43	ASN
18	P	55	GLU
18	P	61	GLN
18	P	69	ASP
18	P	78	VAL
18	P	98	GLN
19	Q	3	ASN
19	Q	7	GLN
19	Q	21	ARG
19	Q	26	VAL
19	Q	51	ARG
19	Q	65	SER
19	Q	68	GLU
19	Q	92	VAL
19	Q	115	ASN
20	R	6	ARG
20	R	13	ARG
20	R	17	ILE
20	R	24	TYR
20	R	51	ARG
20	R	52	GLN
20	R	109	LEU
21	S	20	VAL
21	S	25	LEU
21	S	38	VAL
21	S	45	GLU
21	S	71	LYS

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Mol	Chain	Res	Type
21	S	72	VAL
21	S	83	TYR
21	S	101	ILE
22	T	12	SER
22	T	28	LYS
22	T	74	ILE
22	T	95	ARG
22	T	98	LYS
23	U	7	LEU
23	U	16	VAL
23	U	17	SER
23	U	48	GLN
23	U	72	GLN
24	V	7	ARG
24	V	34	VAL
24	V	41	LEU
24	V	42	VAL
24	V	68	SER
24	V	83	VAL
24	V	102	THR
25	W	7	GLU
25	W	12	GLN
25	W	61	LEU
25	W	78	GLN
25	W	90	ASP
25	W	92	VAL
26	X	11	ARG
26	X	12	ASN
26	X	21	LEU
26	X	35	SER
26	X	41	ARG
26	X	56	ASP
27	Y	2	SER
27	Y	4	VAL
27	Y	42	SER
27	Y	74	ARG
28	Z	2	LYS
28	Z	16	THR
28	Z	28	LEU
28	Z	44	LYS
28	Z	45	GLN
28	Z	48	ARG

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Mol	Chain	Res	Type
28	Z	56	LEU
29	a	36	VAL
29	a	56	LYS
30	b	4	GLN
30	b	9	THR
30	b	15	MET
30	b	18	SER
30	b	25	VAL
30	b	26	THR
30	b	28	LEU
30	b	32	LYS
30	b	36	GLU
30	b	40	ARG
30	b	46	ASP
30	b	52	ARG
31	c	5	ILE
31	c	6	ARG
31	c	10	LYS
31	c	22	THR
31	c	47	VAL
32	d	1	MET
32	d	12	ARG
32	d	24	THR
32	d	25	LYS
32	d	34	ARG
32	d	41	ARG
33	e	8	ARG
33	e	31	HIS
33	e	32	ILE
33	e	51	SER
34	f	2	LYS
34	f	12	ARG
34	f	36	ARG
35	i	333	ASP
35	i	337	GLN
35	i	369	ASP
35	i	386	LYS
35	i	397	SER
35	i	411	GLN
36	k	36	LEU
36	k	40	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such

sidechains are listed below:

Mol	Chain	Res	Type
5	C	86	ASN
5	C	90	ASN
5	C	200	HIS
5	C	251	GLN
6	D	136	ASN
6	D	140	HIS
7	E	165	HIS
8	F	81	GLN
8	F	127	ASN
10	H	11	ASN
10	H	33	GLN
10	H	43	ASN
12	J	31	GLN
13	K	80	HIS
13	K	86	GLN
14	L	3	GLN
14	L	89	ASN
15	M	104	GLN
16	N	3	GLN
17	O	18	GLN
18	P	100	HIS
19	Q	52	ASN
19	Q	66	ASN
20	R	81	ASN
21	S	82	HIS
22	T	7	HIS
23	U	48	GLN
23	U	59	ASN
26	X	46	HIS
28	Z	39	GLN
28	Z	58	ASN
32	d	26	ASN
32	d	29	GLN
35	i	332	ASN
35	i	381	ASN
35	i	411	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	42/113 (37%)	13 (30%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	2/3 (66%)	1 (50%)	0
3	A	2878/2903 (99%)	518 (17%)	19 (0%)
4	B	119/120 (99%)	13 (10%)	0
All	All	3041/3139 (96%)	545 (17%)	19 (0%)

All (545) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	33	C
1	1	36	U
1	1	37	U
1	1	38	U
1	1	39	A
1	1	41	C
1	1	42	A
1	1	43	G
1	1	46	C
1	1	57	G
1	1	58	G
1	1	67	A
1	1	70	G
2	2	76	A
3	A	10	A
3	A	12	U
3	A	33	C
3	A	34	U
3	A	35	G
3	A	45	G
3	A	46	G
3	A	49	A
3	A	50	U
3	A	51	G
3	A	62	U
3	A	63	A
3	A	65	U
3	A	71	A
3	A	72	U
3	A	74	A
3	A	75	G
3	A	84	A
3	A	93	G
3	A	96	C

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Mol	Chain	Res	Type
3	A	101	A
3	A	102	U
3	A	103	A
3	A	110	G
3	A	118	A
3	A	119	A
3	A	120	U
3	A	136	G
3	A	137	U
3	A	138	U
3	A	139	U
3	A	142	A
3	A	156	A
3	A	162	U
3	A	181	A
3	A	188	G
3	A	196	A
3	A	199	A
3	A	215	G
3	A	216	A
3	A	220	G
3	A	221	A
3	A	222	A
3	A	226	A
3	A	248	G
3	A	266	G
3	A	272	A
3	A	275	C
3	A	276	U
3	A	285	G
3	A	291	G
3	A	302	C
3	A	311	A
3	A	329	G
3	A	330	A
3	A	335	C
3	A	349	U
3	A	353	C
3	A	356	G
3	A	361	G
3	A	362	A
3	A	372	G

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Mol	Chain	Res	Type
3	A	386	G
3	A	396	G
3	A	399	U
3	A	411	G
3	A	419	U
3	A	424	G
3	A	454	A
3	A	455	C
3	A	475	C
3	A	477	A
3	A	479	A
3	A	480	A
3	A	481	G
3	A	491	G
3	A	504	A
3	A	505	A
3	A	509	C
3	A	510	C
3	A	513	A
3	A	518	G
3	A	529	A
3	A	531	C
3	A	532	A
3	A	533	G
3	A	543	G
3	A	544	C
3	A	550	C
3	A	552	U
3	A	558	U
3	A	563	A
3	A	567	U
3	A	568	U
3	A	573	U
3	A	575	A
3	A	586	A
3	A	603	A
3	A	613	A
3	A	614	A
3	A	615	U
3	A	627	A
3	A	632	A
3	A	634	C

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Mol	Chain	Res	Type
3	A	637	A
3	A	645	C
3	A	646	U
3	A	647	G
3	A	653	U
3	A	654	A
3	A	655	A
3	A	668	A
3	A	685	A
3	A	686	U
3	A	711	G
3	A	712	G
3	A	713	G
3	A	718	A
3	A	730	A
3	A	747	U
3	A	753	A
3	A	757	G
3	A	763	G
3	A	764	A
3	A	765	C
3	A	775	G
3	A	777	G
3	A	782	A
3	A	784	G
3	A	785	G
3	A	788	A
3	A	789	A
3	A	790	U
3	A	791	C
3	A	793	A
3	A	794	A
3	A	801	G
3	A	805	G
3	A	812	C
3	A	827	U
3	A	828	U
3	A	831	G
3	A	846	U
3	A	859	G
3	A	865	C
3	A	869	G

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Mol	Chain	Res	Type
3	A	878	A
3	A	896	A
3	A	897	C
3	A	899	A
3	A	907	G
3	A	910	A
3	A	914	G
3	A	915	C
3	A	932	U
3	A	933	A
3	A	946	C
3	A	953	G
3	A	957	C
3	A	961	C
3	A	974	G
3	A	983	A
3	A	990	A
3	A	996	A
3	A	999	U
3	A	1005	C
3	A	1009	A
3	A	1012	U
3	A	1013	C
3	A	1022	G
3	A	1023	U
3	A	1027	A
3	A	1033	U
3	A	1040	A
3	A	1046	A
3	A	1056	G
3	A	1057	A
3	A	1070	A
3	A	1071	G
3	A	1073	A
3	A	1083	U
3	A	1087	G
3	A	1088	A
3	A	1090	A
3	A	1101	U
3	A	1111	A
3	A	1112	G
3	A	1116	G

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Mol	Chain	Res	Type
3	A	1129	A
3	A	1130	U
3	A	1132	U
3	A	1133	A
3	A	1135	C
3	A	1136	G
3	A	1139	G
3	A	1142	A
3	A	1143	A
3	A	1155	A
3	A	1173	U
3	A	1179	G
3	A	1182	G
3	A	1206	G
3	A	1212	G
3	A	1218	G
3	A	1236	G
3	A	1238	G
3	A	1247	A
3	A	1249	U
3	A	1252	G
3	A	1253	A
3	A	1256	G
3	A	1262	A
3	A	1271	G
3	A	1272	A
3	A	1294	U
3	A	1300	G
3	A	1301	A
3	A	1302	A
3	A	1308	A
3	A	1329	U
3	A	1332	G
3	A	1337	G
3	A	1338	G
3	A	1345	C
3	A	1346	G
3	A	1365	A
3	A	1379	U
3	A	1383	A
3	A	1395	A
3	A	1403	A

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Mol	Chain	Res	Type
3	A	1416	G
3	A	1417	C
3	A	1424	G
3	A	1428	C
3	A	1434	A
3	A	1437	C
3	A	1449	G
3	A	1451	C
3	A	1452	G
3	A	1453	A
3	A	1482	G
3	A	1489	C
3	A	1491	G
3	A	1493	C
3	A	1494	A
3	A	1495	A
3	A	1497	U
3	A	1498	C
3	A	1509	A
3	A	1510	G
3	A	1515	A
3	A	1524	G
3	A	1529	G
3	A	1533	C
3	A	1535	A
3	A	1536	C
3	A	1537	G
3	A	1554	U
3	A	1560	G
3	A	1566	A
3	A	1569	A
3	A	1576	U
3	A	1578	U
3	A	1581	G
3	A	1583	A
3	A	1585	C
3	A	1606	C
3	A	1607	C
3	A	1608	A
3	A	1616	A
3	A	1634	A
3	A	1639	C

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Mol	Chain	Res	Type
3	A	1647	U
3	A	1648	U
3	A	1649	G
3	A	1660	G
3	A	1674	G
3	A	1677	A
3	A	1715	G
3	A	1722	A
3	A	1725	U
3	A	1729	U
3	A	1730	C
3	A	1738	G
3	A	1744	A
3	A	1757	A
3	A	1764	C
3	A	1773	A
3	A	1782	U
3	A	1786	A
3	A	1791	A
3	A	1800	C
3	A	1801	A
3	A	1802	A
3	A	1808	A
3	A	1809	A
3	A	1811	G
3	A	1816	C
3	A	1829	A
3	A	1847	A
3	A	1849	G
3	A	1850	G
3	A	1870	C
3	A	1871	A
3	A	1872	A
3	A	1876	A
3	A	1896	G
3	A	1906	G
3	A	1920	C
3	A	1927	A
3	A	1929	G
3	A	1930	G
3	A	1931	U
3	A	1934	C

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Mol	Chain	Res	Type
3	A	1936	A
3	A	1937	A
3	A	1939	U
3	A	1955	U
3	A	1956	U
3	A	1960	A
3	A	1962	C
3	A	1966	A
3	A	1967	C
3	A	1970	A
3	A	1971	U
3	A	1972	G
3	A	1974	C
3	A	1982	U
3	A	1991	U
3	A	1992	G
3	A	1993	U
3	A	1997	C
3	A	2021	C
3	A	2023	C
3	A	2030	A
3	A	2031	A
3	A	2033	A
3	A	2043	C
3	A	2050	C
3	A	2054	A
3	A	2055	C
3	A	2056	G
3	A	2060	A
3	A	2061	G
3	A	2062	A
3	A	2069	G
3	A	2072	C
3	A	2093	G
3	A	2097	A
3	A	2101	A
3	A	2103	C
3	A	2104	C
3	A	2105	U
3	A	2106	U
3	A	2111	U
3	A	2112	G

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Mol	Chain	Res	Type
3	A	2113	U
3	A	2116	G
3	A	2117	A
3	A	2118	U
3	A	2119	A
3	A	2120	G
3	A	2123	G
3	A	2126	A
3	A	2128	G
3	A	2131	U
3	A	2132	U
3	A	2133	G
3	A	2134	A
3	A	2145	C
3	A	2146	C
3	A	2147	A
3	A	2148	G
3	A	2159	G
3	A	2160	C
3	A	2161	C
3	A	2163	A
3	A	2164	C
3	A	2165	C
3	A	2167	U
3	A	2168	G
3	A	2169	A
3	A	2170	A
3	A	2171	A
3	A	2172	U
3	A	2173	A
3	A	2174	C
3	A	2177	C
3	A	2178	C
3	A	2185	U
3	A	2187	U
3	A	2190	G
3	A	2198	A
3	A	2203	U
3	A	2204	G
3	A	2211	A
3	A	2212	A
3	A	2225	A

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Mol	Chain	Res	Type
3	A	2238	G
3	A	2239	G
3	A	2250	G
3	A	2268	A
3	A	2278	A
3	A	2280	G
3	A	2283	C
3	A	2287	A
3	A	2288	A
3	A	2297	A
3	A	2305	U
3	A	2308	G
3	A	2322	A
3	A	2325	G
3	A	2331	G
3	A	2336	A
3	A	2345	G
3	A	2347	C
3	A	2350	C
3	A	2354	C
3	A	2357	G
3	A	2366	A
3	A	2383	G
3	A	2385	C
3	A	2402	U
3	A	2403	C
3	A	2406	A
3	A	2420	C
3	A	2421	G
3	A	2422	C
3	A	2423	U
3	A	2424	C
3	A	2425	A
3	A	2427	C
3	A	2429	G
3	A	2430	A
3	A	2431	U
3	A	2432	A
3	A	2434	A
3	A	2435	A
3	A	2440	C
3	A	2441	U

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Mol	Chain	Res	Type
3	A	2445	G
3	A	2448	A
3	A	2464	G
3	A	2475	C
3	A	2476	A
3	A	2478	A
3	A	2491	U
3	A	2492	U
3	A	2497	A
3	A	2502	G
3	A	2504	U
3	A	2505	G
3	A	2506	U
3	A	2507	C
3	A	2513	A
3	A	2514	U
3	A	2518	A
3	A	2520	C
3	A	2529	G
3	A	2566	A
3	A	2567	G
3	A	2578	G
3	A	2582	G
3	A	2585	U
3	A	2586	U
3	A	2602	A
3	A	2603	G
3	A	2609	U
3	A	2613	U
3	A	2615	U
3	A	2621	G
3	A	2623	G
3	A	2624	G
3	A	2629	U
3	A	2630	G
3	A	2636	C
3	A	2638	G
3	A	2669	G
3	A	2682	A
3	A	2689	U
3	A	2690	U
3	A	2714	G

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Mol	Chain	Res	Type
3	A	2716	C
3	A	2726	A
3	A	2733	A
3	A	2739	U
3	A	2744	G
3	A	2748	A
3	A	2757	A
3	A	2765	A
3	A	2778	A
3	A	2779	U
3	A	2780	G
3	A	2791	G
3	A	2792	A
3	A	2798	U
3	A	2799	A
3	A	2801	G
3	A	2820	A
3	A	2821	A
3	A	2825	G
3	A	2833	U
3	A	2835	A
3	A	2836	U
3	A	2849	U
3	A	2860	A
3	A	2861	U
3	A	2867	G
3	A	2870	C
3	A	2873	A
3	A	2879	A
3	A	2880	C
3	A	2883	A
3	A	2884	U
3	A	2885	G
3	A	2886	A
3	A	2888	C
3	A	2891	U
4	B	24	G
4	B	25	U
4	B	35	C
4	B	41	G
4	B	45	A
4	B	56	G

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Mol	Chain	Res	Type
4	B	66	A
4	B	67	G
4	B	71	C
4	B	88	C
4	B	89	U
4	B	90	C
4	B	109	A

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	A	100	U
3	A	613	A
3	A	645	C
3	A	653	U
3	A	784	G
3	A	827	U
3	A	830	G
3	A	1110	G
3	A	1344	U
3	A	1494	A
3	A	1721	G
3	A	1939	U
3	A	2127	G
3	A	2158	A
3	A	2422	C
3	A	2424	C
3	A	2430	A
3	A	2602	A
3	A	2756	U

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 432 ligands modelled in this entry, 432 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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.