



Full wwPDB EM Validation Report ⓘ

Mar 1, 2026 – 02:55 PM UTC

PDB ID : 5A2Q / pdb_00005a2q
EMDB ID : EMD-3019
Title : Structure of the HCV IRES bound to the human ribosome
Authors : Quade, N.; Leiundgut, M.; Boehringer, D.; Heuvel, J.v.d.; Ban, N.
Deposited on : 2015-05-21
Resolution : 3.90 Å(reported)
Based on initial model : 4W23

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

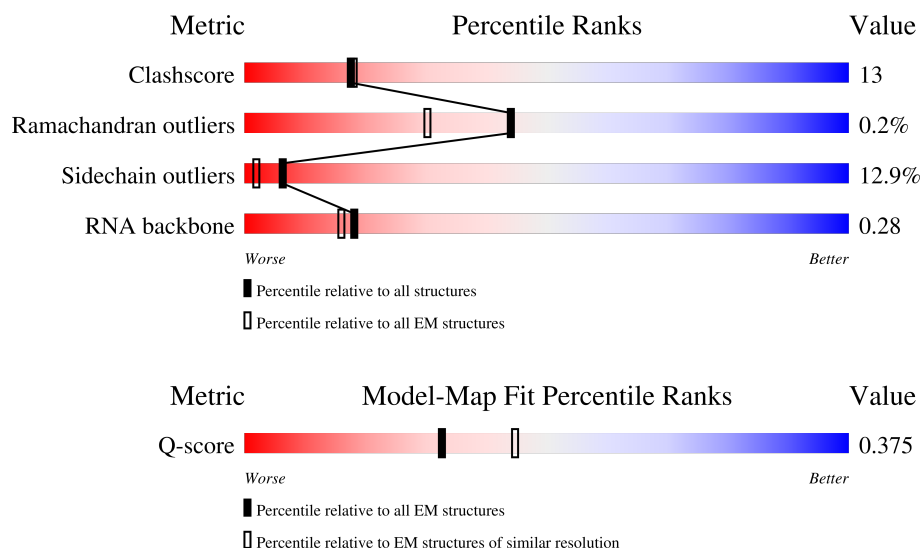
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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.



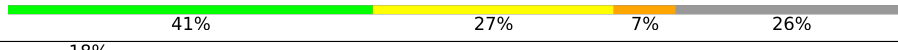
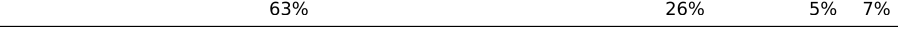
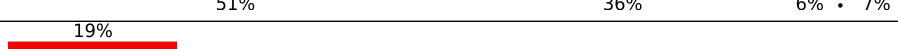
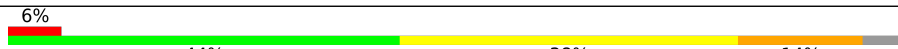
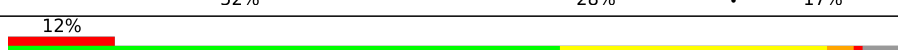
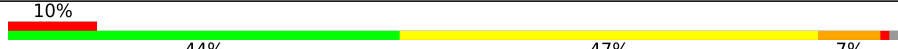
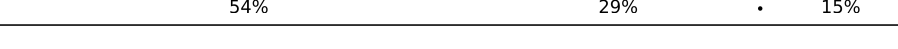
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8855 (3.40 - 4.40)

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

Mol	Chain	Length	Quality of chain
1	2	1868	
2	3	257	
3	A	295	

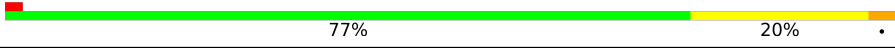
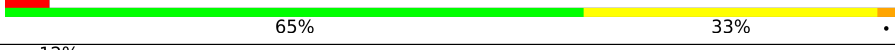
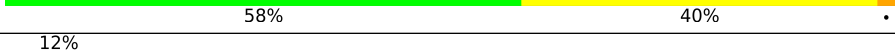
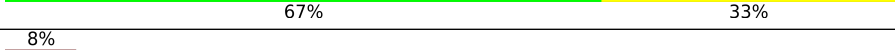
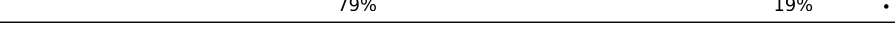
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Mol	Chain	Length	Quality of chain
4	B	264	
5	C	293	
6	D	243	
7	E	263	
8	F	204	
9	G	249	
10	H	194	
11	I	208	
12	J	194	
13	K	165	
14	L	158	
15	M	132	
16	N	151	
17	O	151	
18	P	145	
19	Q	146	
20	R	135	
21	S	152	
22	T	146	
23	U	119	
24	V	83	
25	W	130	
26	X	143	
27	Y	130	
28	Z	125	

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Mol	Chain	Length	Quality of chain
29	a	101	
30	b	82	
31	c	61	
32	d	55	
33	e	56	
34	f	72	
35	g	315	
36	h	24	
37	r	13	
38	w	62	

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 80749 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 18S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1665	Total	C	N	O	P	0	0
			35552	15869	6385	11633	1665		

- Molecule 2 is a RNA chain called HCV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	257	Total	C	N	O	P	0	0
			5485	2444	979	1805	257		

- Molecule 3 is a protein called RIBOSOMAL PROTEIN US2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	216	Total	C	N	O	S	0	0
			1705	1083	299	315	8		

- Molecule 4 is a protein called RIBOSOMAL PROTEIN ES1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 5 is a protein called RIBOSOMAL PROTEIN US5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	218	Total	C	N	O	S	0	0
			1690	1094	289	297	10		

- Molecule 6 is a protein called RIBOSOMAL PROTEIN US3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	225	Total	C	N	O	S	0	0
			1752	1117	315	313	7		

- Molecule 7 is a protein called RIBOSOMAL PROTEIN ES4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 8 is a protein called RIBOSOMAL PROTEIN US7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 9 is a protein called RIBOSOMAL PROTEIN ES6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	230	Total	C	N	O	S	0	0
			1864	1164	373	320	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	221	ARG	LYS	conflict	UNP P62753

- Molecule 10 is a protein called RIBOSOMAL PROTEIN ES7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	186	Total	C	N	O	S	0	0
			1501	957	276	267	1		

- Molecule 11 is a protein called RIBOSOMAL PROTEIN ES8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 12 is a protein called RIBOSOMAL PROTEIN US4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 13 is a protein called RIBOSOMAL PROTEIN ES10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	95	Total	C	N	O	S	0	0
			800	522	142	131	5		

- Molecule 14 is a protein called RIBOSOMAL PROTEIN US17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	151	Total	C	N	O	S	0	0
			1229	782	230	211	6		

- Molecule 15 is a protein called RIBOSOMAL PROTEIN ES12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	123	Total	C	N	O	S	0	0
			953	598	169	177	9		

- Molecule 16 is a protein called RIBOSOMAL PROTEIN US15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 17 is a protein called RIBOSOMAL PROTEIN US11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	135	Total	C	N	O	S	0	0
			1010	618	198	188	6		

- Molecule 18 is a protein called RIBOSOMAL PROTEIN US19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	120	Total	C	N	O	S	0	0
			984	625	184	168	7		

- Molecule 19 is a protein called RIBOSOMAL PROTEIN US9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	139	Total	C	N	O	S	0	0
			1109	704	210	192	3		

- Molecule 20 is a protein called RIBOSOMAL PROTEIN ES17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	132	Total	C	N	O	S	0	0
			1066	669	199	194	4		

- Molecule 21 is a protein called RIBOSOMAL PROTEIN US13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	143	Total	C	N	O	S	0	0
			1184	743	240	200	1		

- Molecule 22 is a protein called RIBOSOMAL PROTEIN ES19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	145	Total	C	N	O	S	0	0
			1128	706	218	201	3		

- Molecule 23 is a protein called RIBOSOMAL PROTEIN US10.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 24 is a protein called RIBOSOMAL PROTEIN ES21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	82	Total	C	N	O	S	0	0
			625	384	116	120	5		

- Molecule 25 is a protein called RIBOSOMAL PROTEIN US8.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 26 is a protein called RIBOSOMAL PROTEIN US12.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 27 is a protein called RIBOSOMAL PROTEIN ES24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 28 is a protein called RIBOSOMAL PROTEIN ES25.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 29 is a protein called RIBOSOMAL PROTEIN ES26.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	101	Total	C	N	O	S	0	0
			816	509	170	132	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	78	VAL	ALA	conflict	UNP P62854

- Molecule 30 is a protein called RIBOSOMAL PROTEIN ES27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 31 is a protein called RIBOSOMAL PROTEIN ES28.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	61	Total	C	N	O	S	0	0
			479	292	95	90	2		

- Molecule 32 is a protein called RIBOSOMAL PROTEIN US14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	55	Total	C	N	O	S	0	0
			458	286	94	73	5		

- Molecule 33 is a protein called RIBOSOMAL PROTEIN ES30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	56	Total	C	N	O	S	0	0
			442	273	96	72	1		

- Molecule 34 is a protein called RIBOSOMAL PROTEIN ES31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	72	Total	C	N	O	S	0	0
			585	366	114	97	8		

- Molecule 35 is a protein called RIBOSOMAL PROTEIN RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 36 is a protein called RIBOSOMAL PROTEIN EL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	24	Total	C	N	O	S	0	0
			231	140	63	26	2		

- Molecule 37 is a protein called RIBOSOMAL PROTEIN EL19.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	r	13	Total	C	N	O	0	0
			118	68	31	19		

- Molecule 38 is a protein called RIBOSOMAL PROTEIN EL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	w	62	Total	C	N	O	S	0	0
			452	279	92	80	1		

- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
39	2	98	Total	Mg	0
			98	98	

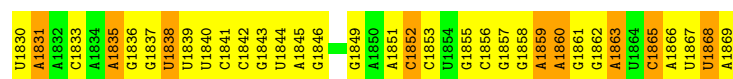
- Molecule 40 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
40	a	1	Total 1	Zn 1	0
40	d	1	Total 1	Zn 1	0
40	f	1	Total 1	Zn 1	0

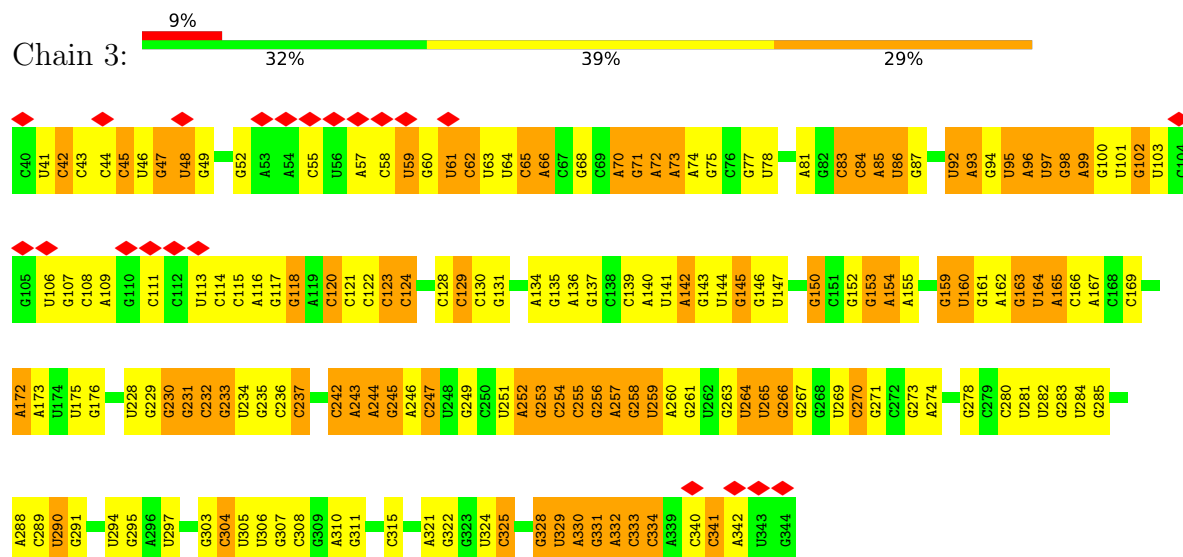
- Molecule 41 is water.

Mol	Chain	Residues	Atoms		AltConf
41	2	141	Total 141	O 141	0
41	C	2	Total 2	O 2	0
41	e	1	Total 1	O 1	0

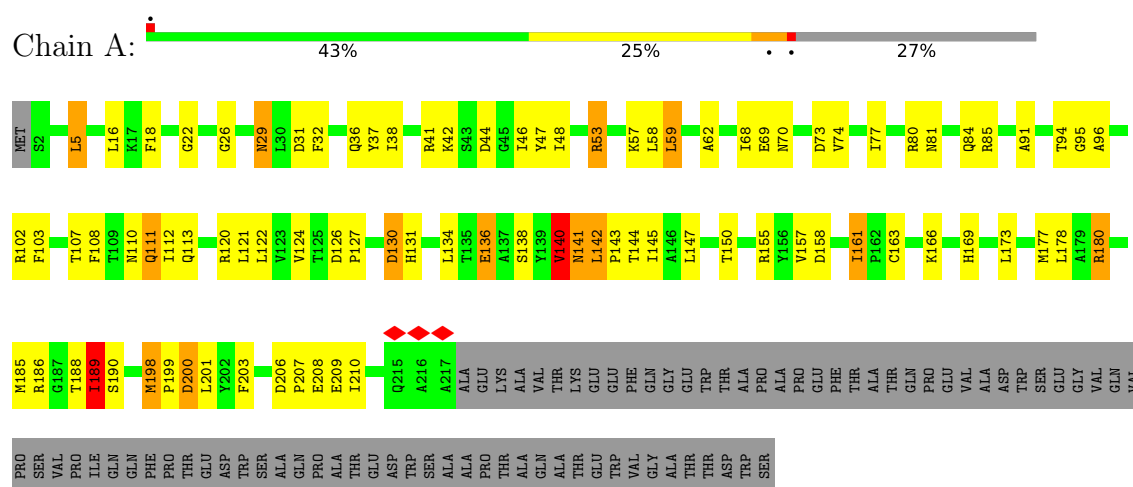
G1734	G1656	A1589	C1526	A1454	C1309	G1245	G1171	G1097	U1015	C941	G868	G
A1735	G1657	C1590	G1526	A1455	U1310	A1246	U1177	C1098	U1016	G942	A869	G
G1736	G1658	C1591	C1527	U1462	C1311	C1247	U1178	G1099	U1017	G943	A870	C
G1737	U1659	C1592	G1528	U1463	G1312	U1248	G1179	A1100	U1018	A944	U871	C791
C1738	C1660	C1593	C1529	U1464	A1313	C1249	C1180	U101	U945	G946	A872	C792
U1741	A1661	A1594	U1590	A1465	U1314	A1250	G1181	A1023	A1023	G874	A794	C793
U1662	U1662	A1595	A1531	G1466	U1315	A1251	A1182	G1109	C1026	C877	A795	A796
A1663	A1663	C1597	C1532	G1467	C1316	A1252	A1181	U1110	A1030	C878	G796	G797
G1742	A1664	A1533	A1533	G1468	C1317	A1253	A1182	U1111	A1031	G879	G797	G798
G1743	G1665	U1598	U1535	A1469	G1320	G1254	A1190	U1112	U954	G880	U799	U799
A1744	G1666	A1599	U1536	A1470	G1321	G1255	A1191	C1032	A1032	G881	U806	U806
U1746	U1667	G1600	G1536	C1470	G1322	A1258	A1192	U1113	A1033	U882	G807	G807
U1761	A1668	A1601	A1537	U1471	U1400	A1259	U1193	U1114	A1034	U887	A808	A808
C	G1670	U1602	A1542	G1473	A1401	A1260	A1194	U1115	A1035	U888	A810	A810
G	U1671	G1603	U1543	A1474	A1402	A1261	A1195	C1116	A1036	U889	A811	A811
G	U1672	G1604	C1544	G1475	C1403	C1262	A1199	U1117	G1037	U890	A812	A812
C	U1673	G1605	A1545	A1476	U1405	U1263	G1207	U1118	A1041	U897	A816	A816
C	A1674	G1606	U1546	U1477	A1406	G1264	A1208	U1119	G1043	U898	G817	G817
A	A1675	U1608	C1547	U1478	G1406	G1265	A1209	U1120	U1045	C900	A818	A818
C	U1676	G1609	C1548	G1479	U1407	C1266	G1210	U1121	U1046	G901	G819	G819
C	U1677	G1610	U1549	A1480	U1414	C1267	G1211	G1122	A1048	G902	U820	U820
C	U1678	G1611	U1550	A1481	C1415	C1268	G1212	C1123	A1049	A903	U822	U822
A1679	A1679	G1612	U1551	G1482	C	G1269	A1203	C1124	U1052	G904	U823	U823
G1680	G1680	G1613	G	G1491	C	C1270	G1209	G1125	C1064	G971	G824	C824
U1681	U1681	A1614	C	A1486	U1341	C1271	G1210	U1126	G976	G976	G828	G828
C1682	C1682	U1615	C	A1487	U1342	C1272	G1211	G1127	C977	C977	C829	C829
G1683	U1683	G1616	U	G1488	U1343	C1273	G1212	A1133	G978	G978	C830	C830
U1684	U1684	G1617	A	A1489	U1344	C1274	G1213	G1134	A980	A980	G831	G831
G1686	G1686	C1618	C	G1490	A1344	A1275	G1214	U1135	A1058	A1058	C834	C834
G1687	G1687	U1621	C	G1491	U1345	G1276	G1215	C1136	A981	A981	C	C
C1688	C1688	U1622	C1558	C1492	U1346	C1277	G1216	U1137	A917	A917	A	A
C1689	C1689	A1623	C1559	U1426	G1348	A1278	G1217	C1138	A920	A920	G	G
U1690	U1690	G1624	U1560	U1427	U1349	A1279	G1218	U1139	A921	A921	C	C
U1691	U1691	C1625	C1561	G1495	G1354	A1280	G1219	U1140	A990	A990	G841	G841
U1692	U1692	U1626	C1562	G1496	C1355	A1281	A1220	C1139	A991	A991	C842	C842
G1693	G1693	C1627	C1563	U1431	C1356	A1282	G1221	U1141	A992	A992	U844	U844
U1694	U1694	C1628	C1564	U1432	G1357	A1283	G1222	C1063	A993	A993	G845	G845
A1695	A1695	G1629	C1565	U1433	U1358	G1284	G1223	U1065	A994	A994	G846	G846
U1699	U1699	A1630	G1566	C	U1359	A1285	G1224	C1066	A995	A995	A847	A847
A1699	A1699	U1631	G1567	U1505	U1360	A1286	G1225	U1067	A996	A996	G852	G852
G1798	G1798	G1632	C1568	A1506	U1361	U1287	G1226	U1068	A997	A997	C856	C856
G1799	G1799	A1633	C1569	U1507	U1362	U1288	G1227	U1069	A998	A998	U857	U857
A1800	A1800	U1642	C1570	G1508	U1363	U1289	G1228	C1070	A999	A999	A858	A858
A1801	A1801	A1634	C1571	U1509	U1364	A1290	G1229	U1071	A1000	A1000	A861	A861
G1805	G1805	U1643	C1572	G1510	U1365	G1291	G1230	U1072	U1001	U1001	U938	U938
A1806	A1806	C1644	G1573	U1511	U1366	A1292	G1231	C1073	U1002	U1002	U940	U940
C1807	C1807	U1645	C1574	C1512	U1367	G1293	G1232	C1074	U1003	U1003		
G1814	G1814	G1646	G1577	U1513	U1371	G1294	G1233	C1075	U1004	U1004		
A1815	A1815	C1647	U1578	G1514	U1372	U1297	G1234	U1076	A1008	A1008		
G1816	G1816	U1648	A1579	U1515	C1373	G1298	G1235	U1077	A1009	A1009		
G1817	G1817	C1580	A1580	U1516	U1374	U1299	G1236	C1078	A1010	A1010		
A1818	A1818	U1649	C1581	U1517	C1375	A1301	G1237	U1079	U1011	U1011		
U1729	U1729	A1650	C1582	G1518	U1376	G1302	U1238	U1080	A1012	A1012		
U1730	U1730	U1651	C1583	U1519	U1377	C1303	U1239	U1081				
A1824	A1824	G1652	U1584	U1520	U1378	U1304	U1240	U1082				
A1825	A1825	U1653	U1585	C1521	A1379	C1305	A1241	U1083				
G1826	G1826	G1654	U1586	A1522	C1380	C1306	U1242	U1084				
G1829	G1829	C1655	A1587	G1524	U1381	U1307	U1243	U1085				
			A1588		A1382	U1308	U1244	G1096				



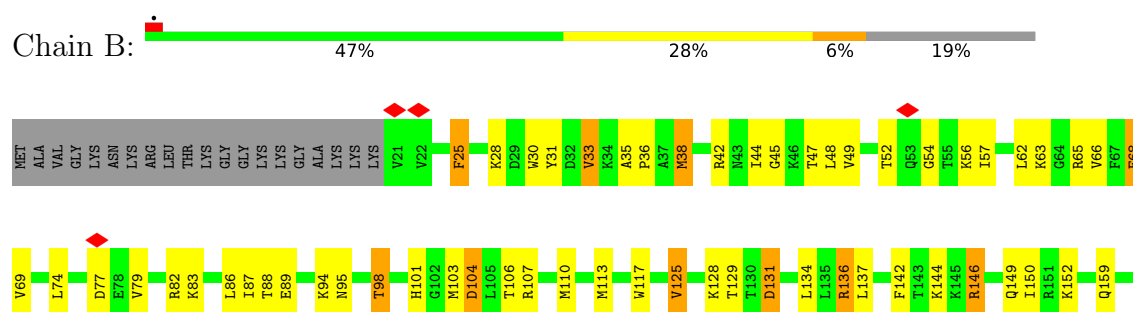
• Molecule 2: HCV IRES



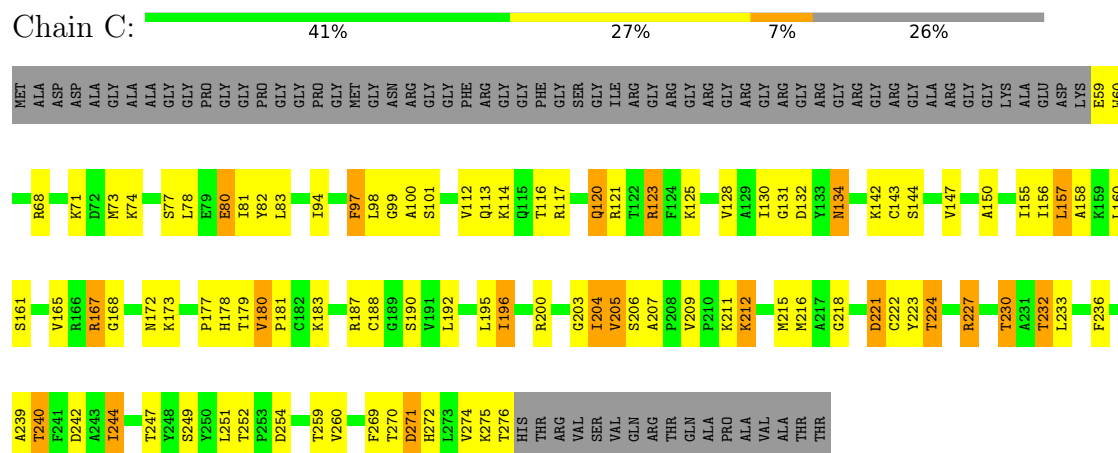
• Molecule 3: RIBOSOMAL PROTEIN US2



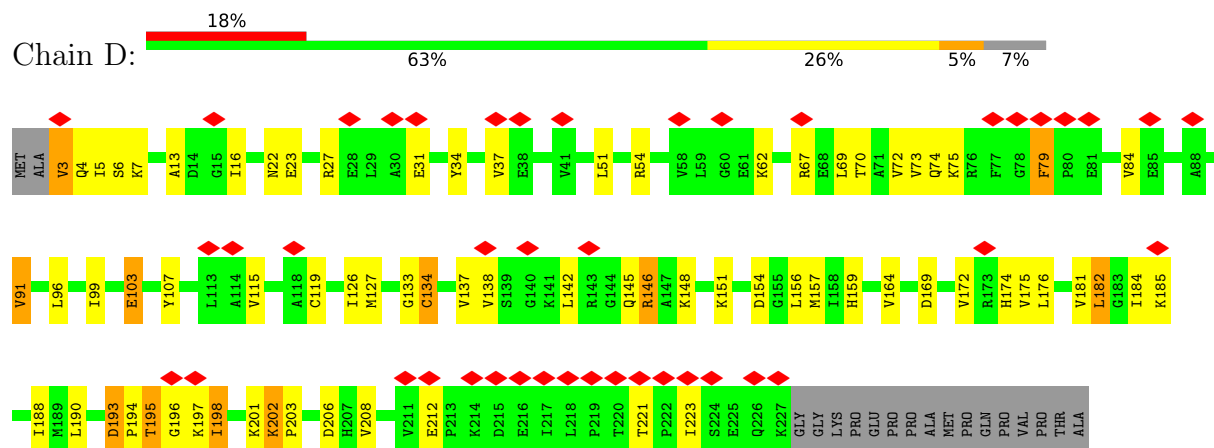
• Molecule 4: RIBOSOMAL PROTEIN ES1



- Molecule 5: RIBOSOMAL PROTEIN US5

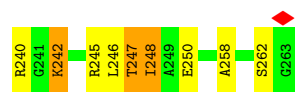


- Molecule 6: RIBOSOMAL PROTEIN US3

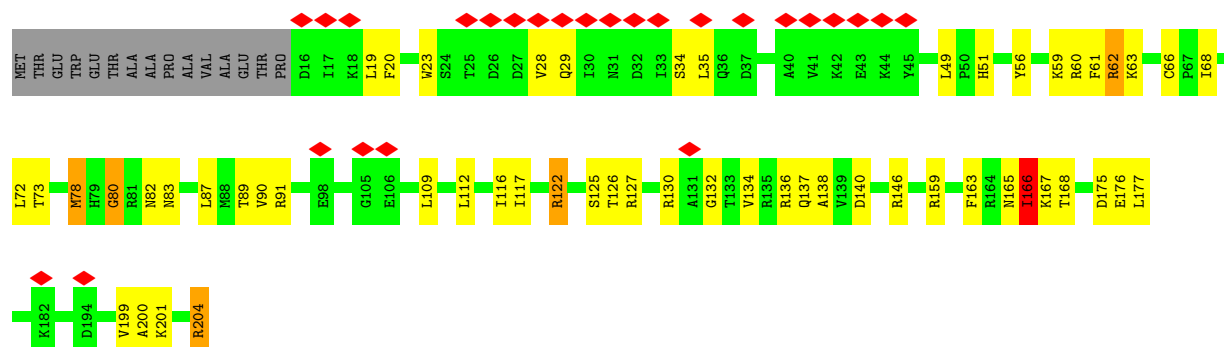


- Molecule 7: RIBOSOMAL PROTEIN ES4

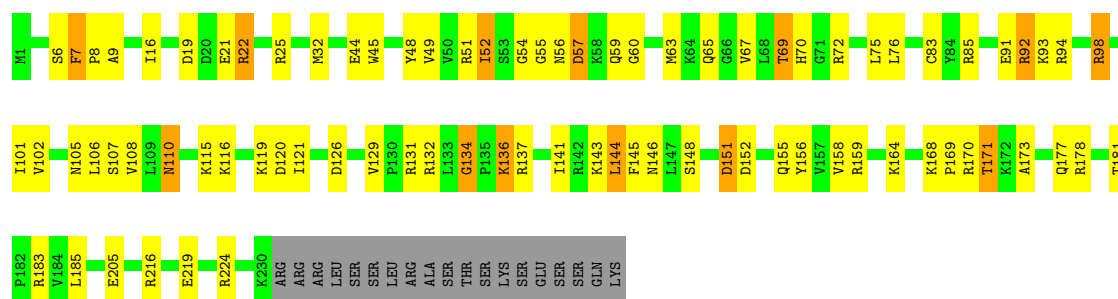




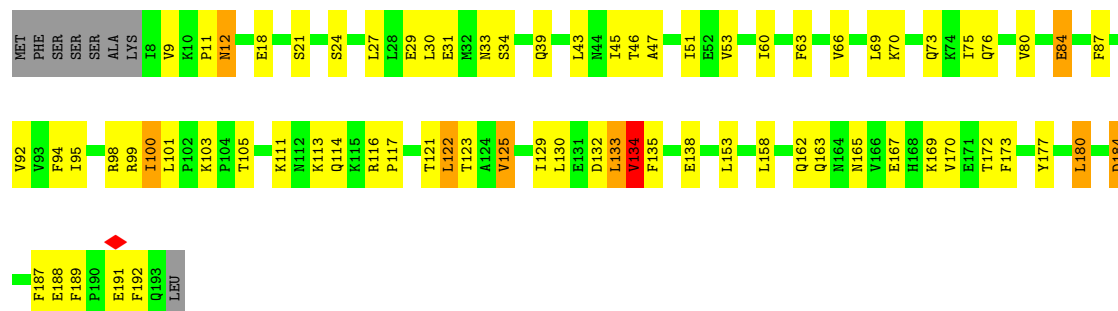
• Molecule 8: RIBOSOMAL PROTEIN US7



• Molecule 9: RIBOSOMAL PROTEIN ES6

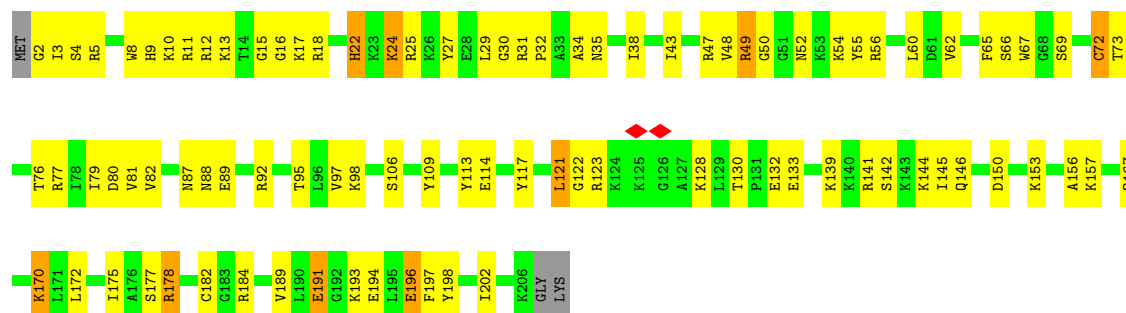


• Molecule 10: RIBOSOMAL PROTEIN ES7



• Molecule 11: RIBOSOMAL PROTEIN ES8

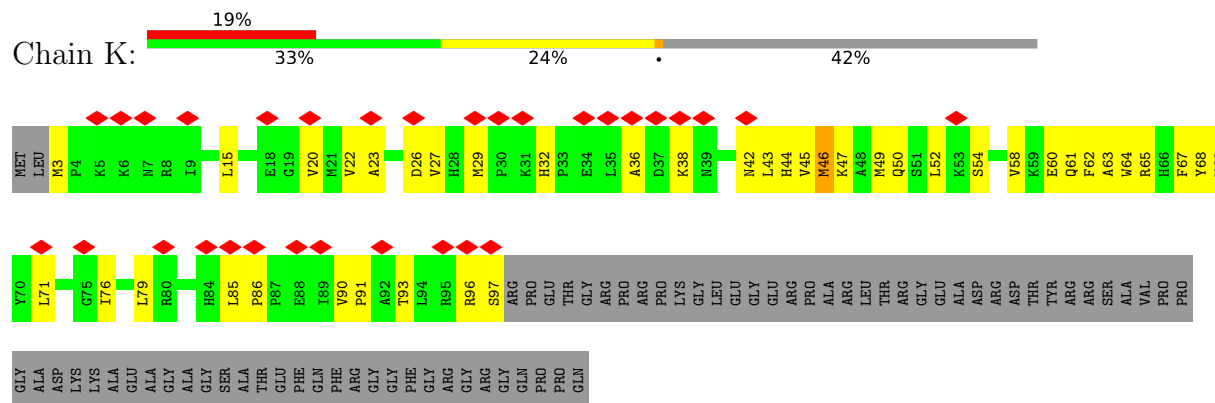




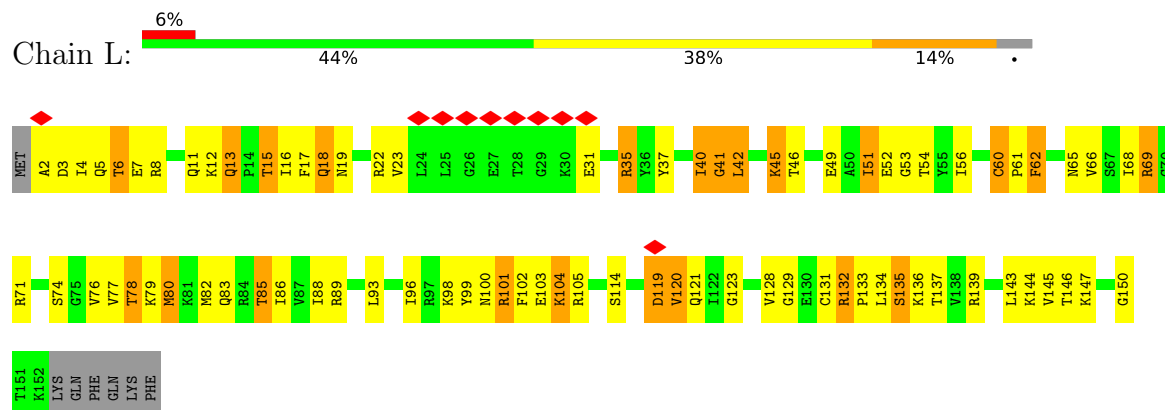
• Molecule 12: RIBOSOMAL PROTEIN US4



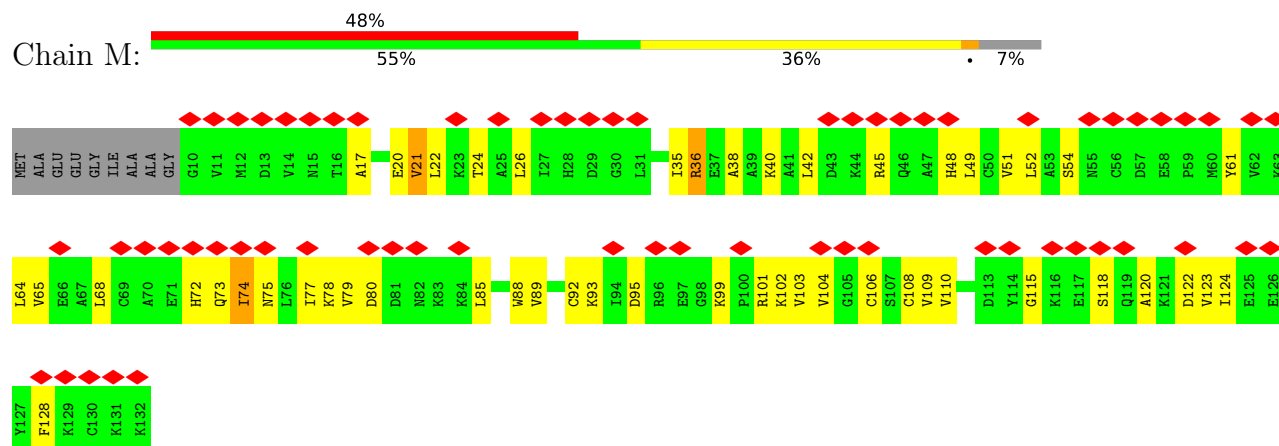
• Molecule 13: RIBOSOMAL PROTEIN ES10



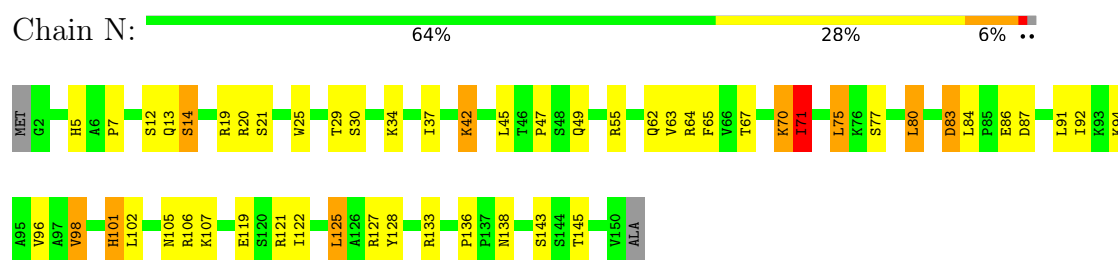
• Molecule 14: RIBOSOMAL PROTEIN US17



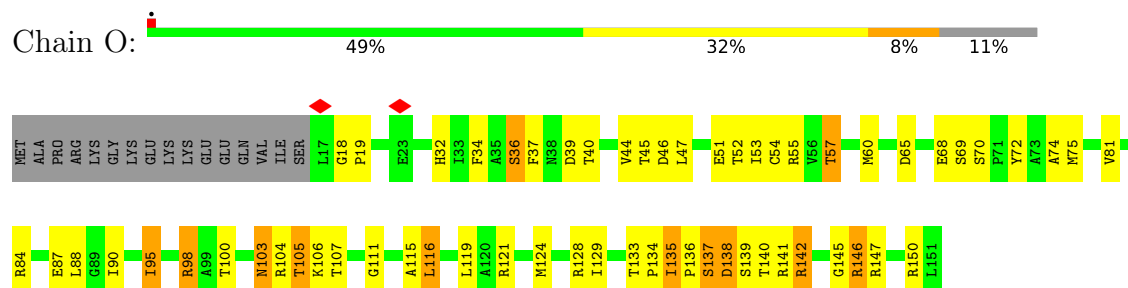
• Molecule 15: RIBOSOMAL PROTEIN ES12



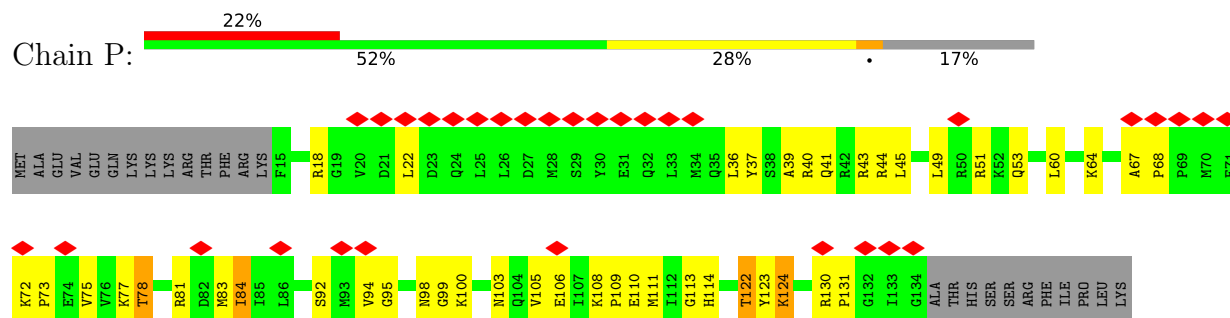
• Molecule 16: RIBOSOMAL PROTEIN US15



• Molecule 17: RIBOSOMAL PROTEIN US11

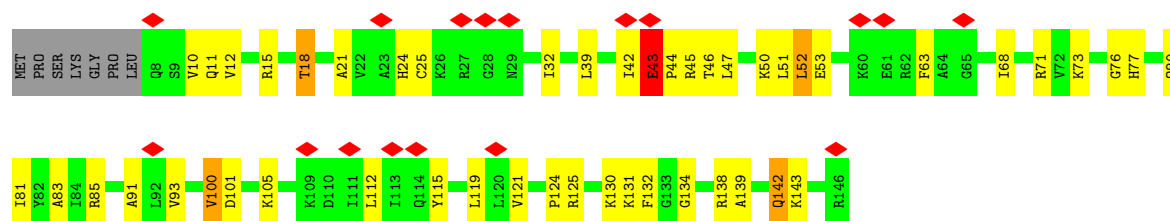


• Molecule 18: RIBOSOMAL PROTEIN US19

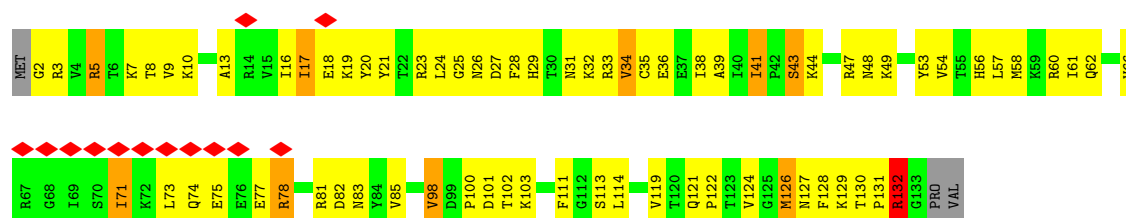
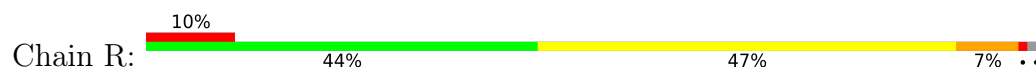


• Molecule 19: RIBOSOMAL PROTEIN US9

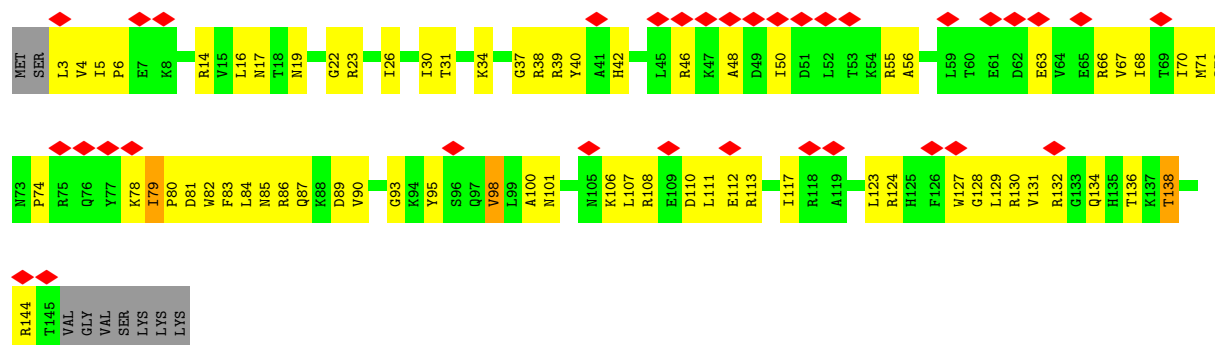




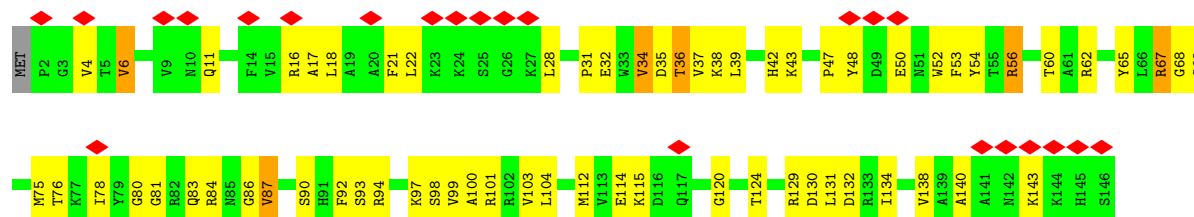
• Molecule 20: RIBOSOMAL PROTEIN ES17



• Molecule 21: RIBOSOMAL PROTEIN US13

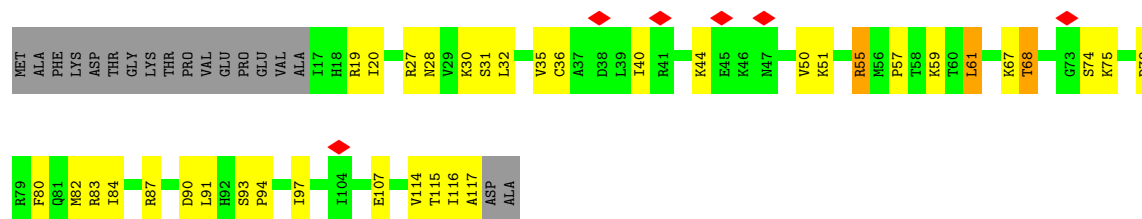


• Molecule 22: RIBOSOMAL PROTEIN ES19



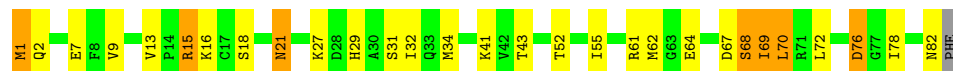
• Molecule 23: RIBOSOMAL PROTEIN US10





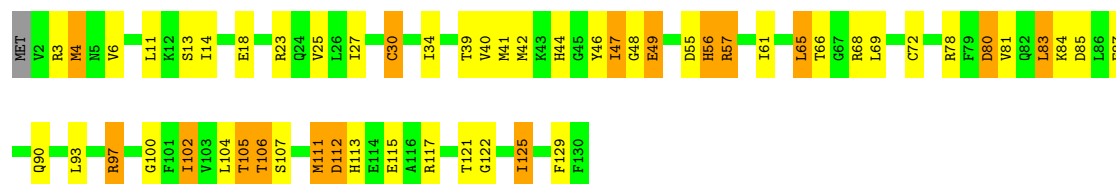
• Molecule 24: RIBOSOMAL PROTEIN ES21

Chain V: 64% 27% 8%



• Molecule 25: RIBOSOMAL PROTEIN US8

Chain W: 57% 30% 12%



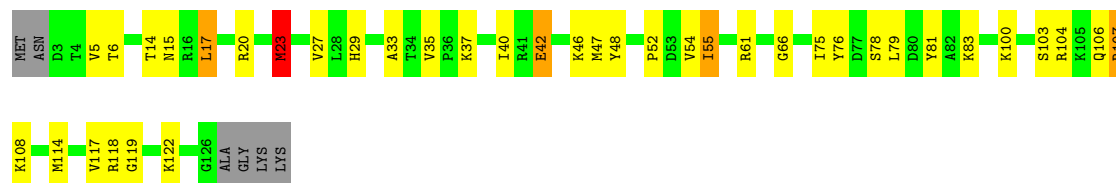
• Molecule 26: RIBOSOMAL PROTEIN US12

Chain X: 65% 28% 5%



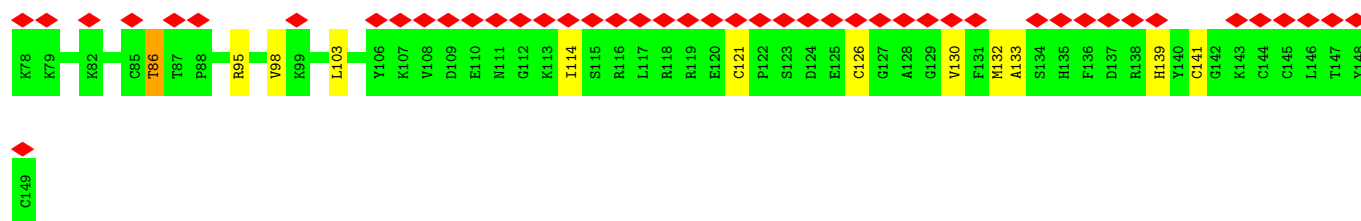
• Molecule 27: RIBOSOMAL PROTEIN ES24

Chain Y: 65% 26% 5%

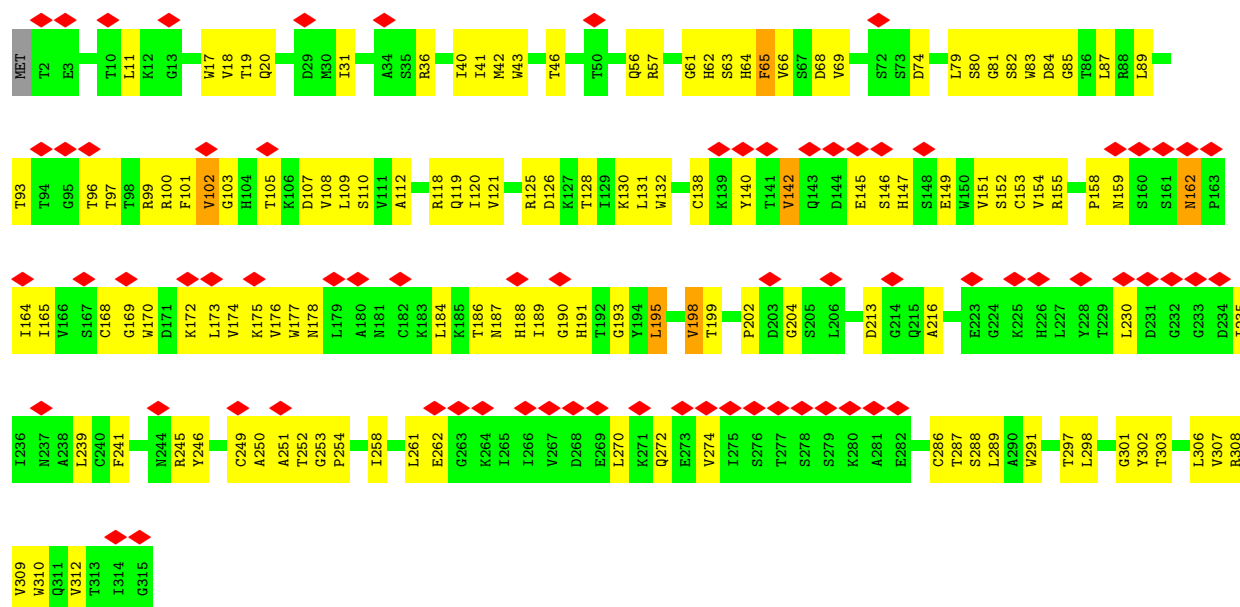


• Molecule 28: RIBOSOMAL PROTEIN ES25

Chain Z: 10% 34% 21% 42%



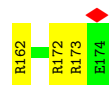
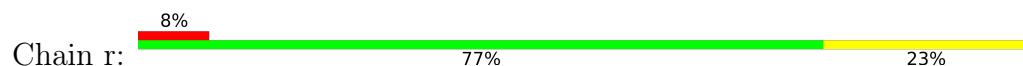
• Molecule 35: RIBOSOMAL PROTEIN RACK1



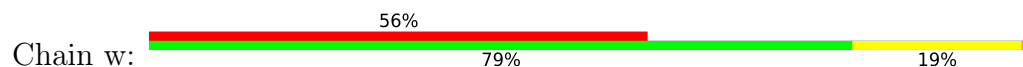
• Molecule 36: RIBOSOMAL PROTEIN EL41

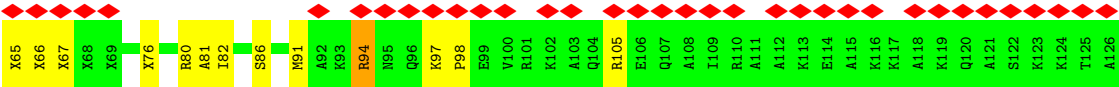


• Molecule 37: RIBOSOMAL PROTEIN EL19



• Molecule 38: RIBOSOMAL PROTEIN EL24





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	404357	Depositor
Resolution determination method	Not provided	
CTF correction method	INDIVIDUAL FRAMES	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20.00	Depositor
Minimum defocus (nm)	1500.00	Depositor
Maximum defocus (nm)	3400.00	Depositor
Magnification	100719	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.475	Depositor
Minimum map value	-0.256	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	300.24, 300.24, 300.24	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	0.38	0/39755	0.55	8/61954 (0.0%)
2	3	0.23	0/6127	0.46	0/9547
3	A	0.63	0/1742	1.01	5/2367 (0.2%)
4	B	0.64	0/1756	1.00	1/2350 (0.0%)
5	C	0.77	0/1726	1.06	3/2332 (0.1%)
6	D	0.50	0/1780	0.90	4/2397 (0.2%)
7	E	0.69	0/2118	1.08	14/2849 (0.5%)
8	F	0.44	0/1516	0.91	4/2037 (0.2%)
9	G	0.54	0/1887	0.97	6/2513 (0.2%)
10	H	0.57	1/1524 (0.1%)	1.03	6/2042 (0.3%)
11	I	0.62	0/1711	1.02	5/2282 (0.2%)
12	J	0.69	0/1524	1.02	6/2035 (0.3%)
13	K	0.46	0/824	0.87	3/1112 (0.3%)
14	L	0.74	0/1250	1.11	5/1673 (0.3%)
15	M	0.49	0/963	0.82	0/1291
16	N	0.66	0/1226	1.00	5/1649 (0.3%)
17	O	0.66	0/1023	1.15	7/1372 (0.5%)
18	P	0.48	0/1003	0.87	4/1341 (0.3%)
19	Q	0.49	0/1126	1.00	6/1506 (0.4%)
20	R	0.52	0/1080	0.93	2/1449 (0.1%)
21	S	0.46	0/1202	0.83	2/1610 (0.1%)
22	T	0.50	0/1148	0.87	1/1538 (0.1%)
23	U	0.46	0/813	0.86	0/1092
24	V	0.66	0/631	1.02	2/844 (0.2%)
25	W	0.80	0/1051	1.06	4/1406 (0.3%)
26	X	0.75	0/1116	1.11	2/1490 (0.1%)
27	Y	0.62	0/1031	0.94	2/1370 (0.1%)
28	Z	0.41	0/580	0.78	1/780 (0.1%)
29	a	0.71	0/830	0.97	0/1112
30	b	0.67	0/653	1.05	1/876 (0.1%)
31	c	0.51	0/481	0.93	1/643 (0.2%)
32	d	0.46	0/469	0.93	1/623 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	0.61	0/447	0.90	0/587
34	f	0.42	0/595	0.88	2/785 (0.3%)
35	g	0.46	0/2497	0.85	3/3399 (0.1%)
36	h	0.64	0/232	0.94	0/295
37	r	0.35	0/117	0.65	0/149
38	w	0.56	0/368	0.76	0/485
All	All	0.49	1/85922 (0.0%)	0.76	116/125182 (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
6	D	0	1
10	H	0	1
26	X	0	2
27	Y	0	1
35	g	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	H	66	VAL	CA-CB	-5.93	1.51	1.54

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Q	43	GLU	CA-C-N	-10.91	107.80	120.13
19	Q	43	GLU	C-N-CA	-10.91	107.80	120.13
26	X	85	VAL	CA-C-N	9.86	129.49	119.24
26	X	85	VAL	C-N-CA	9.86	129.49	119.24
10	H	111	LYS	N-CA-C	-8.96	102.36	113.38
9	G	134	GLY	CA-C-N	8.75	129.29	119.93
9	G	134	GLY	C-N-CA	8.75	129.29	119.93
3	A	161	ILE	CA-C-N	8.33	130.25	119.84
3	A	161	ILE	C-N-CA	8.33	130.25	119.84
14	L	41	GLY	N-CA-C	8.16	124.78	114.66
31	c	23	SER	N-CA-C	-8.04	102.11	111.03
3	A	140	VAL	N-CA-C	7.76	120.52	112.83
7	E	29	PRO	N-CA-C	7.63	123.40	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Q	134	GLY	CA-C-N	7.34	126.97	119.56
19	Q	134	GLY	C-N-CA	7.34	126.97	119.56
12	J	144	ILE	CA-C-N	7.26	126.79	119.24
12	J	144	ILE	C-N-CA	7.26	126.79	119.24
16	N	136	PRO	CA-C-N	-7.07	111.00	119.84
16	N	136	PRO	C-N-CA	-7.07	111.00	119.84
12	J	15	THR	CA-C-N	6.93	126.92	119.78
12	J	15	THR	C-N-CA	6.93	126.92	119.78
4	B	45	GLY	N-CA-C	6.89	120.17	110.74
32	d	35	GLY	N-CA-C	-6.76	105.31	115.32
8	F	80	GLY	N-CA-C	6.62	120.66	112.64
5	C	134	ASN	N-CA-C	6.57	124.80	110.80
9	G	85	ARG	CA-C-N	6.51	126.27	119.76
9	G	85	ARG	C-N-CA	6.51	126.27	119.76
14	L	13	GLN	CA-C-N	6.49	127.96	119.84
14	L	13	GLN	C-N-CA	6.49	127.96	119.84
8	F	49	LEU	CA-C-N	6.43	126.19	119.05
8	F	49	LEU	C-N-CA	6.43	126.19	119.05
7	E	23	LEU	N-CA-C	6.33	120.73	112.89
7	E	136	ILE	CA-C-N	6.21	126.12	119.85
7	E	136	ILE	C-N-CA	6.21	126.12	119.85
20	R	43	SER	CB-CA-C	-6.09	108.55	115.79
9	G	7	PHE	CA-C-N	6.06	125.27	118.97
9	G	7	PHE	C-N-CA	6.06	125.27	118.97
10	H	135	PHE	CA-C-N	-6.03	113.41	119.56
10	H	135	PHE	C-N-CA	-6.03	113.41	119.56
7	E	41	CYS	N-CA-C	6.01	119.18	109.86
17	O	145	GLY	N-CA-C	-5.94	102.43	111.10
7	E	34	GLY	CA-C-N	5.91	125.61	119.05
7	E	34	GLY	C-N-CA	5.91	125.61	119.05
27	Y	66	GLY	N-CA-C	5.89	123.49	115.30
1	2	1253	A	P-O3'-C3'	5.85	128.98	120.20
27	Y	23	MET	N-CA-C	5.82	117.09	108.60
30	b	7	LEU	N-CA-C	-5.77	105.73	112.89
18	P	124	LYS	CA-C-N	5.76	126.10	119.93
18	P	124	LYS	C-N-CA	5.76	126.10	119.93
10	H	66	VAL	CB-CA-C	-5.73	108.25	113.70
6	D	202	LYS	CA-C-N	5.70	125.90	120.31
6	D	202	LYS	C-N-CA	5.70	125.90	120.31
14	L	129	GLY	N-CA-C	-5.68	102.49	110.96
1	2	1253	A	C2'-C3'-O3'	5.68	118.02	109.50
1	2	1835	A	P-O3'-C3'	5.63	128.64	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	70	ILE	N-CA-C	5.61	116.51	108.93
11	I	157	LYS	N-CA-C	-5.61	100.18	108.99
34	f	121	CYS	CA-C-N	5.61	125.23	119.56
34	f	121	CYS	C-N-CA	5.61	125.23	119.56
11	I	139	LYS	CB-CA-C	-5.58	108.52	116.34
5	C	100	ALA	N-CA-C	-5.54	106.48	113.18
3	A	77	ILE	N-CA-C	5.51	116.06	108.12
13	K	90	VAL	N-CA-C	5.51	114.55	108.05
11	I	139	LYS	N-CA-C	5.51	116.15	108.00
25	W	65	LEU	N-CA-C	5.49	117.85	108.90
14	L	62	PHE	N-CA-C	5.48	118.08	111.40
17	O	138	ASP	N-CA-C	5.46	118.36	108.69
1	2	1838	U	P-O3'-C3'	5.45	128.38	120.20
5	C	99	GLY	N-CA-C	-5.45	97.49	113.30
12	J	147	PHE	N-CA-C	-5.44	98.34	108.02
24	V	13	VAL	CA-C-N	5.43	125.40	120.03
24	V	13	VAL	C-N-CA	5.43	125.40	120.03
19	Q	45	ARG	N-CA-C	-5.42	106.66	113.28
6	D	79	PHE	CA-C-N	5.42	125.42	119.89
6	D	79	PHE	C-N-CA	5.42	125.42	119.89
11	I	24	LYS	N-CA-C	5.42	117.88	110.24
17	O	107	THR	CA-C-N	-5.40	114.41	120.14
17	O	107	THR	C-N-CA	-5.40	114.41	120.14
35	g	191	HIS	N-CA-C	5.37	118.48	109.95
1	2	1835	A	C2'-C3'-O3'	5.36	117.55	109.50
13	K	96	ARG	N-CA-C	5.36	115.94	108.00
16	N	71	ILE	N-CA-C	5.36	115.80	110.23
7	E	151	ASP	CA-C-N	5.34	125.05	119.82
7	E	151	ASP	C-N-CA	5.34	125.05	119.82
18	P	130	ARG	CA-C-N	5.31	125.31	120.21
18	P	130	ARG	C-N-CA	5.31	125.31	120.21
12	J	144	ILE	N-CA-C	5.30	116.08	107.71
35	g	162	ASN	CA-C-N	5.29	125.30	119.90
35	g	162	ASN	C-N-CA	5.29	125.30	119.90
11	I	67	TRP	CA-CB-CG	5.27	123.62	113.60
7	E	233	LYS	CA-C-N	5.27	125.03	119.76
7	E	233	LYS	C-N-CA	5.27	125.03	119.76
1	2	114	G	C2'-C3'-O3'	5.26	117.39	109.50
10	H	189	PHE	CA-C-N	5.24	125.18	119.78
10	H	189	PHE	C-N-CA	5.24	125.18	119.78
16	N	7	PRO	CA-C-N	5.22	124.93	119.92
16	N	7	PRO	C-N-CA	5.22	124.93	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	T	6	VAL	N-CA-C	5.21	116.56	110.62
13	K	96	ARG	CB-CA-C	-5.21	109.05	116.34
28	Z	66	LYS	CB-CA-C	-5.19	110.17	117.23
20	R	132	ARG	N-CA-C	5.18	117.54	110.24
17	O	135	ILE	CA-C-N	-5.17	114.66	120.14
17	O	135	ILE	C-N-CA	-5.17	114.66	120.14
7	E	4	GLY	CA-C-N	5.16	125.14	120.03
7	E	4	GLY	C-N-CA	5.16	125.14	120.03
17	O	139	SER	N-CA-C	5.16	117.51	110.55
1	2	1838	U	C2'-C3'-O3'	5.15	117.22	109.50
25	W	100	GLY	N-CA-C	-5.14	106.11	112.33
21	S	79	ILE	CA-C-N	5.13	125.13	119.90
21	S	79	ILE	C-N-CA	5.13	125.13	119.90
8	F	62	ARG	N-CA-C	-5.09	107.02	113.18
25	W	111	MET	N-CA-C	5.07	114.52	107.73
1	2	408	A	P-O3'-C3'	5.04	127.76	120.20
25	W	93	LEU	N-CA-C	5.01	117.86	111.69
19	Q	12	VAL	N-CA-C	5.01	114.65	108.53
3	A	141	ASN	N-CA-C	5.01	118.63	111.92

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	D	193	ASP	Peptide
10	H	134	VAL	Peptide
26	X	107	ARG	Peptide
26	X	112	VAL	Peptide
27	Y	118	ARG	Peptide
35	g	190	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	35552	0	17948	749	0
2	3	5485	0	2776	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1705	0	1706	57	0
4	B	1729	0	1803	63	0
5	C	1690	0	1777	57	0
6	D	1752	0	1848	60	0
7	E	2076	0	2177	84	0
8	F	1495	0	1549	37	0
9	G	1864	0	2018	69	0
10	H	1501	0	1593	42	0
11	I	1682	0	1769	58	0
12	J	1499	0	1618	63	0
13	K	800	0	818	27	0
14	L	1229	0	1302	51	0
15	M	953	0	990	29	0
16	N	1202	0	1289	37	0
17	O	1010	0	1034	48	0
18	P	984	0	1028	34	0
19	Q	1109	0	1174	35	0
20	R	1066	0	1116	55	0
21	S	1184	0	1244	65	0
22	T	1128	0	1158	58	0
23	U	803	0	873	29	0
24	V	625	0	628	17	0
25	W	1034	0	1080	33	0
26	X	1098	0	1167	38	0
27	Y	1014	0	1082	24	0
28	Z	574	0	627	26	0
29	a	816	0	867	41	0
30	b	640	0	665	18	0
31	c	479	0	507	13	0
32	d	458	0	448	21	0
33	e	442	0	487	20	0
34	f	585	0	615	10	0
35	g	2440	0	2396	90	0
36	h	231	0	277	6	0
37	r	118	0	132	2	0
38	w	452	0	493	11	0
39	2	98	0	0	0	0
40	a	1	0	0	0	0
40	d	1	0	0	0	0
40	f	1	0	0	0	0
41	2	141	0	0	14	0
41	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	e	1	0	0	0	0
All	All	80749	0	62079	1911	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 13.

All (1911) 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)
35:g:245:ARG:HH12	35:g:312:VAL:HG11	1.24	1.02
15:M:20:GLU:HB3	15:M:120:ALA:HB2	1.50	0.94
1:2:1622:U:H3	18:P:122:THR:HG1	1.11	0.90
22:T:69:GLY:HA2	22:T:120:GLY:HA3	1.55	0.89
1:2:1256:G:H21	1:2:1659:U:H5'	1.37	0.89
1:2:560:A:H5'	12:J:174:LYS:HG3	1.56	0.88
1:2:1496:U:H4'	32:d:24:CYS:HB2	1.55	0.87
1:2:958:G:N2	17:O:68:GLU:OE2	2.08	0.86
1:2:1337:C:H2'	1:2:1338:G:H8	1.42	0.85
12:J:136:ARG:HD2	12:J:160:SER:HA	1.57	0.85
21:S:50:ILE:HD12	21:S:67:VAL:CG2	2.06	0.84
1:2:384:U:O4	11:I:5:ARG:NH2	2.11	0.83
4:B:87:ILE:HG12	4:B:101:HIS:HB2	1.60	0.83
1:2:589:G:N2	41:2:2001:HOH:O	2.08	0.83
25:W:80:ASP:N	25:W:80:ASP:OD1	2.11	0.83
1:2:909:G:OP2	37:r:172:ARG:NH1	2.12	0.82
22:T:76:THR:HG22	22:T:94:ARG:HB3	1.61	0.82
1:2:76:U:H5'	9:G:159:ARG:HH22	1.41	0.82
11:I:141:ARG:HD3	11:I:146:GLN:HA	1.60	0.82
26:X:67:ARG:NH2	26:X:114:ASP:OD2	2.10	0.81
9:G:59:GLN:HG3	9:G:72:ARG:NH2	1.95	0.81
20:R:34:VAL:HG13	20:R:38:ILE:HD12	1.63	0.81
1:2:297:A:H5'	7:E:132:GLY:HA2	1.63	0.81
1:2:685:A:H62	1:2:918:U:H3	1.26	0.80
1:2:64:A:H2	1:2:83:A:H62	1.23	0.80
1:2:1241:A:HO2'	1:2:1266:C:HO2'	1.26	0.80
26:X:68:LYS:HB3	26:X:91:LEU:HD22	1.63	0.79
26:X:93:PHE:O	26:X:140:ARG:NH1	2.16	0.79
1:2:1601:A:H4'	1:2:1602:U:H5'	1.62	0.79
1:2:587:A:N3	41:2:2005:HOH:O	2.14	0.79
1:2:943:U:OP1	4:B:214:LYS:NZ	2.15	0.79
25:W:57:ARG:NH2	30:b:26:GLN:OE1	2.14	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1579:A:H4'	1:2:1581:C:H5	1.49	0.79
1:2:115:U:OP1	1:2:382:C:O2'	2.01	0.78
1:2:551:U:O2'	33:e:44:ASN:ND2	2.17	0.78
29:a:73:TYR:HB3	29:a:78:VAL:HG22	1.66	0.78
2:3:71:G:O6	2:3:94:G:O2'	2.02	0.78
21:S:86:ARG:HD2	21:S:106:LYS:HD3	1.66	0.77
2:3:42:C:H42	2:3:120:C:H42	1.32	0.77
1:2:1649:U:OP2	1:2:1674:G:N1	2.16	0.77
1:2:499:G:H2'	1:2:501:C:H5	1.48	0.77
1:2:1521:C:OP2	21:S:124:ARG:NH1	2.18	0.77
4:B:144:LYS:HB2	4:B:208:HIS:HB2	1.65	0.76
1:2:1865:C:H5	29:a:6:ARG:H	1.31	0.76
11:I:122:GLY:HA2	11:I:167:GLN:HG2	1.67	0.76
29:a:51:ARG:HH12	31:c:40:ARG:HH21	1.31	0.76
18:P:44:ARG:HD2	18:P:84:ILE:HD11	1.65	0.76
1:2:121:U:H5''	7:E:77:ARG:HH21	1.49	0.76
1:2:1446:A:OP1	23:U:57:PRO:HA	1.86	0.76
21:S:17:ASN:HD22	21:S:101:ASN:HD21	1.34	0.76
35:g:87:LEU:HB3	35:g:101:PHE:HB2	1.68	0.76
1:2:925:G:H2'	1:2:926:A:H5''	1.66	0.75
29:a:33:ASP:OD1	29:a:34:LYS:N	2.19	0.75
1:2:1068:G:N7	41:2:2008:HOH:O	2.20	0.74
1:2:1310:U:OP2	15:M:36:ARG:NH2	2.19	0.74
1:2:103:A:OP2	1:2:356:C:N4	2.20	0.74
1:2:1333:U:H2'	1:2:1334:G:H8	1.51	0.74
12:J:47:LYS:HA	12:J:102:ILE:HD11	1.70	0.74
33:e:50:GLY:HA3	33:e:52:LYS:HE3	1.70	0.74
12:J:121:LYS:H	12:J:125:HIS:HD2	1.35	0.74
6:D:96:LEU:HD12	6:D:198:ILE:HG21	1.67	0.74
21:S:34:LYS:HB2	21:S:100:ALA:HA	1.68	0.74
4:B:198:GLU:HB2	4:B:210:VAL:HG11	1.70	0.74
1:2:1738:C:OP1	9:G:92:ARG:NH2	2.21	0.73
32:d:17:GLY:HA2	32:d:27:ARG:HD3	1.70	0.73
2:3:150:G:H1	2:3:242:C:H42	1.36	0.73
13:K:27:VAL:HG13	13:K:43:LEU:HD13	1.71	0.73
15:M:21:VAL:HG21	15:M:124:ILE:HD12	1.69	0.73
1:2:1015:U:OP2	30:b:20:LYS:NZ	2.20	0.73
1:2:190:G:O2'	1:2:209:A:N6	2.22	0.73
5:C:60:TRP:O	5:C:71:LYS:NZ	2.21	0.73
16:N:101:HIS:CE1	16:N:105:ASN:HD22	2.06	0.73
18:P:41:GLN:NE2	18:P:113:GLY:O	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:390:C:H4'	14:L:8:ARG:HH22	1.52	0.73
1:2:525:A:N7	41:2:2009:HOH:O	2.21	0.73
1:2:1542:C:H4'	22:T:11:GLN:HB2	1.70	0.73
1:2:1818:A:H5''	36:h:16:LYS:NZ	2.04	0.72
2:3:92:U:H5'	2:3:93:A:H2'	1.69	0.72
4:B:101:HIS:O	4:B:217:MET:HG3	1.88	0.72
2:3:70:A:H61	2:3:97:U:H3	1.37	0.72
20:R:31:ASN:HA	20:R:34:VAL:HB	1.71	0.72
29:a:51:ARG:HH11	31:c:62:GLU:HG2	1.54	0.72
1:2:1395:C:OP1	19:Q:15:ARG:NH1	2.22	0.72
1:2:925:G:H1	1:2:1017:U:H3	1.37	0.72
6:D:208:VAL:HG12	20:R:41:ILE:HG22	1.71	0.72
1:2:171:A:H5''	9:G:177:GLN:HG2	1.72	0.72
23:U:51:LYS:HB2	23:U:90:ASP:HB2	1.72	0.72
7:E:48:LEU:HD22	7:E:70:ILE:HD11	1.70	0.72
14:L:131:CYS:SG	14:L:132:ARG:N	2.63	0.72
1:2:1478:U:H2'	1:2:1479:G:C8	2.25	0.71
8:F:127:ARG:HH22	8:F:132:GLY:H	1.38	0.71
19:Q:53:GLU:OE1	19:Q:85:ARG:NH2	2.23	0.71
1:2:387:C:OP2	11:I:10:LYS:NZ	2.24	0.71
2:3:70:A:H3'	2:3:71:G:H5'	1.71	0.71
6:D:27:ARG:HG3	13:K:63:ALA:HB2	1.72	0.71
1:2:1337:C:H2'	1:2:1338:G:C8	2.26	0.71
6:D:67:ARG:NH1	13:K:93:THR:O	2.23	0.71
12:J:88:ASP:OD1	12:J:88:ASP:N	2.23	0.71
6:D:172:VAL:HG22	6:D:185:LYS:HG2	1.71	0.71
1:2:446:G:OP2	11:I:47:ARG:NH2	2.23	0.70
26:X:140:ARG:HD2	26:X:141:PRO:HD2	1.74	0.70
14:L:22:ARG:HH22	14:L:31:GLU:HG3	1.55	0.70
1:2:381:C:H5'	11:I:49:ARG:HB2	1.73	0.70
1:2:1309:C:H4'	34:f:133:ALA:HB2	1.73	0.70
1:2:1326:U:O4	32:d:28:HIS:ND1	2.24	0.70
5:C:134:ASN:HA	5:C:218:GLY:HA3	1.74	0.70
35:g:42:MET:HB3	35:g:57:ARG:H	1.55	0.70
1:2:1534:C:H4'	1:2:1535:U:O5'	1.91	0.69
12:J:109:ARG:NH2	12:J:146:SER:OG	2.24	0.69
15:M:21:VAL:HG23	15:M:120:ALA:HB1	1.74	0.69
1:2:1269:G:H1	1:2:1513:C:H42	1.40	0.69
1:2:475:C:OP2	41:2:2002:HOH:O	2.10	0.69
1:2:619:A:N1	26:X:114:ASP:HB2	2.08	0.69
1:2:9:U:OP2	41:2:2003:HOH:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1866:A:C6	29:a:87:ARG:NH1	2.60	0.69
2:3:92:U:O4	2:3:93:A:N6	2.26	0.69
1:2:996:A:H2'	1:2:997:A:C8	2.28	0.69
20:R:41:ILE:HD13	20:R:47:ARG:HB2	1.74	0.69
1:2:615:C:O2'	1:2:616:A:O4'	2.11	0.69
1:2:1399:C:H5''	35:g:100:ARG:NH1	2.08	0.69
14:L:80:MET:HB3	14:L:86:ILE:HG22	1.75	0.69
21:S:50:ILE:CD1	21:S:67:VAL:CG2	2.70	0.69
5:C:271:ASP:OD1	5:C:271:ASP:N	2.26	0.68
1:2:65:C:OP1	9:G:136:LYS:NZ	2.26	0.68
1:2:688:U:H5	10:H:103:LYS:H	1.41	0.68
35:g:120:ILE:HB	35:g:132:TRP:HB2	1.75	0.68
5:C:209:VAL:HG21	5:C:233:LEU:HD11	1.75	0.68
11:I:69:SER:OG	11:I:191:GLU:OE1	2.08	0.68
1:2:1332:A:O2'	6:D:145:GLN:OE1	2.11	0.68
7:E:11:ARG:NH2	7:E:24:THR:OG1	2.27	0.68
9:G:159:ARG:HH11	9:G:171:THR:HG21	1.57	0.68
29:a:26:CYS:HB3	29:a:28:ARG:H	1.57	0.68
35:g:172:LYS:HE2	35:g:193:GLY:H	1.58	0.68
1:2:643:A:OP1	12:J:39:ASN:ND2	2.27	0.68
1:2:1721:U:H4'	1:2:1722:G:H5''	1.76	0.68
25:W:81:VAL:HG21	25:W:125:ILE:HG13	1.76	0.68
8:F:138:ALA:O	31:c:63:ARG:NH1	2.27	0.68
18:P:18:ARG:HG3	18:P:36:LEU:HB3	1.75	0.68
27:Y:78:SER:HB3	27:Y:81:TYR:HD2	1.59	0.68
1:2:617:G:H4'	26:X:88:ASP:HB3	1.77	0.67
1:2:145:G:H2'	1:2:146:G:C8	2.30	0.67
18:P:98:ASN:ND2	18:P:103:ASN:OD1	2.28	0.67
21:S:50:ILE:CD1	21:S:67:VAL:HG23	2.23	0.67
2:3:146:G:H1	2:3:247:C:H42	1.43	0.67
3:A:85:ARG:HH21	3:A:201:LEU:HD12	1.58	0.67
10:H:9:VAL:HG12	10:H:11:PRO:HD3	1.77	0.67
22:T:22:LEU:HB3	22:T:54:TYR:HD1	1.58	0.67
35:g:11:LEU:HB2	35:g:307:VAL:HB	1.76	0.67
1:2:499:G:H2'	1:2:501:C:C5	2.30	0.67
1:2:1661:A:OP2	32:d:32:ARG:NH1	2.26	0.67
22:T:140:ALA:HA	22:T:143:LYS:HE2	1.77	0.67
1:2:1649:U:O2'	1:2:1650:A:OP1	2.13	0.67
35:g:176:VAL:HB	35:g:186:THR:HB	1.76	0.67
3:A:53:ARG:NH2	24:V:82:ASN:O	2.27	0.66
1:2:1048:G:OP2	41:2:2004:HOH:O	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1333:U:H2'	1:2:1334:G:C8	2.29	0.66
1:2:1579:A:H4'	1:2:1581:C:C5	2.31	0.66
1:2:76:U:H3'	1:2:77:A:H5'	1.77	0.66
4:B:65:ARG:NH2	17:O:51:GLU:OE2	2.18	0.66
35:g:251:ALA:HB2	35:g:289:LEU:HD22	1.77	0.66
8:F:35:LEU:HD21	8:F:146:ARG:HD2	1.78	0.66
12:J:104:ASP:OD1	12:J:104:ASP:N	2.28	0.66
6:D:157:MET:HG3	6:D:159:HIS:CE1	2.30	0.66
1:2:309:G:OP2	11:I:55:TYR:OH	2.11	0.66
20:R:27:ASP:O	20:R:31:ASN:ND2	2.28	0.66
21:S:16:LEU:HD21	21:S:72:GLN:HE22	1.58	0.66
1:2:993:G:N7	29:a:15:ARG:NH1	2.43	0.66
35:g:11:LEU:HB3	35:g:43:TRP:CH2	2.31	0.66
2:3:329:U:O2'	2:3:330:A:O5'	2.10	0.66
35:g:241:PHE:HE1	35:g:261:LEU:HD11	1.61	0.66
35:g:147:HIS:HD2	35:g:151:VAL:HG22	1.60	0.65
1:2:1857:G:N7	17:O:146:ARG:NH1	2.43	0.65
9:G:69:THR:HG22	9:G:70:HIS:H	1.61	0.65
1:2:996:A:O2'	1:2:997:A:O4'	2.10	0.65
8:F:72:LEU:HD22	8:F:112:LEU:HD11	1.76	0.65
30:b:31:TYR:O	30:b:48:SER:HB2	1.96	0.65
8:F:78:MET:H	8:F:159:ARG:HH22	1.44	0.65
29:a:78:VAL:CG1	29:a:83:VAL:HB	2.27	0.65
1:2:1342:U:H4'	1:2:1343:U:O5'	1.96	0.65
6:D:195:THR:HG22	6:D:201:LYS:HE2	1.79	0.65
17:O:103:ASN:N	17:O:103:ASN:OD1	2.28	0.65
1:2:1622:U:O4	18:P:81:ARG:NH2	2.30	0.65
2:3:252:A:H4'	2:3:253:G:H5'	1.79	0.65
2:3:330:A:O2'	2:3:331:G:O5'	2.15	0.65
14:L:68:ILE:HG21	14:L:143:LEU:HD11	1.77	0.65
2:3:144:U:H2'	2:3:145:G:H8	1.60	0.65
2:3:333:C:O2'	2:3:334:C:OP1	2.14	0.65
1:2:632:C:OP2	41:2:2006:HOH:O	2.14	0.64
29:a:51:ARG:HH12	31:c:40:ARG:NH2	1.95	0.64
9:G:54:GLY:H	9:G:110:ASN:HB2	1.62	0.64
1:2:841:G:H2'	1:2:842:C:H6	1.62	0.64
1:2:1543:U:O2'	19:Q:43:GLU:OE2	2.15	0.64
11:I:123:ARG:NH1	11:I:133:GLU:OE2	2.28	0.64
12:J:169:ARG:HE	12:J:175:ARG:HH21	1.43	0.64
22:T:52:TRP:O	22:T:56:ARG:HB2	1.98	0.64
1:2:1284:A:O4'	1:2:1312:G:N2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1453:C:OP1	20:R:48:ASN:ND2	2.26	0.64
1:2:640:A:H2'	1:2:641:A:C8	2.32	0.64
1:2:1599:U:C4	8:F:166:ILE:HD12	2.33	0.64
12:J:169:ARG:HH21	12:J:175:ARG:HH22	1.46	0.63
1:2:918:U:H3'	16:N:64:ARG:HH22	1.63	0.63
13:K:60:GLU:HG2	13:K:69:TRP:CD1	2.34	0.63
22:T:75:MET:HB3	22:T:100:ALA:HB1	1.80	0.63
2:3:232:C:H2'	2:3:233:G:H5''	1.79	0.63
2:3:243:A:O2'	2:3:244:A:OP1	2.16	0.63
3:A:42:LYS:HE2	3:A:46:ILE:HB	1.79	0.63
1:2:1428:G:O6	19:Q:71:ARG:NH2	2.30	0.63
1:2:1606:G:H5'	22:T:86:GLY:HA2	1.79	0.63
14:L:119:ASP:O	14:L:147:LYS:NZ	2.30	0.63
1:2:1277:C:H2'	1:2:1278:A:H8	1.64	0.63
3:A:198:MET:HG2	3:A:200:ASP:HB2	1.80	0.63
1:2:639:C:HO2'	1:2:640:A:H8	1.46	0.63
1:2:1598:G:H3'	28:Z:80:ARG:HG2	1.81	0.63
7:E:122:LYS:NZ	7:E:143:ASP:OD2	2.29	0.63
1:2:816:A:P	12:J:10:ARG:HH22	2.22	0.63
1:2:925:G:C2'	1:2:926:A:H5''	2.28	0.63
1:2:1139:C:H5	1:2:1149:A:H62	1.47	0.63
5:C:259:THR:HG21	24:V:16:LYS:H	1.62	0.63
28:Z:79:ILE:HG23	28:Z:83:LEU:HD23	1.80	0.63
1:2:808:A:O2'	1:2:809:A:O5'	2.15	0.63
29:a:78:VAL:HG12	29:a:83:VAL:HB	1.80	0.63
1:2:1650:A:OP1	19:Q:138:ARG:HB2	1.99	0.62
5:C:179:THR:OG1	5:C:180:VAL:N	2.31	0.62
35:g:169:GLY:O	35:g:195:LEU:HB2	1.99	0.62
1:2:1590:C:H41	19:Q:77:HIS:CE1	2.16	0.62
18:P:72:LYS:NZ	18:P:106:GLU:OE2	2.32	0.62
1:2:75:G:H22	9:G:155:GLN:HG3	1.63	0.62
1:2:114:G:OP1	14:L:69:ARG:NH1	2.32	0.62
13:K:23:ALA:HB3	13:K:67:PHE:HB2	1.81	0.62
23:U:61:LEU:HD11	23:U:84:ILE:HD11	1.80	0.62
1:2:71:G:O2'	1:2:79:A:N6	2.32	0.62
1:2:1567:G:H2'	22:T:37:VAL:HG21	1.81	0.62
1:2:1857:G:OP2	17:O:141:ARG:NH2	2.32	0.62
1:2:559:G:HO2'	1:2:560:A:H8	1.46	0.62
1:2:843:C:H2'	1:2:844:U:O4'	1.99	0.62
1:2:1277:C:H2'	1:2:1278:A:C8	2.35	0.62
1:2:1498:A:OP2	6:D:27:ARG:NH1	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1866:A:C5	29:a:87:ARG:NH1	2.68	0.62
5:C:178:HIS:H	5:C:178:HIS:CD2	2.17	0.62
1:2:980:A:H2'	1:2:981:A:C8	2.34	0.62
1:2:919:A:OP2	16:N:64:ARG:NH1	2.32	0.62
1:2:1237:C:H2'	1:2:1238:U:O4'	1.99	0.62
1:2:1824:A:OP2	26:X:61:GLN:NE2	2.33	0.62
5:C:206:SER:HB3	5:C:224:THR:HB	1.81	0.62
1:2:943:U:OP2	4:B:216:LYS:NZ	2.28	0.62
1:2:1512:C:O2'	32:d:7:TYR:O	2.16	0.62
1:2:1616:U:OP2	18:P:43:ARG:NH2	2.33	0.62
1:2:1859:A:H5'	1:2:1860:A:OP2	1.99	0.62
11:I:72:CYS:SG	11:I:73:THR:N	2.72	0.61
35:g:121:VAL:HG12	35:g:154:VAL:HG11	1.81	0.61
1:2:618:C:OP1	26:X:87:ASN:HA	2.01	0.61
1:2:816:A:OP2	12:J:10:ARG:NH2	2.33	0.61
1:2:870:A:H4'	1:2:871:U:H5'	1.81	0.61
1:2:1190:A:H2'	1:2:1191:C:O4'	2.00	0.61
1:2:1589:A:OP1	22:T:80:GLY:HA3	2.00	0.61
1:2:1605:G:OP1	22:T:84:ARG:NH2	2.33	0.61
1:2:1605:G:O2'	1:2:1634:A:N6	2.32	0.61
21:S:22:GLY:HA2	21:S:56:ALA:HB3	1.83	0.61
25:W:55:ASP:OD1	25:W:56:HIS:N	2.33	0.61
1:2:1380:C:O2'	3:A:113:GLN:OE1	2.14	0.61
2:3:165:A:N6	2:3:237:C:O2'	2.33	0.61
35:g:153:CYS:SG	35:g:155:ARG:NH1	2.74	0.61
35:g:249:CYS:HB2	35:g:291:TRP:HZ3	1.65	0.61
35:g:270:LEU:HB3	35:g:310:TRP:CZ2	2.36	0.61
1:2:1395:C:H1'	1:2:1474:A:C4	2.35	0.61
1:2:1518:C:OP1	1:2:1520:G:H8	1.82	0.61
1:2:1565:C:OP2	22:T:101:ARG:NH1	2.33	0.61
3:A:41:ARG:HB2	3:A:47:TYR:CE1	2.35	0.61
1:2:683:G:H4'	25:W:4:MET:HB3	1.83	0.61
1:2:1036:A:N3	1:2:1844:U:O2'	2.33	0.61
21:S:68:ILE:HG23	21:S:72:GLN:HE21	1.66	0.61
17:O:98:ARG:HH11	17:O:98:ARG:HG3	1.65	0.61
8:F:35:LEU:HD12	8:F:117:ILE:HG12	1.83	0.61
1:2:73:C:O2'	1:2:74:G:O4'	2.19	0.60
1:2:1016:U:H5''	16:N:14:SER:HB3	1.83	0.60
35:g:245:ARG:NH1	35:g:312:VAL:HG11	2.06	0.60
1:2:634:A:H2'	1:2:635:G:C8	2.37	0.60
6:D:212:GLU:HG2	20:R:19:LYS:HZ3	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:127:ARG:HH22	8:F:132:GLY:N	1.98	0.60
9:G:148:SER:OG	9:G:151:ASP:OD1	2.18	0.60
1:2:940:U:H2'	1:2:941:C:C6	2.36	0.60
1:2:76:U:OP1	9:G:159:ARG:NH1	2.27	0.60
1:2:792:C:H2'	1:2:793:G:C8	2.37	0.60
1:2:841:G:H2'	1:2:842:C:C6	2.37	0.60
1:2:963:A:H2'	1:2:964:A:C8	2.36	0.60
2:3:253:G:O2'	2:3:254:C:H5'	2.02	0.60
4:B:136:ARG:HG3	4:B:218:LEU:HD11	1.84	0.60
13:K:58:VAL:HG12	13:K:71:LEU:HD23	1.82	0.60
1:2:1231:C:H2'	1:2:1232:U:O4'	2.02	0.60
10:H:9:VAL:HG23	10:H:24:SER:HB3	1.83	0.60
22:T:42:HIS:CG	22:T:81:GLY:HA3	2.36	0.60
1:2:1207:G:N2	2:3:341:C:OP2	2.33	0.60
2:3:233:G:C4	30:b:80:ARG:NH1	2.70	0.60
1:2:163:U:O3'	9:G:83:CYS:HA	2.02	0.60
1:2:164:A:H3'	1:2:165:G:N2	2.17	0.60
1:2:1224:G:H2'	1:2:1225:U:C6	2.37	0.60
5:C:59:GLU:OE2	5:C:71:LYS:NZ	2.30	0.60
6:D:115:VAL:HG21	6:D:142:LEU:HD22	1.83	0.60
1:2:91:A:H5''	1:2:92:A:H5''	1.84	0.60
1:2:1566:G:H1'	1:2:1570:G:N2	2.17	0.60
5:C:259:THR:HG21	24:V:15:ARG:HA	1.84	0.60
7:E:42:LEU:HD13	7:E:47:PHE:HB2	1.82	0.60
11:I:31:ARG:HB3	11:I:32:PRO:HD2	1.83	0.60
14:L:82:MET:HB3	14:L:85:THR:HG23	1.83	0.60
21:S:23:ARG:HB2	28:Z:48:VAL:HG21	1.82	0.60
1:2:1857:G:H3'	17:O:146:ARG:NH2	2.17	0.60
7:E:66:MET:HE1	7:E:78:THR:HB	1.83	0.60
7:E:102:ILE:HD12	7:E:239:PRO:HD3	1.84	0.60
1:2:128:U:O2'	1:2:130:G:O6	2.21	0.59
6:D:96:LEU:HD12	6:D:198:ILE:HD13	1.84	0.59
17:O:106:LYS:NZ	17:O:135:ILE:HG13	2.17	0.59
20:R:57:LEU:HD11	20:R:66:VAL:HG11	1.84	0.59
22:T:18:LEU:HD13	22:T:134:ILE:HD13	1.84	0.59
1:2:1001:A:H8	1:2:1001:A:H5''	1.66	0.59
1:2:1480:A:OP1	19:Q:131:LYS:NZ	2.35	0.59
1:2:1589:A:N3	1:2:1653:U:O2'	2.34	0.59
1:2:1863:A:OP2	29:a:4:LYS:NZ	2.33	0.59
4:B:146:ARG:HA	4:B:146:ARG:HH11	1.67	0.59
15:M:72:HIS:O	15:M:73:GLN:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:44:PRO:HG2	19:Q:47:LEU:HB2	1.83	0.59
35:g:18:VAL:HB	35:g:301:GLY:HA3	1.84	0.59
7:E:43:PRO:HG2	7:E:46:ILE:HD13	1.84	0.59
12:J:136:ARG:HD3	12:J:158:ASP:HB2	1.84	0.59
1:2:1240:A:C4	18:P:100:LYS:HB2	2.37	0.59
1:2:1629:C:H5'	21:S:39:ARG:HG2	1.83	0.59
23:U:20:ILE:HG23	23:U:116:ILE:HG12	1.84	0.59
7:E:181:CYS:SG	7:E:195:ILE:HG13	2.43	0.59
22:T:42:HIS:CD2	22:T:43:LYS:HG3	2.37	0.59
1:2:294:U:C4	14:L:65:ASN:HB2	2.37	0.59
1:2:1015:U:P	30:b:20:LYS:NZ	2.76	0.59
1:2:1623:A:C8	21:S:132:ARG:HD2	2.38	0.59
20:R:5:ARG:HG3	20:R:10:LYS:HE2	1.85	0.59
1:2:1470:C:OP2	8:F:59:LYS:NZ	2.35	0.59
26:X:71:ARG:HD2	26:X:82:THR:HG22	1.84	0.59
1:2:525:A:H2'	1:2:526:A:C8	2.37	0.58
2:3:163:G:O2'	2:3:164:U:H4'	2.02	0.58
8:F:59:LYS:HG3	8:F:62:ARG:HB2	1.84	0.58
12:J:169:ARG:HH21	12:J:175:ARG:NH2	2.01	0.58
5:C:131:GLY:HA3	5:C:216:MET:HB3	1.84	0.58
2:3:61:U:O2'	2:3:62:C:OP1	2.19	0.58
21:S:85:ASN:HD22	21:S:98:VAL:HB	1.68	0.58
7:E:179:ASN:HD22	7:E:231:GLY:H	1.51	0.58
12:J:21:GLU:CD	12:J:24:ARG:HB2	2.29	0.58
12:J:77:LEU:HA	12:J:80:ARG:HH11	1.67	0.58
13:K:64:TRP:HZ3	32:d:22:ARG:HD2	1.67	0.58
14:L:22:ARG:NH2	14:L:31:GLU:HG3	2.17	0.58
20:R:33:ARG:NH1	20:R:36:GLU:OE1	2.35	0.58
1:2:638:C:O4'	33:e:56:ASN:ND2	2.37	0.58
1:2:1746:U:H4'	9:G:65:GLN:NE2	2.19	0.58
1:2:641:A:OP2	33:e:34:ARG:NH2	2.36	0.58
1:2:1126:G:OP2	20:R:129:LYS:NZ	2.26	0.58
7:E:127:ARG:NH2	7:E:142:HIS:HB2	2.19	0.58
14:L:60:CYS:HB2	14:L:114:SER:HB2	1.84	0.58
15:M:118:SER:O	15:M:122:ASP:HB2	2.04	0.58
29:a:7:ASN:ND2	29:a:10:ARG:O	2.37	0.58
1:2:1608:U:H4'	21:S:130:ARG:NH1	2.18	0.58
9:G:44:GLU:HA	9:G:119:LYS:HD2	1.85	0.58
35:g:105:THR:OG1	35:g:126:ASP:OD2	2.21	0.58
1:2:172:U:OP1	1:2:314:U:O2'	2.22	0.58
1:2:926:A:H2'	1:2:927:C:O4'	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:76:GLN:HE22	10:H:94:PHE:HB2	1.68	0.58
17:O:95:ILE:HB	17:O:129:ILE:HD13	1.85	0.58
23:U:19:ARG:HG3	23:U:117:ALA:HA	1.86	0.58
4:B:62:LEU:HA	4:B:65:ARG:HE	1.69	0.57
35:g:173:LEU:HD12	35:g:175:LYS:NZ	2.19	0.57
1:2:979:C:H2'	1:2:980:A:C8	2.39	0.57
6:D:13:ALA:HA	6:D:16:ILE:HD12	1.86	0.57
20:R:57:LEU:O	20:R:61:ILE:HG13	2.04	0.57
21:S:80:PRO:HB2	21:S:83:PHE:HD2	1.69	0.57
1:2:64:A:H2	1:2:83:A:N6	1.99	0.57
1:2:525:A:H2'	1:2:526:A:H8	1.69	0.57
19:Q:25:CYS:SG	19:Q:91:ALA:HB1	2.44	0.57
35:g:245:ARG:HH12	35:g:312:VAL:CG1	2.08	0.57
1:2:407:G:H2'	1:2:407:G:N3	2.19	0.57
12:J:169:ARG:HE	12:J:175:ARG:NH2	2.03	0.57
20:R:25:GLY:O	20:R:31:ASN:ND2	2.33	0.57
1:2:1275:G:N2	1:2:1506:A:OP2	2.36	0.57
5:C:212:LYS:HG3	5:C:216:MET:HE2	1.86	0.57
14:L:135:SER:OG	14:L:136:LYS:N	2.38	0.57
1:2:1392:U:OP1	23:U:83:ARG:NH1	2.31	0.57
8:F:137:GLN:HE21	31:c:63:ARG:HH22	1.53	0.57
1:2:1217:A:H2'	1:2:1218:C:C6	2.39	0.57
1:2:1537:A:O2'	1:2:1604:G:OP1	2.22	0.57
1:2:1612:G:H1'	21:S:87:GLN:HG3	1.86	0.57
8:F:125:SER:HB3	8:F:136:ARG:HB3	1.86	0.57
11:I:132:GLU:CD	11:I:132:GLU:H	2.13	0.57
17:O:54:CYS:HB3	17:O:81:VAL:HG23	1.86	0.57
25:W:18:GLU:OE1	25:W:65:LEU:HD13	2.04	0.57
32:d:19:ARG:HH11	32:d:32:ARG:HD2	1.69	0.57
1:2:1241:A:H2'	1:2:1242:U:H4'	1.85	0.57
11:I:11:ARG:HB3	11:I:15:GLY:HA2	1.87	0.57
21:S:68:ILE:O	21:S:72:GLN:HG2	2.05	0.57
35:g:216:ALA:HB3	35:g:230:LEU:HB2	1.87	0.57
1:2:1137:U:O2'	1:2:1138:C:OP1	2.21	0.57
2:3:150:G:H1	2:3:242:C:N4	2.01	0.57
12:J:89:GLU:OE1	12:J:89:GLU:N	2.37	0.57
25:W:42:MET:HE2	25:W:49:GLU:HA	1.86	0.57
1:2:146:G:OP1	9:G:143:LYS:NZ	2.38	0.57
1:2:376:A:H2'	1:2:377:G:O4'	2.05	0.57
4:B:38:MET:HE1	4:B:182:LYS:O	2.05	0.57
1:2:1374:C:H2'	1:2:1375:G:O4'	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:13:LYS:HG3	14:L:137:THR:HG21	1.85	0.56
29:a:51:ARG:NH1	31:c:62:GLU:HG2	2.20	0.56
35:g:298:LEU:HB2	35:g:310:TRP:HB2	1.87	0.56
1:2:1785:C:O2'	1:2:1786:U:O5'	2.20	0.56
27:Y:55:ILE:HG22	27:Y:75:ILE:HG23	1.87	0.56
1:2:589:G:N2	41:2:2015:HOH:O	2.37	0.56
1:2:798:G:H3'	1:2:799:U:C5'	2.35	0.56
2:3:256:G:H5'	2:3:257:A:H5''	1.86	0.56
7:E:11:ARG:NH1	7:E:20:LEU:HD22	2.21	0.56
7:E:87:MET:HE2	7:E:123:LEU:H	1.70	0.56
17:O:36:SER:OG	17:O:37:PHE:N	2.35	0.56
26:X:100:VAL:HG13	26:X:122:VAL:HG13	1.86	0.56
35:g:239:LEU:HD23	35:g:250:ALA:HA	1.86	0.56
1:2:1287:A:H5''	34:f:95:ARG:HH12	1.70	0.56
7:E:136:ILE:HG12	7:E:149:TYR:HE1	1.70	0.56
11:I:80:ASP:OD1	11:I:81:VAL:N	2.39	0.56
32:d:19:ARG:NH1	32:d:32:ARG:HD2	2.20	0.56
1:2:165:G:H2'	1:2:166:A:H8	1.69	0.56
1:2:1334:G:O2'	6:D:174:HIS:HD2	1.88	0.56
2:3:144:U:H2'	2:3:145:G:C8	2.39	0.56
7:E:97:GLU:OE2	7:E:113:ARG:NH1	2.37	0.56
21:S:78:LYS:NZ	22:T:32:GLU:O	2.32	0.56
23:U:40:ILE:O	23:U:44:LYS:HB2	2.05	0.56
11:I:141:ARG:HD3	11:I:146:GLN:CA	2.34	0.56
15:M:24:THR:HB	15:M:115:GLY:HA3	1.86	0.56
20:R:111:PHE:O	20:R:114:LEU:HG	2.06	0.56
1:2:1001:A:H5''	1:2:1001:A:C8	2.41	0.56
2:3:81:A:N6	2:3:84:C:O2'	2.39	0.56
5:C:187:ARG:HD3	5:C:192:LEU:HD23	1.88	0.56
1:2:1428:G:H4'	1:2:1429:G:C5'	2.36	0.56
1:2:1498:A:P	6:D:27:ARG:HH12	2.29	0.56
4:B:28:LYS:HB3	4:B:48:LEU:HD11	1.86	0.56
7:E:85:GLY:O	7:E:88:ASP:HB2	2.05	0.56
12:J:132:GLN:HB3	12:J:134:HIS:CD2	2.40	0.56
1:2:958:G:O2'	1:2:959:G:O5'	2.24	0.56
2:3:294:U:H2'	2:3:295:G:H2'	1.87	0.56
3:A:198:MET:HG3	3:A:199:PRO:HD2	1.88	0.56
9:G:44:GLU:CD	9:G:44:GLU:H	2.14	0.56
35:g:245:ARG:NH1	35:g:312:VAL:HG21	2.21	0.56
1:2:122:G:H21	7:E:146:THR:HG21	1.70	0.56
7:E:179:ASN:HD21	7:E:230:LYS:HD2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:166:ILE:HD13	8:F:166:ILE:N	2.21	0.56
11:I:9:HIS:CG	11:I:9:HIS:O	2.59	0.56
16:N:87:ASP:N	16:N:87:ASP:OD1	2.37	0.56
38:w:65:UNK:HG2	38:w:66:UNK:HG3	1.86	0.56
15:M:93:LYS:HB2	15:M:102:LYS:HB3	1.88	0.55
17:O:72:TYR:O	17:O:75:MET:HB2	2.05	0.55
20:R:26:ASN:OD1	20:R:58:MET:HE2	2.05	0.55
1:2:585:C:OP1	12:J:179:LYS:NZ	2.39	0.55
1:2:1818:A:H5''	36:h:16:LYS:HZ1	1.71	0.55
4:B:52:THR:HG22	4:B:54:GLY:H	1.71	0.55
7:E:138:HIS:CD2	7:E:148:ARG:HB3	2.42	0.55
24:V:21:ASN:O	24:V:21:ASN:ND2	2.37	0.55
12:J:136:ARG:HB3	12:J:160:SER:HB3	1.88	0.55
35:g:20:GLN:HE22	35:g:155:ARG:HH22	1.53	0.55
35:g:158:PRO:HG2	35:g:202:PRO:HA	1.88	0.55
1:2:1578:U:O2'	6:D:6:SER:HA	2.05	0.55
12:J:77:LEU:HA	12:J:80:ARG:NH1	2.21	0.55
34:f:126:CYS:HB2	34:f:130:VAL:HB	1.87	0.55
1:2:84:A:H4'	27:Y:119:GLY:O	2.07	0.55
1:2:1225:U:H1'	19:Q:142:GLN:HE22	1.71	0.55
1:2:1284:A:H5''	1:2:1286:G:O4'	2.07	0.55
1:2:1475:G:H5'	19:Q:124:PRO:HG3	1.89	0.55
21:S:6:PRO:HG2	28:Z:49:LEU:HD13	1.89	0.55
21:S:74:PRO:HA	21:S:79:ILE:HD12	1.88	0.55
35:g:128:THR:HG21	35:g:130:LYS:HE2	1.89	0.55
1:2:85:A:H2'	1:2:86:C:H6	1.71	0.55
1:2:1546:G:H5'	19:Q:18:THR:HG21	1.89	0.55
4:B:104:ASP:OD1	4:B:104:ASP:N	2.40	0.55
1:2:639:C:O2'	1:2:640:A:H8	1.90	0.55
1:2:1392:U:H3	1:2:1478:U:H3	1.55	0.55
14:L:133:PRO:HB3	14:L:139:ARG:NH1	2.20	0.55
20:R:20:TYR:HD2	20:R:23:ARG:HD2	1.72	0.55
22:T:22:LEU:HD22	22:T:28:LEU:HD12	1.89	0.55
22:T:75:MET:HG3	22:T:104:LEU:HD11	1.89	0.55
1:2:533:A:H2'	1:2:534:G:O4'	2.06	0.55
1:2:634:A:H2'	1:2:635:G:H8	1.72	0.55
1:2:917:U:O2'	1:2:918:U:O5'	2.25	0.55
1:2:1511:U:H2'	1:2:1512:C:C6	2.42	0.55
16:N:62:GLN:HB2	16:N:65:PHE:CD2	2.40	0.55
27:Y:15:ASN:HB3	27:Y:17:LEU:HD12	1.89	0.55
1:2:217:A:H5'	1:2:218:U:OP2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:551:U:H2'	1:2:552:G:C8	2.42	0.54
1:2:1736:G:H2'	1:2:1737:G:C8	2.41	0.54
9:G:159:ARG:HB3	9:G:171:THR:HG23	1.89	0.54
35:g:42:MET:O	35:g:56:GLN:N	2.40	0.54
1:2:145:G:H2'	1:2:146:G:H8	1.71	0.54
1:2:1428:G:H4'	1:2:1429:G:H5'	1.87	0.54
1:2:1590:C:H41	19:Q:77:HIS:HE1	1.55	0.54
21:S:98:VAL:HG11	21:S:106:LYS:HD2	1.89	0.54
27:Y:103:SER:HB3	27:Y:106:GLN:HG2	1.90	0.54
1:2:92:A:H4'	1:2:93:U:OP2	2.06	0.54
1:2:1546:G:H1	1:2:1655:C:HO2'	1.55	0.54
1:2:1866:A:C2	29:a:87:ARG:NH1	2.73	0.54
27:Y:78:SER:HB3	27:Y:81:TYR:CD2	2.42	0.54
1:2:797:C:O2'	1:2:798:G:OP1	2.21	0.54
1:2:1719:A:N6	1:2:1814:G:O2'	2.41	0.54
1:2:65:C:O2'	1:2:67:C:OP2	2.25	0.54
1:2:1272:C:H42	1:2:1510:G:H1	1.55	0.54
1:2:1731:A:H2'	1:2:1732:G:C8	2.43	0.54
3:A:143:PRO:HG3	24:V:32:ILE:HG23	1.87	0.54
6:D:74:GLN:HE21	6:D:84:VAL:HG12	1.72	0.54
7:E:124:CYS:HB3	7:E:141:THR:HB	1.89	0.54
10:H:184:ASP:N	10:H:184:ASP:OD1	2.40	0.54
12:J:119:LEU:HB3	12:J:159:PHE:CE1	2.42	0.54
17:O:57:THR:H	17:O:60:MET:HE2	1.72	0.54
19:Q:112:LEU:HD22	19:Q:119:LEU:HD13	1.89	0.54
1:2:591:U:O2'	1:2:592:C:H3'	2.08	0.54
1:2:1259:A:H61	1:2:1519:U:C5'	2.20	0.54
1:2:1415:C:H5''	22:T:129:ARG:HG3	1.90	0.54
1:2:1493:C:OP1	1:2:1494:U:O2'	2.22	0.54
1:2:1565:C:H3'	1:2:1566:G:H5''	1.89	0.54
1:2:1613:G:H5''	18:P:39:ALA:HB2	1.88	0.54
1:2:1615:U:O4	18:P:40:ARG:NH1	2.41	0.54
3:A:155:ARG:HD2	24:V:61:ARG:O	2.08	0.54
8:F:122:ARG:CZ	31:c:59:LEU:HD21	2.38	0.54
1:2:1384:C:H4'	6:D:157:MET:O	2.08	0.54
1:2:1597:C:H3'	1:2:1598:G:C8	2.43	0.54
2:3:150:G:N2	2:3:242:C:N3	2.53	0.54
7:E:151:ASP:OD2	9:G:216:ARG:NH2	2.40	0.54
21:S:84:LEU:HD12	21:S:95:TYR:HB3	1.88	0.54
1:2:830:A:C2	1:2:831:G:C8	2.96	0.54
8:F:87:LEU:HA	8:F:90:VAL:HG22	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:78:LEU:HD13	12:J:92:MET:O	2.07	0.54
16:N:63:VAL:HG21	16:N:71:ILE:HD11	1.90	0.54
25:W:3:ARG:HD3	25:W:6:VAL:HG22	1.89	0.54
32:d:10:HIS:CG	32:d:11:PRO:HD2	2.43	0.54
2:3:84:C:O2'	2:3:85:A:O5'	2.26	0.54
23:U:31:SER:O	23:U:35:VAL:HG23	2.08	0.54
1:2:51:U:H2'	1:2:52:G:C8	2.42	0.54
1:2:70:G:N2	1:2:80:G:N3	2.55	0.54
1:2:1271:C:H5'	1:2:1301:A:H2	1.72	0.54
1:2:1528:G:O2'	1:2:1666:C:OP1	2.25	0.54
3:A:134:LEU:HD21	3:A:144:THR:HG21	1.89	0.54
9:G:131:ARG:HG3	38:w:80:ARG:HH11	1.73	0.54
11:I:66:SER:O	11:I:189:VAL:HG23	2.08	0.54
1:2:589:G:O2'	1:2:590:A:OP2	2.19	0.53
1:2:1041:G:H5'	1:2:1042:A:OP2	2.08	0.53
1:2:1222:G:H5''	8:F:78:MET:HE3	1.90	0.53
3:A:141:ASN:ND2	24:V:29:HIS:O	2.41	0.53
4:B:209:ASP:HB3	4:B:211:PHE:HE1	1.73	0.53
1:2:388:U:H2'	1:2:389:A:H8	1.73	0.53
1:2:554:A:H4'	1:2:555:A:OP1	2.07	0.53
5:C:204:ILE:HG23	5:C:222:CYS:HB3	1.91	0.53
1:2:559:G:H3'	12:J:177:ASN:ND2	2.23	0.53
1:2:944:A:H5''	17:O:134:PRO:HB3	1.90	0.53
1:2:1217:A:H2'	1:2:1218:C:H6	1.74	0.53
1:2:1643:U:H2'	1:2:1644:C:C6	2.43	0.53
12:J:127:ARG:HD3	33:e:31:ARG:HD3	1.90	0.53
14:L:99:TYR:O	14:L:101:ARG:HG2	2.09	0.53
17:O:98:ARG:HH11	17:O:98:ARG:CG	2.21	0.53
26:X:82:THR:O	26:X:118:VAL:HG13	2.08	0.53
26:X:119:ARG:HB2	26:X:120:PHE:CE1	2.44	0.53
29:a:26:CYS:CB	29:a:28:ARG:H	2.21	0.53
1:2:520:A:H5''	12:J:12:THR:OG1	2.09	0.53
1:2:594:A:H61	1:2:643:A:H5''	1.73	0.53
1:2:1223:A:H4'	1:2:1651:A:H4'	1.91	0.53
1:2:1455:A:OP2	20:R:56:HIS:ND1	2.41	0.53
5:C:221:ASP:OD1	5:C:221:ASP:N	2.42	0.53
9:G:55:GLY:HA3	9:G:63:MET:SD	2.48	0.53
10:H:101:LEU:O	10:H:116:ARG:NH1	2.41	0.53
1:2:941:C:H5''	4:B:136:ARG:NH2	2.24	0.53
4:B:87:ILE:HG22	4:B:88:THR:O	2.08	0.53
6:D:79:PHE:CE1	6:D:84:VAL:HB	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:127:MET:HE3	6:D:154:ASP:HB3	1.89	0.53
13:K:32:HIS:NE2	13:K:45:VAL:HG11	2.23	0.53
1:2:77:A:H5''	1:2:77:A:H8	1.73	0.53
1:2:1239:U:H4'	18:P:124:LYS:HB3	1.91	0.53
1:2:1858:G:OP2	17:O:146:ARG:NH2	2.41	0.53
10:H:80:VAL:O	10:H:84:GLU:HB2	2.08	0.53
14:L:104:LYS:HZ1	26:X:8:ARG:HD3	1.72	0.53
26:X:73:GLN:HG3	26:X:80:LYS:HG3	1.91	0.53
1:2:70:G:C2	1:2:80:G:C2	2.96	0.53
2:3:260:A:C2	2:3:261:G:H1'	2.44	0.53
12:J:95:ASP:N	12:J:95:ASP:OD1	2.41	0.53
35:g:109:LEU:HD13	35:g:152:SER:HA	1.90	0.53
2:3:86:U:H5''	17:O:72:TYR:CZ	2.44	0.53
2:3:254:C:H4'	2:3:255:C:OP1	2.08	0.53
6:D:31:GLU:HG2	6:D:107:TYR:HE2	1.74	0.53
14:L:7:GLU:HB2	14:L:11:GLN:HE21	1.74	0.53
14:L:37:TYR:CG	14:L:51:ILE:HG22	2.44	0.53
1:2:1651:A:H2'	1:2:1652:G:H8	1.74	0.53
13:K:62:PHE:CZ	13:K:65:ARG:HA	2.44	0.53
23:U:78:ASP:HB3	23:U:80:PHE:HE1	1.74	0.53
1:2:1259:A:H61	1:2:1519:U:H5'	1.73	0.52
1:2:75:G:N2	9:G:155:GLN:HG3	2.24	0.52
1:2:1224:G:H2'	1:2:1225:U:H6	1.73	0.52
1:2:1584:G:C4	1:2:1586:U:H1'	2.44	0.52
1:2:1596:U:OP2	28:Z:85:ARG:NH2	2.42	0.52
1:2:1830:U:OP2	2:3:342:A:O2'	2.27	0.52
8:F:56:TYR:HB3	8:F:63:LYS:HA	1.91	0.52
8:F:112:LEU:HD13	8:F:177:LEU:HD21	1.91	0.52
9:G:7:PHE:HE1	9:G:9:ALA:HB3	1.74	0.52
9:G:110:ASN:OD1	9:G:110:ASN:N	2.42	0.52
18:P:44:ARG:HH21	18:P:53:GLN:HE22	1.58	0.52
21:S:83:PHE:HE2	22:T:36:THR:HG23	1.74	0.52
1:2:317:C:OP2	9:G:183:ARG:NH2	2.42	0.52
1:2:601:G:O2'	1:2:602:G:O4'	2.26	0.52
8:F:28:VAL:HG12	8:F:29:GLN:H	1.75	0.52
23:U:27:ARG:NH1	32:d:51:GLY:HA3	2.24	0.52
24:V:64:GLU:O	24:V:68:SER:OG	2.27	0.52
1:2:1229:G:H21	22:T:87:VAL:HG12	1.74	0.52
1:2:1643:U:O2'	19:Q:142:GLN:HG2	2.10	0.52
3:A:207:PRO:HA	3:A:210:ILE:HD12	1.91	0.52
5:C:200:ARG:O	12:J:54:ARG:NH2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:83:ASP:OD1	16:N:83:ASP:N	2.41	0.52
1:2:205:G:H2'	1:2:206:G:O4'	2.08	0.52
1:2:1060:A:O2'	1:2:1062:A:N7	2.40	0.52
4:B:128:LYS:HG3	4:B:134:LEU:HD13	1.92	0.52
6:D:23:GLU:O	6:D:27:ARG:HG2	2.10	0.52
22:T:28:LEU:HD21	22:T:53:PHE:CE1	2.45	0.52
1:2:60:A:H2	1:2:61:A:C2	2.28	0.52
1:2:621:C:OP1	26:X:107:ARG:HD2	2.08	0.52
1:2:808:A:H5''	7:E:219:ALA:O	2.09	0.52
1:2:969:U:P	1:2:970:G:H5'	2.49	0.52
1:2:1818:A:H5''	36:h:16:LYS:HZ3	1.71	0.52
10:H:163:GLN:O	10:H:167:GLU:HB2	2.10	0.52
33:e:11:LYS:O	33:e:15:GLN:HB2	2.10	0.52
35:g:258:ILE:HD11	35:g:298:LEU:HD11	1.92	0.52
1:2:69:C:N4	1:2:70:G:O6	2.42	0.52
1:2:112:U:H5''	1:2:113:G:H2'	1.92	0.52
1:2:380:G:C6	1:2:382:C:H5''	2.45	0.52
1:2:1293:A:H2'	1:2:1294:G:C8	2.44	0.52
23:U:50:VAL:HG12	23:U:91:LEU:HD22	1.91	0.52
28:Z:91:LEU:HD22	28:Z:96:LEU:HD12	1.91	0.52
1:2:912:C:C2	1:2:914:U:H1'	2.44	0.52
17:O:106:LYS:HZ3	17:O:135:ILE:HA	1.74	0.52
1:2:579:C:O2	27:Y:61:ARG:NH2	2.42	0.52
1:2:1159:G:H1'	25:W:4:MET:HE3	1.92	0.52
9:G:98:ARG:NH2	9:G:101:ILE:O	2.41	0.52
26:X:77:ASN:OD1	26:X:77:ASN:N	2.29	0.52
1:2:1101:U:H2'	1:2:1102:G:C8	2.45	0.52
27:Y:37:LYS:HA	27:Y:40:ILE:HG22	1.90	0.52
1:2:89:C:N4	41:2:2019:HOH:O	2.42	0.51
1:2:1269:G:H1	1:2:1513:C:N4	2.07	0.51
1:2:1284:A:O2'	15:M:106:CYS:SG	2.65	0.51
9:G:151:ASP:OD1	9:G:151:ASP:N	2.43	0.51
24:V:55:ILE:HD11	24:V:69:ILE:HG12	1.92	0.51
35:g:288:SER:OG	35:g:289:LEU:N	2.42	0.51
1:2:319:C:O2'	1:2:320:G:OP1	2.25	0.51
2:3:305:U:O2'	2:3:325:C:N4	2.41	0.51
3:A:26:GLY:HA3	3:A:150:THR:HG23	1.93	0.51
7:E:106:LYS:HD2	7:E:108:ARG:NH2	2.25	0.51
15:M:52:LEU:O	15:M:78:LYS:HA	2.10	0.51
22:T:37:VAL:HG22	22:T:38:LYS:N	2.25	0.51
28:Z:58:LEU:HD12	28:Z:62:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:g:17:TRP:CE2	35:g:303:THR:HG23	2.44	0.51
35:g:20:GLN:HB2	35:g:68:ASP:HA	1.92	0.51
1:2:625:G:O6	26:X:63:ASN:HB2	2.10	0.51
1:2:957:A:H2'	1:2:958:G:H5'	1.93	0.51
1:2:1298:G:H4'	18:P:77:LYS:O	2.11	0.51
1:2:1414:A:N6	1:2:1425:G:O6	2.42	0.51
4:B:68:GLU:HG3	4:B:83:LYS:HE2	1.93	0.51
5:C:236:PHE:O	5:C:240:THR:HG22	2.10	0.51
38:w:67:UNK:O	38:w:67:UNK:HG2	2.09	0.51
1:2:1542:C:OP1	22:T:62:ARG:NH1	2.41	0.51
2:3:172:A:H2'	2:3:173:A:C8	2.44	0.51
3:A:108:PHE:HB3	3:A:140:VAL:HG21	1.93	0.51
21:S:50:ILE:HD12	21:S:67:VAL:HG21	1.87	0.51
1:2:4:C:H5'	5:C:230:THR:HG21	1.91	0.51
1:2:684:G:H1'	1:2:920:A:C2	2.44	0.51
1:2:1217:A:C2	1:2:1218:C:C2	2.99	0.51
1:2:1800:A:H5''	1:2:1801:A:OP2	2.11	0.51
6:D:195:THR:H	6:D:201:LYS:HE2	1.75	0.51
7:E:258:ALA:O	7:E:262:SER:OG	2.25	0.51
14:L:35:ARG:NH1	14:L:53:GLY:O	2.44	0.51
17:O:37:PHE:HE2	17:O:105:THR:HG21	1.75	0.51
25:W:44:HIS:NE2	25:W:112:ASP:OD2	2.40	0.51
1:2:345:U:H5''	7:E:37:LYS:HG2	1.92	0.51
1:2:434:G:H2'	1:2:435:A:C8	2.45	0.51
1:2:559:G:O2'	1:2:560:A:H8	1.94	0.51
3:A:134:LEU:CD2	3:A:144:THR:HG21	2.41	0.51
11:I:141:ARG:HH22	11:I:153:LYS:HZ1	1.56	0.51
30:b:67:THR:HG22	30:b:68:GLY:H	1.75	0.51
1:2:1528:G:H2'	1:2:1529:C:H6	1.75	0.51
4:B:217:MET:HE1	4:B:220:LYS:HG2	1.91	0.51
12:J:15:THR:HG22	12:J:44:TRP:CZ3	2.46	0.51
12:J:160:SER:O	12:J:162:ARG:N	2.44	0.51
15:M:79:VAL:HG12	15:M:80:ASP:H	1.75	0.51
27:Y:104:ARG:O	27:Y:108:LYS:HB2	2.10	0.51
1:2:70:G:C6	1:2:71:G:C4	2.99	0.51
3:A:189:ILE:HG22	3:A:190:SER:H	1.76	0.51
10:H:100:ILE:HD11	10:H:125:VAL:HG11	1.93	0.51
10:H:138:GLU:OE1	16:N:19:ARG:NH1	2.44	0.51
23:U:32:LEU:HD21	23:U:87:ARG:HE	1.75	0.51
1:2:180:G:O2'	1:2:181:A:H5'	2.10	0.51
1:2:1037:G:H4'	1:2:1845:A:H4'	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1228:A:H2'	1:2:1229:G:C8	2.46	0.51
10:H:158:LEU:HD11	10:H:187:PHE:HD2	1.75	0.51
1:2:806:U:C2	1:2:858:A:C2	2.99	0.51
1:2:1650:A:H5'	19:Q:139:ALA:HB2	1.93	0.51
1:2:1692:U:H2'	1:2:1693:G:C8	2.46	0.51
14:L:120:VAL:HG22	14:L:145:VAL:HG11	1.91	0.51
25:W:78:ARG:HG2	25:W:78:ARG:HH11	1.76	0.51
1:2:29:G:H4'	26:X:129:SER:HB3	1.93	0.50
1:2:167:G:N7	41:2:2014:HOH:O	2.35	0.50
1:2:478:G:H2'	1:2:479:C:H6	1.77	0.50
1:2:511:U:H2'	1:2:512:A:H8	1.76	0.50
1:2:869:A:N1	10:H:114:GLN:NE2	2.59	0.50
1:2:1391:C:O3'	23:U:83:ARG:NH2	2.43	0.50
9:G:57:ASP:HA	9:G:107:SER:H	1.75	0.50
10:H:39:GLN:O	10:H:43:LEU:HG	2.11	0.50
20:R:13:ALA:HB3	20:R:53:TYR:HD2	1.76	0.50
20:R:17:ILE:HG12	20:R:54:VAL:HG13	1.93	0.50
21:S:26:ILE:O	21:S:30:ILE:HG12	2.11	0.50
27:Y:79:LEU:HD21	27:Y:83:LYS:HE3	1.93	0.50
35:g:79:LEU:HD12	35:g:89:LEU:HA	1.93	0.50
35:g:173:LEU:HD22	35:g:189:ILE:HG12	1.92	0.50
1:2:1550:G:H21	1:2:1577:G:H21	1.59	0.50
1:2:1599:U:C5	8:F:166:ILE:HD12	2.46	0.50
1:2:1741:U:H2'	1:2:1742:C:O4'	2.11	0.50
6:D:194:PRO:HA	6:D:201:LYS:HD3	1.91	0.50
7:E:73:ASP:HB3	7:E:164:LEU:HD22	1.93	0.50
15:M:36:ARG:HE	15:M:40:LYS:NZ	2.08	0.50
26:X:19:ASP:N	26:X:19:ASP:OD1	2.39	0.50
35:g:253:GLY:HA2	35:g:286:CYS:H	1.77	0.50
1:2:638:C:O2'	1:2:639:C:O5'	2.28	0.50
2:3:153:G:H3'	2:3:154:A:H5'	1.92	0.50
6:D:62:LYS:O	6:D:67:ARG:NH2	2.44	0.50
6:D:127:MET:HE1	6:D:133:GLY:HA2	1.93	0.50
9:G:126:ASP:OD1	9:G:126:ASP:N	2.45	0.50
15:M:77:ILE:HG12	15:M:128:PHE:HZ	1.76	0.50
19:Q:39:LEU:HD13	19:Q:52:LEU:HD23	1.92	0.50
1:2:189:U:H5'	1:2:190:G:OP2	2.12	0.50
1:2:520:A:H2'	1:2:521:A:H8	1.76	0.50
1:2:1234:C:H5'	1:2:1246:A:H61	1.76	0.50
9:G:216:ARG:O	9:G:219:GLU:HG2	2.11	0.50
29:a:10:ARG:NH1	29:a:12:LYS:HD3	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:46:GLU:O	29:a:50:VAL:HG23	2.10	0.50
1:2:85:A:H2'	1:2:86:C:C6	2.46	0.50
1:2:334:C:H5'	1:2:335:G:OP2	2.12	0.50
2:3:64:U:H3	2:3:103:U:H3	1.59	0.50
2:3:263:G:C2	2:3:264:U:H5	2.29	0.50
5:C:272:HIS:HA	5:C:275:LYS:HD2	1.93	0.50
7:E:103:TYR:CG	7:E:189:LEU:HD11	2.46	0.50
21:S:46:ARG:NE	22:T:50:GLU:OE1	2.45	0.50
21:S:50:ILE:HD11	21:S:67:VAL:HG23	1.91	0.50
1:2:164:A:H3'	1:2:165:G:H21	1.75	0.50
1:2:871:U:OP2	1:2:871:U:H4'	2.12	0.50
1:2:979:C:H2'	1:2:980:A:H8	1.77	0.50
1:2:1033:G:H5''	1:2:1034:A:OP1	2.11	0.50
1:2:1136:U:H2'	1:2:1137:U:C6	2.46	0.50
1:2:1597:C:H4'	1:2:1603:G:O6	2.12	0.50
4:B:144:LYS:HB2	4:B:208:HIS:CB	2.38	0.50
6:D:75:LYS:HB3	13:K:22:VAL:HG21	1.93	0.50
15:M:49:LEU:HD22	15:M:75:ASN:HB2	1.92	0.50
21:S:55:ARG:NH2	28:Z:82:SER:OG	2.45	0.50
1:2:581:U:OP1	12:J:133:ARG:NH2	2.43	0.50
1:2:1719:A:H2'	1:2:1720:U:O4'	2.12	0.50
3:A:144:THR:H	3:A:158:ASP:HB2	1.76	0.50
4:B:35:ALA:HB1	4:B:36:PRO:HD2	1.93	0.50
8:F:34:SER:HA	31:c:55:VAL:HG13	1.94	0.50
14:L:77:VAL:HA	14:L:88:ILE:HG22	1.94	0.50
15:M:92:CYS:SG	15:M:103:VAL:HG22	2.51	0.50
35:g:165:ILE:HG13	35:g:177:TRP:HB2	1.94	0.50
1:2:389:A:H2'	1:2:390:C:H6	1.77	0.50
1:2:435:A:H8	1:2:435:A:OP2	1.94	0.50
1:2:1578:U:O2	6:D:6:SER:HB2	2.11	0.50
2:3:146:G:H1	2:3:247:C:N4	2.08	0.50
16:N:5:HIS:HD1	16:N:121:ARG:HG3	1.76	0.50
23:U:78:ASP:HB3	23:U:80:PHE:CE1	2.47	0.50
36:h:21:ARG:HA	36:h:25:LYS:HD2	1.92	0.50
1:2:44:U:O2'	1:2:45:A:H2'	2.12	0.50
4:B:125:VAL:HG22	4:B:169:MET:HG3	1.94	0.50
10:H:191:GLU:O	10:H:192:PHE:HB2	2.11	0.50
21:S:86:ARG:NH2	21:S:110:ASP:OD2	2.44	0.50
1:2:296:U:O2'	7:E:131:VAL:O	2.23	0.49
2:3:98:G:O2'	2:3:99:A:C8	2.62	0.49
4:B:86:LEU:HB3	4:B:98:THR:CG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:35:ARG:HH22	14:L:54:THR:C	2.19	0.49
18:P:18:ARG:HA	21:S:93:GLY:HA3	1.94	0.49
35:g:121:VAL:HG11	35:g:165:ILE:HD12	1.94	0.49
1:2:795:A:C2	1:2:796:G:H1'	2.46	0.49
1:2:828:G:H4'	7:E:23:LEU:HD22	1.94	0.49
1:2:1643:U:H2'	1:2:1644:C:H6	1.77	0.49
3:A:122:LEU:HD22	3:A:142:LEU:HD12	1.94	0.49
4:B:146:ARG:N	4:B:149:GLN:OE1	2.44	0.49
5:C:254:ASP:HB3	24:V:1:MET:HG3	1.94	0.49
7:E:44:LEU:HB3	7:E:80:ILE:O	2.13	0.49
7:E:86:PHE:CE2	7:E:87:MET:HG2	2.47	0.49
9:G:49:VAL:HB	9:G:115:LYS:HB2	1.94	0.49
21:S:128:GLY:O	21:S:144:ARG:NH2	2.45	0.49
28:Z:92:LEU:HD21	28:Z:109:TYR:HE1	1.76	0.49
1:2:70:G:N2	1:2:80:G:C2	2.80	0.49
1:2:870:A:H4'	1:2:871:U:C5'	2.42	0.49
3:A:29:ASN:N	3:A:29:ASN:OD1	2.42	0.49
5:C:130:ILE:HG22	5:C:158:ALA:HB1	1.94	0.49
7:E:127:ARG:HH21	7:E:142:HIS:HB2	1.78	0.49
11:I:142:SER:H	11:I:145:ILE:HD12	1.77	0.49
14:L:77:VAL:O	14:L:123:GLY:N	2.38	0.49
17:O:39:ASP:HA	17:O:69:SER:HA	1.95	0.49
21:S:86:ARG:HB3	21:S:89:ASP:OD1	2.12	0.49
26:X:59:ALA:HB1	26:X:114:ASP:OD1	2.12	0.49
1:2:1161:U:H2'	1:2:1162:C:C6	2.48	0.49
1:2:1284:A:H61	1:2:1313:A:H2'	1.77	0.49
1:2:1284:A:N6	1:2:1313:A:H2'	2.27	0.49
1:2:1515:G:N2	18:P:99:GLY:O	2.44	0.49
2:3:233:G:O5'	30:b:43:ILE:HG21	2.13	0.49
5:C:77:SER:O	5:C:80:GLU:HG2	2.12	0.49
6:D:137:VAL:HG22	6:D:151:LYS:HG3	1.93	0.49
12:J:137:VAL:HG12	12:J:138:ARG:HG3	1.94	0.49
15:M:42:LEU:HG	15:M:74:ILE:HD13	1.95	0.49
18:P:22:LEU:HD11	18:P:109:PRO:HB3	1.94	0.49
20:R:16:ILE:HD11	20:R:39:ALA:HB2	1.95	0.49
28:Z:50:PHE:CZ	28:Z:58:LEU:HD22	2.46	0.49
1:2:107:A:C2	1:2:355:G:C2	2.99	0.49
1:2:433:A:H5''	11:I:25:ARG:HH22	1.77	0.49
9:G:22:ARG:HA	9:G:25:ARG:HG2	1.94	0.49
16:N:37:ILE:HD11	16:N:63:VAL:HG11	1.95	0.49
16:N:47:PRO:HG2	16:N:86:GLU:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:51:LEU:HD13	19:Q:81:ILE:HG23	1.94	0.49
20:R:20:TYR:CE2	20:R:38:ILE:HG12	2.47	0.49
22:T:17:ALA:CB	22:T:138:VAL:HG21	2.42	0.49
28:Z:57:LYS:O	28:Z:61:GLU:HB3	2.13	0.49
1:2:168:C:O2'	9:G:132:ARG:O	2.31	0.49
1:2:1232:U:C5	21:S:138:THR:HG21	2.48	0.49
1:2:1354:G:N7	41:2:2013:HOH:O	2.34	0.49
1:2:1733:U:H2'	1:2:1734:G:H5'	1.95	0.49
3:A:18:PHE:O	3:A:22:GLY:N	2.42	0.49
6:D:142:LEU:HB2	6:D:148:LYS:HD2	1.95	0.49
20:R:33:ARG:O	20:R:36:GLU:HG2	2.13	0.49
1:2:587:A:H5'	1:2:592:C:N4	2.27	0.49
1:2:857:U:H5''	7:E:201:HIS:CD2	2.48	0.49
1:2:1392:U:P	23:U:83:ARG:HH12	2.34	0.49
2:3:255:C:H3'	2:3:256:G:H5''	1.94	0.49
2:3:332:A:H3'	2:3:333:C:H5'	1.93	0.49
3:A:42:LYS:HD3	3:A:48:ILE:HD11	1.95	0.49
4:B:129:THR:OG1	4:B:131:ASP:OD1	2.29	0.49
8:F:60:ARG:HG2	8:F:61:PHE:CD2	2.47	0.49
17:O:65:ASP:O	17:O:68:GLU:HB2	2.13	0.49
1:2:63:U:H5''	1:2:64:A:OP2	2.13	0.49
1:2:1149:A:O2'	1:2:1150:A:H5''	2.12	0.49
1:2:1510:G:H2'	1:2:1511:U:C6	2.48	0.49
5:C:168:GLY:HA3	5:C:181:PRO:HA	1.93	0.49
9:G:145:PHE:HD2	9:G:156:TYR:HB3	1.78	0.49
20:R:23:ARG:NH2	35:g:149:GLU:OE2	2.45	0.49
35:g:246:TYR:CE2	35:g:262:GLU:HG3	2.48	0.49
1:2:309:G:O2'	1:2:310:C:OP2	2.28	0.49
1:2:792:C:H2'	1:2:793:G:H8	1.76	0.49
1:2:1293:A:H2'	1:2:1294:G:H8	1.77	0.49
1:2:1592:C:O2'	19:Q:43:GLU:O	2.31	0.49
1:2:1597:C:H4'	1:2:1603:G:C6	2.47	0.49
5:C:77:SER:HA	5:C:97:PHE:HE1	1.78	0.49
6:D:134:CYS:HB2	6:D:188:ILE:HD13	1.95	0.49
6:D:138:VAL:HG12	6:D:182:LEU:HD22	1.95	0.49
10:H:60:ILE:HB	10:H:92:VAL:HG22	1.94	0.49
17:O:116:LEU:HD22	29:a:53:ILE:HD11	1.95	0.49
1:2:1003:U:H2'	1:2:1004:U:H6	1.78	0.49
1:2:1143:A:H5''	1:2:1144:A:OP2	2.13	0.49
1:2:1547:C:H2'	1:2:1548:G:O4'	2.12	0.49
1:2:1816:G:H2'	1:2:1817:G:H8	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:328:G:C6	2:3:329:U:C4	3.00	0.49
4:B:30:TRP:CE2	4:B:48:LEU:HD13	2.46	0.49
10:H:134:VAL:HG11	10:H:158:LEU:HD22	1.94	0.49
11:I:22:HIS:HB2	11:I:25:ARG:NH2	2.27	0.49
35:g:249:CYS:HB2	35:g:291:TRP:CZ3	2.47	0.49
1:2:60:A:O2'	1:2:61:A:O5'	2.26	0.48
1:2:586:G:N7	12:J:172:ARG:HD3	2.28	0.48
1:2:1063:C:OP1	41:2:2007:HOH:O	2.20	0.48
5:C:188:CYS:HB3	5:C:239:ALA:HB2	1.94	0.48
6:D:34:TYR:OH	6:D:37:VAL:HG23	2.13	0.48
12:J:81:LEU:HD23	12:J:84:ILE:HD11	1.93	0.48
14:L:15:THR:O	14:L:16:ILE:HD13	2.12	0.48
18:P:44:ARG:HH21	18:P:53:GLN:NE2	2.11	0.48
22:T:67:ARG:HG3	22:T:68:GLY:O	2.13	0.48
1:2:190:G:C6	1:2:208:G:C6	3.01	0.48
1:2:220:U:H2'	1:2:221:A:C8	2.48	0.48
1:2:596:U:H2'	1:2:597:G:O4'	2.13	0.48
1:2:818:A:H5''	1:2:819:G:OP2	2.13	0.48
1:2:1045:U:H2'	1:2:1046:U:O4'	2.12	0.48
1:2:1204:A:OP1	5:C:117:ARG:HB3	2.13	0.48
1:2:1244:U:H3	1:2:1257:G:H22	1.59	0.48
2:3:164:U:H2'	2:3:165:A:H1'	1.95	0.48
2:3:263:G:N3	2:3:264:U:H5	2.11	0.48
5:C:78:LEU:HD12	5:C:81:ILE:HD12	1.95	0.48
7:E:100:ARG:HB2	7:E:114:ILE:HD12	1.95	0.48
1:2:209:A:H2'	1:2:210:U:H5'	1.94	0.48
1:2:553:U:C4	1:2:554:A:N7	2.82	0.48
1:2:1267:C:H2'	1:2:1268:C:C6	2.48	0.48
1:2:1735:A:C4	1:2:1800:A:C2	3.00	0.48
2:3:134:A:H61	2:3:290:U:H3	1.61	0.48
18:P:45:LEU:HD23	18:P:49:LEU:HD21	1.95	0.48
22:T:42:HIS:HD2	22:T:43:LYS:HG3	1.78	0.48
24:V:76:ASP:HB3	24:V:78:ILE:HG13	1.94	0.48
1:2:72:C:H5	9:G:170:ARG:HH22	1.60	0.48
1:2:1210:G:N2	1:2:1690:U:C2	2.82	0.48
5:C:196:ILE:HG13	5:C:223:TYR:O	2.12	0.48
11:I:48:VAL:HG22	11:I:52:ASN:O	2.13	0.48
11:I:79:ILE:HG22	11:I:80:ASP:HB2	1.96	0.48
20:R:28:PHE:HD2	20:R:29:HIS:CE1	2.30	0.48
22:T:42:HIS:ND1	22:T:81:GLY:HA3	2.29	0.48
1:2:70:G:N2	1:2:79:A:N6	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1181:A:O2'	1:2:1182:A:O4'	2.31	0.48
1:2:1463:U:H4'	1:2:1464:C:H5'	1.95	0.48
2:3:83:C:H5	2:3:84:C:C4	2.32	0.48
7:E:95:THR:HB	7:E:97:GLU:HG3	1.94	0.48
15:M:54:SER:OG	15:M:78:LYS:HB3	2.14	0.48
16:N:98:VAL:O	16:N:102:LEU:HB2	2.13	0.48
20:R:132:ARG:H	20:R:132:ARG:HG3	1.38	0.48
1:2:171:A:N7	1:2:173:A:C5	2.82	0.48
1:2:665:G:N2	1:2:1163:C:H1'	2.28	0.48
1:2:918:U:H5''	16:N:64:ARG:NH2	2.28	0.48
5:C:203:GLY:O	5:C:221:ASP:HA	2.14	0.48
7:E:211:LYS:HE2	7:E:215:GLY:HA2	1.94	0.48
9:G:146:ASN:ND2	38:w:94:ARG:HG2	2.28	0.48
17:O:44:VAL:HG12	17:O:53:ILE:HD12	1.94	0.48
30:b:47:PHE:HD2	30:b:49:HIS:O	1.97	0.48
1:2:946:U:H4'	1:2:1046:U:OP1	2.14	0.48
1:2:1258:A:C2	1:2:1663:A:H2'	2.48	0.48
1:2:1558:C:H4'	1:2:1559:C:OP1	2.14	0.48
1:2:1856:C:OP2	17:O:146:ARG:HB2	2.14	0.48
3:A:102:ARG:HG3	3:A:103:PHE:O	2.13	0.48
4:B:25:PHE:CE2	17:O:88:LEU:HD13	2.49	0.48
4:B:159:GLN:HE22	4:B:162:ARG:NH1	2.12	0.48
5:C:183:LYS:HB3	5:C:196:ILE:HG23	1.96	0.48
11:I:89:GLU:HG2	11:I:92:ARG:NH2	2.28	0.48
25:W:112:ASP:N	25:W:112:ASP:OD1	2.46	0.48
35:g:42:MET:HB3	35:g:56:GLN:HB3	1.95	0.48
1:2:958:G:H22	17:O:68:GLU:CD	2.17	0.48
1:2:1207:G:O2'	1:2:1837:G:N2	2.46	0.48
1:2:1398:G:O2'	35:g:61:GLY:O	2.30	0.48
1:2:1745:A:O2'	1:2:1746:U:O4'	2.21	0.48
1:2:1868:U:O2	29:a:97:PRO:HB2	2.13	0.48
2:3:252:A:H4'	2:3:253:G:C5'	2.44	0.48
2:3:258:G:H1'	2:3:273:G:C6	2.49	0.48
3:A:121:LEU:HD12	3:A:143:PRO:HB2	1.95	0.48
4:B:30:TRP:HE1	17:O:18:GLY:HA2	1.79	0.48
7:E:136:ILE:HG12	7:E:149:TYR:CE1	2.48	0.48
16:N:45:LEU:HB3	16:N:49:GLN:HB2	1.95	0.48
27:Y:20:ARG:HB3	27:Y:76:TYR:CD1	2.49	0.48
35:g:57:ARG:NH1	35:g:93:THR:O	2.47	0.48
35:g:102:VAL:HG12	35:g:103:GLY:H	1.79	0.48
35:g:107:ASP:OD2	35:g:125:ARG:NH1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:563:G:N7	1:2:586:G:N2	2.62	0.48
1:2:587:A:H5'	1:2:592:C:H41	1.79	0.48
1:2:872:A:C8	1:2:874:G:C8	3.02	0.48
1:2:913:A:H2	10:H:99:ARG:H	1.60	0.48
1:2:1546:G:H2'	1:2:1547:C:C6	2.49	0.48
1:2:1658:G:OP2	1:2:1660:C:N4	2.47	0.48
2:3:72:A:H2'	2:3:73:A:O4'	2.13	0.48
7:E:245:ARG:HG2	7:E:246:LEU:H	1.78	0.48
10:H:9:VAL:HG22	10:H:45:ILE:HG12	1.95	0.48
16:N:101:HIS:HE1	16:N:105:ASN:HD22	1.56	0.48
1:2:130:G:H1	1:2:182:C:H42	1.61	0.48
1:2:380:G:P	11:I:56:ARG:HH22	2.37	0.48
1:2:1320:G:H2'	1:2:1321:G:H5'	1.95	0.48
4:B:150:ILE:HG22	20:R:132:ARG:HE	1.79	0.48
22:T:37:VAL:HG22	22:T:38:LYS:H	1.79	0.48
1:2:316:G:H2'	1:2:317:C:H6	1.78	0.47
1:2:465:A:H5'	1:2:466:G:C5	2.49	0.47
1:2:582:U:H1'	27:Y:33:ALA:HB2	1.95	0.47
1:2:1154:U:H5''	1:2:1156:U:O4'	2.14	0.47
1:2:1256:G:N2	1:2:1659:U:H5'	2.16	0.47
1:2:1866:A:N1	29:a:87:ARG:NH1	2.62	0.47
2:3:244:A:H1'	2:3:245:G:P	2.54	0.47
4:B:164:ILE:HD13	4:B:207:LEU:HD11	1.96	0.47
5:C:207:ALA:O	5:C:211:LYS:HB2	2.13	0.47
11:I:79:ILE:HG13	11:I:170:LYS:NZ	2.29	0.47
12:J:64:ASP:OD1	12:J:65:GLU:N	2.47	0.47
15:M:61:TYR:OH	15:M:108:CYS:SG	2.65	0.47
38:w:97:LYS:HB3	38:w:98:PRO:HD2	1.96	0.47
1:2:1287:A:H5''	34:f:95:ARG:NH1	2.29	0.47
1:2:1338:G:OP1	23:U:67:LYS:HD2	2.14	0.47
5:C:128:VAL:HG11	5:C:155:ILE:HG12	1.96	0.47
11:I:60:LEU:HD23	11:I:60:LEU:HA	1.63	0.47
14:L:40:ILE:HA	14:L:40:ILE:HD13	1.59	0.47
14:L:60:CYS:SG	14:L:62:PHE:N	2.85	0.47
22:T:42:HIS:HA	22:T:83:GLN:OE1	2.14	0.47
25:W:111:MET:HB2	25:W:115:GLU:OE1	2.13	0.47
27:Y:37:LYS:O	27:Y:40:ILE:HG22	2.14	0.47
35:g:112:ALA:HB2	35:g:154:VAL:O	2.15	0.47
1:2:608:C:H42	1:2:635:G:H1	1.61	0.47
1:2:1603:G:N2	22:T:48:TYR:OH	2.47	0.47
1:2:1608:U:H5''	21:S:130:ARG:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1610:G:N2	21:S:85:ASN:O	2.47	0.47
1:2:1611:G:O2'	21:S:86:ARG:HG2	2.15	0.47
7:E:38:LEU:HG	7:E:39:ARG:N	2.28	0.47
16:N:5:HIS:CE1	16:N:121:ARG:HG3	2.50	0.47
22:T:22:LEU:HB3	22:T:54:TYR:CD1	2.45	0.47
23:U:32:LEU:HD21	23:U:87:ARG:HG3	1.95	0.47
1:2:389:A:H2'	1:2:390:C:C6	2.48	0.47
1:2:943:U:O2	17:O:137:SER:HB3	2.14	0.47
1:2:1011:A:H2'	1:2:1012:A:O4'	2.14	0.47
5:C:244:ILE:H	5:C:244:ILE:HG12	1.55	0.47
7:E:112:HIS:CE1	7:E:239:PRO:HA	2.48	0.47
10:H:63:PHE:HA	10:H:95:ILE:O	2.14	0.47
11:I:141:ARG:HH22	11:I:153:LYS:NZ	2.12	0.47
17:O:142:ARG:HG2	17:O:142:ARG:HH11	1.79	0.47
18:P:78:THR:HG22	18:P:95:GLY:O	2.14	0.47
19:Q:93:VAL:HG12	19:Q:105:LYS:HE3	1.97	0.47
1:2:1224:G:H21	19:Q:142:GLN:NE2	2.11	0.47
1:2:1250:A:H4'	1:2:1251:A:OP2	2.13	0.47
1:2:1415:C:O2'	22:T:132:ASP:OD2	2.28	0.47
1:2:1649:U:HO2'	1:2:1650:A:P	2.36	0.47
1:2:1777:G:H2'	1:2:1778:C:O4'	2.14	0.47
2:3:153:G:H4'	2:3:154:A:OP2	2.13	0.47
4:B:33:VAL:HB	4:B:44:ILE:HD11	1.96	0.47
9:G:102:VAL:HG13	9:G:106:LEU:HD12	1.96	0.47
10:H:69:LEU:O	10:H:73:GLN:HG2	2.14	0.47
10:H:130:LEU:HB2	10:H:177:TYR:HE1	1.79	0.47
26:X:11:ARG:HG3	26:X:12:LYS:N	2.30	0.47
29:a:10:ARG:HH11	29:a:12:LYS:HD3	1.79	0.47
35:g:87:LEU:HD13	35:g:108:VAL:HG11	1.96	0.47
35:g:199:THR:OG1	35:g:239:LEU:O	2.24	0.47
1:2:340:C:H2'	1:2:341:C:O4'	2.15	0.47
1:2:656:G:H5'	1:2:662:G:N2	2.30	0.47
1:2:1210:G:C5'	29:a:85:ARG:HH12	2.26	0.47
4:B:49:VAL:HG21	4:B:62:LEU:HB2	1.97	0.47
6:D:157:MET:HG3	6:D:159:HIS:NE2	2.29	0.47
12:J:123:ILE:O	12:J:126:ALA:HB3	2.15	0.47
12:J:132:GLN:HB3	12:J:134:HIS:HD2	1.79	0.47
14:L:98:LYS:HB3	14:L:99:TYR:CD1	2.50	0.47
14:L:150:GLY:HA3	16:N:133:ARG:NH2	2.28	0.47
25:W:90:GLN:HA	25:W:102:ILE:HD11	1.96	0.47
35:g:81:GLY:HA2	35:g:87:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:448:A:H4'	1:2:449:A:H5'	1.97	0.47
1:2:488:U:H6	1:2:488:U:H2'	1.51	0.47
1:2:862:A:N3	25:W:105:THR:OG1	2.48	0.47
1:2:897:U:H2'	1:2:898:U:O4'	2.14	0.47
1:2:925:G:C2	1:2:926:A:C8	3.03	0.47
1:2:1291:A:OP1	32:d:2:GLY:N	2.48	0.47
1:2:1354:G:H5'	1:2:1355:C:OP2	2.15	0.47
1:2:1585:U:H3	19:Q:73:LYS:HE2	1.80	0.47
2:3:65:C:O2'	2:3:66:A:OP1	2.29	0.47
2:3:304:C:N4	2:3:305:U:O4	2.48	0.47
3:A:141:ASN:HD21	24:V:29:HIS:HA	1.80	0.47
6:D:22:ASN:OD1	6:D:34:TYR:OH	2.25	0.47
6:D:27:ARG:HB3	13:K:61:GLN:HE21	1.80	0.47
6:D:212:GLU:HG2	20:R:19:LYS:NZ	2.29	0.47
7:E:184:THR:OG1	7:E:224:ASN:O	2.30	0.47
11:I:198:TYR:O	11:I:202:ILE:HG13	2.14	0.47
16:N:55:ARG:HG2	16:N:55:ARG:HH11	1.79	0.47
17:O:84:ARG:O	17:O:87:GLU:HB3	2.14	0.47
18:P:110:GLU:HB3	21:S:117:ILE:HD11	1.97	0.47
31:c:26:GLN:H	31:c:26:GLN:HG2	1.51	0.47
1:2:14:C:OP2	5:C:232:THR:HG21	2.15	0.47
1:2:403:G:H2'	1:2:404:G:H8	1.79	0.47
1:2:900:C:H2'	1:2:901:G:H8	1.79	0.47
1:2:1252:C:OP1	23:U:75:LYS:NZ	2.34	0.47
1:2:1287:A:C6	1:2:1313:A:C8	3.02	0.47
7:E:6:LYS:HB2	7:E:6:LYS:HE3	1.65	0.47
11:I:114:GLU:OE1	11:I:123:ARG:NH2	2.46	0.47
12:J:136:ARG:HD2	12:J:160:SER:CA	2.38	0.47
14:L:78:THR:OG1	14:L:79:LYS:N	2.48	0.47
26:X:123:VAL:HG12	26:X:124:LYS:N	2.28	0.47
1:2:1234:C:H4'	1:2:1246:A:N1	2.29	0.47
1:2:1656:G:H1	1:2:1668:U:H3	1.62	0.47
2:3:59:U:H2'	2:3:60:G:C8	2.50	0.47
2:3:265:U:O2'	2:3:266:G:OP2	2.31	0.47
10:H:47:ALA:HB3	10:H:63:PHE:HB2	1.97	0.47
11:I:113:TYR:OH	11:I:156:ALA:HB1	2.15	0.47
21:S:90:VAL:HG21	21:S:113:ARG:NH1	2.30	0.47
30:b:8:LEU:HD23	30:b:8:LEU:HA	1.62	0.47
35:g:146:SER:O	35:g:147:HIS:CG	2.67	0.47
1:2:465:A:H5'	1:2:466:G:C4	2.50	0.47
1:2:552:G:OP1	33:e:39:ASN:ND2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:594:A:H4'	1:2:595:U:OP1	2.13	0.47
1:2:1560:U:H4'	1:2:1583:C:O2'	2.15	0.47
1:2:1651:A:H2'	1:2:1652:G:C8	2.50	0.47
3:A:169:HIS:HA	3:A:203:PHE:CE1	2.50	0.47
11:I:48:VAL:HG11	11:I:54:LYS:HD2	1.96	0.47
11:I:117:TYR:CE1	11:I:156:ALA:HB2	2.49	0.47
25:W:102:ILE:HB	25:W:113:HIS:HB3	1.97	0.47
26:X:7:LEU:C	26:X:9:THR:H	2.22	0.47
26:X:7:LEU:O	26:X:9:THR:N	2.48	0.47
35:g:168:CYS:HB3	35:g:198:VAL:HG23	1.95	0.47
1:2:67:C:C5	9:G:164:LYS:HB2	2.50	0.46
1:2:561:A:OP2	12:J:173:VAL:HB	2.15	0.46
1:2:1144:A:H2'	1:2:1145:A:C8	2.50	0.46
1:2:1671:G:H2'	1:2:1672:U:C6	2.50	0.46
2:3:123:C:O2'	2:3:124:C:OP1	2.32	0.46
3:A:206:ASP:OD1	3:A:208:GLU:HG2	2.15	0.46
5:C:116:THR:HG22	5:C:117:ARG:HG2	1.97	0.46
20:R:18:GLU:HA	20:R:71:ILE:CD1	2.45	0.46
35:g:65:PHE:O	35:g:82:SER:OG	2.29	0.46
35:g:162:ASN:HD21	35:g:178:ASN:HD22	1.62	0.46
1:2:80:G:N2	1:2:81:U:C2	2.83	0.46
1:2:332:G:H4'	1:2:333:G:OP1	2.15	0.46
1:2:1577:G:H1'	1:2:1582:C:O2	2.16	0.46
1:2:1609:C:H42	1:2:1630:A:H61	1.62	0.46
1:2:1630:A:OP1	21:S:37:GLY:N	2.38	0.46
1:2:1788:A:H2'	1:2:1789:G:O4'	2.16	0.46
5:C:161:SER:HA	24:V:27:LYS:NZ	2.31	0.46
6:D:146:ARG:HA	6:D:146:ARG:HD2	1.63	0.46
6:D:202:LYS:HA	6:D:203:PRO:HD3	1.75	0.46
12:J:128:VAL:O	12:J:132:GLN:HB2	2.16	0.46
15:M:17:ALA:HB3	15:M:123:VAL:HG11	1.97	0.46
1:2:409:C:C2	1:2:432:G:C2	3.04	0.46
1:2:548:C:H2'	1:2:549:C:C6	2.50	0.46
1:2:920:A:C8	1:2:922:A:C8	3.02	0.46
1:2:1373:C:OP1	20:R:7:LYS:N	2.48	0.46
1:2:1798:C:H4'	11:I:2:GLY:O	2.15	0.46
2:3:263:G:C2	2:3:264:U:C5	3.03	0.46
2:3:270:C:HO2'	2:3:271:G:H8	1.54	0.46
16:N:5:HIS:ND1	16:N:121:ARG:HG3	2.29	0.46
16:N:80:LEU:H	16:N:80:LEU:HD22	1.80	0.46
26:X:51:VAL:HG13	26:X:70:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:g:175:LYS:HE3	35:g:187:ASN:HD21	1.81	0.46
1:2:590:A:OP1	1:2:590:A:H3'	2.15	0.46
1:2:1177:U:H2'	1:2:1178:U:H6	1.80	0.46
4:B:217:MET:HE2	4:B:217:MET:HB3	1.52	0.46
7:E:197:ASN:OD1	7:E:198:ARG:N	2.48	0.46
11:I:34:ALA:HB2	11:I:56:ARG:HD3	1.97	0.46
16:N:125:LEU:O	16:N:128:TYR:HB3	2.15	0.46
25:W:6:VAL:HG12	25:W:34:ILE:HD11	1.97	0.46
29:a:22:ARG:HD3	29:a:29:CYS:SG	2.56	0.46
29:a:67:LEU:HD12	29:a:68:TYR:H	1.81	0.46
35:g:168:CYS:HB2	35:g:195:LEU:HD22	1.96	0.46
1:2:439:A:O2'	1:2:440:G:H5'	2.15	0.46
1:2:976:G:H2'	1:2:977:C:C6	2.51	0.46
1:2:1075:C:H5''	16:N:107:LYS:HZ2	1.80	0.46
1:2:1375:G:H2'	1:2:1376:A:H8	1.80	0.46
1:2:1425:G:H2'	1:2:1426:U:C6	2.51	0.46
4:B:69:VAL:HG11	4:B:74:LEU:HD21	1.97	0.46
5:C:77:SER:HA	5:C:97:PHE:CE1	2.50	0.46
7:E:103:TYR:CD1	7:E:189:LEU:HD11	2.51	0.46
10:H:30:LEU:O	10:H:34:SER:HB2	2.15	0.46
10:H:95:ILE:HA	10:H:132:ASP:OD2	2.16	0.46
11:I:76:THR:HG22	11:I:77:ARG:N	2.30	0.46
33:e:8:ARG:HG2	33:e:8:ARG:NH1	2.31	0.46
1:2:520:A:H2'	1:2:521:A:C8	2.51	0.46
1:2:675:U:H2'	1:2:676:C:H6	1.79	0.46
1:2:1356:G:H2'	1:2:1357:A:C8	2.51	0.46
2:3:230:G:O2'	2:3:231:G:OP1	2.27	0.46
9:G:144:LEU:HD23	9:G:144:LEU:HA	1.77	0.46
35:g:68:ASP:OD1	35:g:69:VAL:N	2.49	0.46
1:2:19:A:H2'	1:2:20:G:O4'	2.14	0.46
1:2:316:G:H2'	1:2:317:C:C6	2.50	0.46
2:3:102:G:OP1	28:Z:65:TYR:HA	2.16	0.46
3:A:85:ARG:HD2	20:R:82:ASP:OD1	2.15	0.46
4:B:30:TRP:CE2	17:O:19:PRO:HG3	2.51	0.46
10:H:27:LEU:O	10:H:31:GLU:HG3	2.15	0.46
19:Q:131:LYS:HB2	19:Q:131:LYS:HE3	1.73	0.46
1:2:68:A:H2'	1:2:69:C:O4'	2.16	0.46
1:2:1086:G:O2'	1:2:1087:A:H5'	2.16	0.46
1:2:1580:A:H5''	23:U:59:LYS:NZ	2.30	0.46
1:2:1628:C:H2'	1:2:1629:C:C6	2.51	0.46
1:2:1833:C:OP1	1:2:1840:U:H4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:231:G:N2	2:3:237:C:C2	2.83	0.46
15:M:101:ARG:HG3	15:M:102:LYS:N	2.30	0.46
21:S:50:ILE:CD1	21:S:67:VAL:HG21	2.44	0.46
33:e:51:LYS:HA	33:e:51:LYS:HD2	1.64	0.46
1:2:481:C:H5''	1:2:482:G:OP2	2.16	0.46
1:2:1040:G:H5'	1:2:1041:G:OP2	2.16	0.46
1:2:1060:A:H4'	1:2:1061:U:O5'	2.16	0.46
2:3:231:G:N2	2:3:237:C:O2	2.49	0.46
7:E:23:LEU:HD12	7:E:23:LEU:HA	1.57	0.46
7:E:247:THR:HG23	7:E:250:GLU:OE2	2.16	0.46
8:F:167:LYS:NZ	8:F:175:ASP:OD2	2.49	0.46
22:T:21:PHE:CD2	22:T:134:ILE:HD11	2.51	0.46
1:2:171:A:C5'	9:G:177:GLN:HG2	2.42	0.46
1:2:1336:C:H2'	1:2:1337:C:O4'	2.16	0.46
4:B:31:TYR:CD2	4:B:94:LYS:HA	2.51	0.46
4:B:186:ASN:HA	4:B:189:ILE:HD12	1.98	0.46
7:E:77:ARG:HG2	7:E:82:TYR:CD2	2.50	0.46
7:E:199:GLU:HG3	7:E:207:VAL:HB	1.98	0.46
9:G:137:ARG:HD3	9:G:178:ARG:HH11	1.80	0.46
16:N:42:LYS:HE3	16:N:42:LYS:HB2	1.69	0.46
17:O:46:ASP:OD1	17:O:47:LEU:N	2.46	0.46
21:S:17:ASN:HD22	21:S:101:ASN:ND2	2.09	0.46
35:g:11:LEU:HB3	35:g:43:TRP:CZ2	2.51	0.46
35:g:19:THR:O	35:g:288:SER:HB2	2.16	0.46
35:g:110:SER:CB	35:g:153:CYS:HA	2.46	0.46
1:2:525:A:N7	1:2:587:A:C2	2.84	0.45
1:2:624:C:H41	26:X:63:ASN:HD22	1.64	0.45
1:2:1109:C:C4	20:R:126:MET:SD	3.09	0.45
1:2:1213:C:H42	1:2:1686:G:H1	1.63	0.45
1:2:1454:A:N7	20:R:3:ARG:HD2	2.31	0.45
1:2:1587:G:H1	22:T:67:ARG:CG	2.29	0.45
2:3:231:G:H5''	2:3:232:C:OP2	2.16	0.45
2:3:290:U:O2'	2:3:315:C:OP2	2.33	0.45
3:A:36:GLN:HE22	24:V:70:LEU:HD12	1.82	0.45
7:E:21:ASP:OD2	7:E:24:THR:OG1	2.24	0.45
7:E:44:LEU:HD21	7:E:70:ILE:HG21	1.98	0.45
9:G:59:GLN:HG3	9:G:72:ARG:HH22	1.78	0.45
10:H:116:ARG:HA	10:H:117:PRO:HD3	1.75	0.45
12:J:124:HIS:HD2	33:e:35:ARG:CZ	2.29	0.45
12:J:174:LYS:HE2	12:J:174:LYS:HB3	1.79	0.45
13:K:20:VAL:HA	13:K:69:TRP:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:26:ASP:HB3	13:K:29:MET:HB2	1.98	0.45
20:R:98:VAL:HG13	20:R:102:THR:HB	1.98	0.45
21:S:5:ILE:HG23	28:Z:50:PHE:O	2.16	0.45
22:T:31:PRO:HB2	22:T:34:VAL:HG23	1.97	0.45
1:2:72:C:O2'	1:2:73:C:H2'	2.16	0.45
1:2:658:U:H4'	1:2:659:G:O5'	2.16	0.45
1:2:917:U:O2'	1:2:918:U:O4'	2.35	0.45
1:2:1309:C:C4'	34:f:133:ALA:HB2	2.44	0.45
3:A:44:ASP:O	3:A:46:ILE:HG13	2.15	0.45
10:H:29:GLU:O	10:H:33:ASN:ND2	2.46	0.45
14:L:93:LEU:HB3	14:L:102:PHE:HB3	1.98	0.45
17:O:54:CYS:SG	17:O:84:ARG:HG2	2.57	0.45
22:T:60:THR:HG23	22:T:75:MET:SD	2.57	0.45
25:W:97:ARG:HB3	25:W:97:ARG:HH11	1.80	0.45
26:X:76:LYS:HG3	26:X:77:ASN:OD1	2.16	0.45
26:X:107:ARG:O	26:X:109:GLY:N	2.50	0.45
35:g:174:VAL:HB	35:g:188:HIS:HB2	1.98	0.45
1:2:981:A:H2'	1:2:982:G:C8	2.51	0.45
1:2:1225:U:H1'	19:Q:142:GLN:NE2	2.31	0.45
1:2:1443:C:H2'	1:2:1444:U:H5'	1.98	0.45
3:A:208:GLU:HG3	3:A:209:GLU:HG3	1.99	0.45
7:E:115:THR:HG22	7:E:117:GLU:HG2	1.98	0.45
7:E:126:VAL:HG22	7:E:158:ASP:O	2.15	0.45
7:E:184:THR:O	7:E:189:LEU:HD13	2.16	0.45
8:F:19:LEU:HG	8:F:20:PHE:HD1	1.81	0.45
10:H:133:LEU:O	10:H:173:PHE:HE1	2.00	0.45
12:J:50:LEU:HD23	12:J:51:ALA:N	2.30	0.45
26:X:37:LYS:HE2	26:X:37:LYS:HB3	1.86	0.45
26:X:67:ARG:HH21	26:X:114:ASP:CG	2.17	0.45
1:2:963:A:H2'	1:2:964:A:H8	1.77	0.45
7:E:179:ASN:ND2	7:E:231:GLY:H	2.15	0.45
9:G:6:SER:O	9:G:8:PRO:HD3	2.17	0.45
10:H:158:LEU:HD11	10:H:187:PHE:CD2	2.51	0.45
18:P:111:MET:HA	18:P:114:HIS:ND1	2.32	0.45
20:R:58:MET:O	20:R:62:GLN:HG2	2.16	0.45
28:Z:78:LYS:HA	28:Z:78:LYS:HD3	1.69	0.45
1:2:123:G:H5''	1:2:124:U:OP2	2.16	0.45
1:2:466:G:H1'	9:G:59:GLN:NE2	2.32	0.45
1:2:949:G:C6	1:2:950:C:C4	3.05	0.45
17:O:90:ILE:O	17:O:124:MET:HE1	2.16	0.45
18:P:108:LYS:HB3	18:P:109:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1289:U:H2'	1:2:1290:G:C8	2.52	0.45
1:2:1337:C:O2'	23:U:68:THR:HB	2.17	0.45
1:2:1394:G:H21	1:2:1475:G:H1'	1.81	0.45
1:2:1858:G:OP1	29:a:20:PRO:HG3	2.17	0.45
7:E:55:ALA:HB1	7:E:60:GLU:HB2	1.98	0.45
7:E:235:TRP:N	7:E:235:TRP:CD1	2.85	0.45
7:E:248:ILE:H	7:E:248:ILE:HG13	1.48	0.45
8:F:73:THR:O	8:F:89:THR:HG21	2.16	0.45
9:G:131:ARG:CG	38:w:80:ARG:NH1	2.80	0.45
12:J:111:GLN:CD	12:J:127:ARG:HB2	2.42	0.45
13:K:76:ILE:HD13	13:K:91:PRO:HG3	1.99	0.45
18:P:37:TYR:HB3	18:P:41:GLN:HB2	1.99	0.45
1:2:913:A:H2	10:H:98:ARG:HA	1.82	0.45
1:2:933:G:H2'	1:2:993:G:N2	2.31	0.45
1:2:1245:G:O2'	1:2:1492:U:OP1	2.34	0.45
1:2:1358:U:OP1	5:C:114:LYS:HB2	2.16	0.45
1:2:1451:G:OP1	20:R:32:LYS:HE2	2.16	0.45
1:2:1583:C:H2'	1:2:1584:G:N7	2.31	0.45
1:2:1657:G:H1	1:2:1667:U:H3	1.64	0.45
4:B:181:LEU:O	4:B:185:VAL:HG23	2.17	0.45
7:E:151:ASP:HA	7:E:152:PRO:HD3	1.81	0.45
11:I:87:ASN:HD22	11:I:88:ASN:N	2.14	0.45
14:L:12:LYS:O	14:L:56:ILE:HD13	2.17	0.45
18:P:122:THR:HG22	18:P:123:TYR:HD2	1.82	0.45
20:R:32:LYS:HG2	20:R:47:ARG:HH21	1.82	0.45
21:S:39:ARG:NH2	22:T:38:LYS:HG3	2.32	0.45
22:T:80:GLY:HA2	22:T:92:PHE:HE1	1.80	0.45
35:g:20:GLN:HG3	35:g:68:ASP:CG	2.42	0.45
1:2:66:G:OP2	1:2:82:G:N2	2.44	0.45
1:2:78:C:OP1	9:G:173:ALA:HB3	2.17	0.45
1:2:373:G:OP1	14:L:135:SER:OG	2.35	0.45
1:2:615:C:H2'	1:2:616:A:C8	2.52	0.45
1:2:1043:G:H2'	1:2:1044:G:O4'	2.16	0.45
1:2:1334:G:H22	1:2:1496:U:H3	1.65	0.45
1:2:1642:U:H2'	1:2:1643:U:C6	2.52	0.45
1:2:1656:G:H2'	1:2:1657:G:H8	1.82	0.45
2:3:256:G:H5'	2:3:257:A:H2'	1.97	0.45
9:G:32:MET:HA	9:G:52:ILE:HG22	1.98	0.45
12:J:142:VAL:HG12	12:J:144:ILE:H	1.82	0.45
25:W:11:LEU:HD13	25:W:72:CYS:SG	2.57	0.45
25:W:46:TYR:HB3	25:W:69:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:b:42:LYS:HA	30:b:42:LYS:HD2	1.84	0.45
1:2:590:A:H3'	1:2:590:A:P	2.57	0.45
1:2:922:A:C2'	1:2:923:G:H5'	2.47	0.45
1:2:1448:A:H2'	1:2:1449:G:O4'	2.17	0.45
1:2:1671:G:H2'	1:2:1672:U:H6	1.82	0.45
1:2:1674:G:OP1	8:F:51:HIS:NE2	2.50	0.45
4:B:110:MET:HE1	4:B:213:ARG:HB2	1.98	0.45
10:H:53:VAL:HG21	10:H:172:THR:HA	1.99	0.45
12:J:13:TYR:CD1	12:J:13:TYR:C	2.95	0.45
20:R:130:THR:HA	20:R:131:PRO:HD3	1.79	0.45
21:S:3:LEU:HD23	21:S:3:LEU:HA	1.81	0.45
23:U:94:PRO:HG2	23:U:97:ILE:HG13	1.99	0.45
2:3:142:A:H2'	2:3:143:G:C8	2.52	0.45
10:H:18:GLU:O	10:H:21:SER:OG	2.33	0.45
1:2:104:A:OP1	11:I:12:ARG:NE	2.50	0.44
1:2:528:A:C2	1:2:558:G:C2	3.06	0.44
1:2:604:A:O2'	1:2:605:A:H5'	2.17	0.44
1:2:655:A:H4'	1:2:656:G:H3'	1.99	0.44
1:2:1015:U:P	30:b:20:LYS:HZ1	2.39	0.44
1:2:1239:U:H5''	18:P:124:LYS:HD3	1.99	0.44
5:C:157:LEU:HD12	5:C:157:LEU:HA	1.70	0.44
7:E:170:THR:OG1	7:E:171:ASP:N	2.50	0.44
11:I:146:GLN:O	11:I:150:ASP:HB2	2.17	0.44
16:N:34:LYS:HE3	16:N:67:THR:HB	1.98	0.44
28:Z:66:LYS:H	28:Z:111:ARG:HD3	1.82	0.44
35:g:83:TRP:C	35:g:85:GLY:H	2.24	0.44
1:2:181:A:H2'	1:2:182:C:H2'	1.98	0.44
1:2:536:A:H2'	1:2:536:A:N3	2.33	0.44
1:2:674:C:O2	1:2:1031:A:N1	2.50	0.44
3:A:81:ASN:HA	3:A:84:GLN:CG	2.47	0.44
4:B:83:LYS:HE2	4:B:83:LYS:HB3	1.82	0.44
6:D:175:VAL:CG1	6:D:182:LEU:HB2	2.46	0.44
10:H:130:LEU:HB2	10:H:177:TYR:CE1	2.51	0.44
12:J:119:LEU:HB3	12:J:159:PHE:HE1	1.82	0.44
13:K:36:ALA:C	13:K:38:LYS:H	2.25	0.44
15:M:64:LEU:HD11	34:f:103:LEU:HA	1.98	0.44
18:P:44:ARG:NH2	18:P:83:MET:HA	2.32	0.44
25:W:69:LEU:HD21	25:W:72:CYS:HB2	1.99	0.44
1:2:28:U:H2'	1:2:29:G:C8	2.52	0.44
1:2:488:U:H3'	1:2:489:A:H5'	2.00	0.44
1:2:926:A:H5'	1:2:926:A:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1499:U:H2'	1:2:1500:G:H8	1.82	0.44
1:2:1791:A:H2'	1:2:1792:G:O4'	2.17	0.44
1:2:1852:C:H2'	1:2:1853:C:H6	1.83	0.44
6:D:72:VAL:HG13	13:K:68:TYR:CE2	2.53	0.44
10:H:133:LEU:HD12	10:H:133:LEU:HA	1.66	0.44
11:I:11:ARG:NH1	11:I:15:GLY:O	2.37	0.44
19:Q:100:VAL:HG12	19:Q:101:ASP:H	1.83	0.44
30:b:43:ILE:HD12	30:b:43:ILE:HA	1.81	0.44
33:e:52:LYS:HE2	33:e:52:LYS:HB3	1.86	0.44
35:g:249:CYS:SG	35:g:258:ILE:HG12	2.58	0.44
38:w:76:UNK:O	38:w:76:UNK:HG2	2.18	0.44
1:2:221:A:H2'	1:2:222:U:H6	1.82	0.44
1:2:1630:A:OP2	21:S:39:ARG:HB3	2.17	0.44
25:W:83:LEU:HD12	25:W:83:LEU:HA	1.62	0.44
35:g:89:LEU:HB3	35:g:99:ARG:HB2	1.99	0.44
1:2:1073:U:H2'	1:2:1074:C:H6	1.82	0.44
1:2:1100:A:C2	1:2:1101:U:C2	3.05	0.44
11:I:27:TYR:HB3	11:I:49:ARG:NH2	2.32	0.44
15:M:68:LEU:HD23	34:f:114:ILE:HD13	2.00	0.44
20:R:29:HIS:HA	20:R:32:LYS:HB3	1.99	0.44
35:g:177:TRP:CZ3	35:g:184:LEU:HB2	2.52	0.44
1:2:60:A:H2	1:2:61:A:N3	2.15	0.44
1:2:1453:C:O3'	20:R:49:LYS:HG2	2.17	0.44
1:2:1856:C:H2'	1:2:1857:G:C8	2.53	0.44
2:3:330:A:O2'	2:3:331:G:H2'	2.17	0.44
3:A:68:ILE:HD13	3:A:120:ARG:HB3	1.99	0.44
3:A:200:ASP:HA	3:A:203:PHE:CE2	2.53	0.44
5:C:125:LYS:HA	5:C:142:LYS:O	2.18	0.44
6:D:16:ILE:HD13	32:d:22:ARG:NH2	2.33	0.44
6:D:96:LEU:CD1	6:D:198:ILE:HG21	2.43	0.44
9:G:21:GLU:O	9:G:25:ARG:HG2	2.18	0.44
9:G:145:PHE:CD2	9:G:156:TYR:HB3	2.52	0.44
13:K:47:LYS:HE3	13:K:50:GLN:OE1	2.18	0.44
19:Q:85:ARG:HE	19:Q:119:LEU:HD21	1.83	0.44
21:S:82:TRP:CZ2	22:T:36:THR:HG21	2.52	0.44
30:b:30:SER:HB3	30:b:49:HIS:CD2	2.53	0.44
33:e:13:ARG:HG2	33:e:13:ARG:NH1	2.33	0.44
1:2:963:A:P	17:O:65:ASP:HB2	2.57	0.44
1:2:1192:U:OP2	26:X:119:ARG:NH2	2.47	0.44
1:2:1563:G:OP1	22:T:115:LYS:HE3	2.17	0.44
1:2:1599:U:N3	8:F:166:ILE:HD12	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1670:C:H2'	1:2:1671:G:C8	2.52	0.44
1:2:1672:U:H2'	1:2:1673:U:C6	2.52	0.44
1:2:1866:A:N6	29:a:84:VAL:HG13	2.33	0.44
2:3:95:U:C2'	2:3:96:A:H5'	2.48	0.44
3:A:70:ASN:HB3	3:A:73:ASP:OD2	2.18	0.44
4:B:225:LEU:O	4:B:229:MET:HG2	2.17	0.44
5:C:167:ARG:HB2	5:C:177:PRO:HB2	2.00	0.44
6:D:72:VAL:HG22	13:K:20:VAL:HG11	1.99	0.44
11:I:8:TRP:NE1	11:I:22:HIS:HE1	2.16	0.44
12:J:48:PHE:CZ	12:J:52:LYS:HE3	2.53	0.44
31:c:32:VAL:HB	31:c:42:ILE:O	2.18	0.44
1:2:72:C:N4	1:2:79:A:N7	2.60	0.44
1:2:1630:A:H5'	21:S:37:GLY:N	2.33	0.44
3:A:5:LEU:HD21	24:V:41:LYS:HA	2.00	0.44
4:B:198:GLU:HB2	4:B:210:VAL:CG1	2.42	0.44
14:L:6:THR:HG23	14:L:7:GLU:HG2	2.00	0.44
14:L:61:PRO:HA	14:L:66:VAL:CG2	2.47	0.44
17:O:74:ALA:HB1	17:O:115:ALA:HB2	1.99	0.44
21:S:63:GLU:HA	21:S:66:ARG:HG2	2.00	0.44
25:W:47:ILE:HG12	25:W:48:GLY:N	2.33	0.44
1:2:475:C:O2'	1:2:507:G:N3	2.48	0.44
1:2:1611:G:N2	1:2:1629:C:O2	2.51	0.44
2:3:61:U:HO2'	2:3:62:C:P	2.39	0.44
2:3:245:G:OP1	2:3:245:G:C8	2.70	0.44
3:A:110:ASN:CG	3:A:113:GLN:HE21	2.26	0.44
3:A:208:GLU:HG3	3:A:209:GLU:N	2.32	0.44
4:B:38:MET:HB3	4:B:38:MET:HE2	1.57	0.44
5:C:233:LEU:HD12	5:C:233:LEU:HA	1.52	0.44
8:F:136:ARG:HH11	8:F:199:VAL:HG11	1.82	0.44
11:I:97:VAL:HG23	11:I:98:LYS:O	2.18	0.44
11:I:193:LYS:HA	11:I:196:GLU:OE1	2.18	0.44
12:J:81:LEU:HD23	12:J:81:LEU:HA	1.77	0.44
13:K:46:MET:HE2	13:K:46:MET:HB3	1.90	0.44
1:2:70:G:H2'	1:2:71:G:O4'	2.16	0.43
1:2:494:C:N4	1:2:509:G:H21	2.16	0.43
1:2:533:A:C6	1:2:534:G:C5	3.06	0.43
1:2:958:G:C6	1:2:959:G:C2	3.06	0.43
1:2:1270:G:OP2	34:f:86:THR:HG21	2.18	0.43
1:2:1464:C:H2'	1:2:1465:A:C8	2.53	0.43
3:A:91:ALA:O	3:A:95:GLY:N	2.50	0.43
4:B:63:LYS:HE3	4:B:89:GLU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:188:LEU:HD23	4:B:188:LEU:HA	1.76	0.43
6:D:79:PHE:HE1	6:D:84:VAL:HB	1.80	0.43
9:G:45:TRP:CD1	9:G:45:TRP:H	2.35	0.43
9:G:151:ASP:CG	38:w:105:ARG:HD2	2.42	0.43
12:J:161:LEU:O	12:J:167:GLY:HA3	2.17	0.43
14:L:82:MET:HE2	14:L:85:THR:OG1	2.18	0.43
20:R:77:GLU:HG3	20:R:81:ARG:HE	1.83	0.43
20:R:121:GLN:HA	20:R:122:PRO:HD2	1.85	0.43
22:T:112:MET:HE2	22:T:112:MET:HB3	1.87	0.43
27:Y:20:ARG:HD3	27:Y:76:TYR:HE1	1.83	0.43
29:a:22:ARG:HD2	29:a:27:ALA:O	2.18	0.43
1:2:60:A:HO2'	1:2:61:A:P	2.41	0.43
1:2:360:A:C2	1:2:362:C:C2	3.05	0.43
1:2:749:U:O4	1:2:750:C:N4	2.51	0.43
1:2:1530:U:H2'	1:2:1531:A:O4'	2.18	0.43
1:2:1677:U:H2'	1:2:1678:A:H8	1.84	0.43
3:A:69:GLU:HB2	5:C:270:THR:HG21	1.99	0.43
4:B:168:MET:O	4:B:172:MET:HG2	2.17	0.43
18:P:60:LEU:HD22	18:P:92:SER:OG	2.17	0.43
21:S:81:ASP:O	21:S:87:GLN:NE2	2.49	0.43
21:S:108:ARG:O	21:S:112:GLU:HG2	2.18	0.43
22:T:62:ARG:HA	22:T:65:TYR:HB3	2.01	0.43
35:g:302:TYR:HE2	35:g:308:ARG:HB2	1.83	0.43
36:h:23:ARG:HD2	36:h:23:ARG:HA	1.84	0.43
1:2:551:U:HO2'	33:e:44:ASN:ND2	2.12	0.43
1:2:1272:C:N4	1:2:1510:G:H1	2.16	0.43
2:3:45:C:O2	2:3:118:G:N2	2.50	0.43
3:A:41:ARG:HB2	3:A:47:TYR:CD1	2.53	0.43
4:B:42:ARG:HD3	4:B:42:ARG:HA	1.71	0.43
5:C:270:THR:O	5:C:274:VAL:HG23	2.18	0.43
6:D:69:LEU:O	6:D:73:VAL:HG23	2.18	0.43
8:F:56:TYR:CD1	8:F:66:CYS:HB3	2.53	0.43
11:I:196:GLU:HG2	11:I:197:PHE:N	2.33	0.43
14:L:17:PHE:CE1	14:L:19:ASN:HB2	2.52	0.43
21:S:123:LEU:HD22	21:S:127:TRP:CZ2	2.53	0.43
28:Z:48:VAL:HG22	28:Z:80:ARG:HH11	1.83	0.43
29:a:43:ASN:OD1	29:a:43:ASN:N	2.50	0.43
1:2:126:G:H1'	1:2:180:G:N2	2.32	0.43
1:2:395:G:H5'	14:L:82:MET:SD	2.59	0.43
1:2:1065:G:H2'	1:2:1066:U:C6	2.53	0.43
6:D:3:VAL:HG12	6:D:4:GLN:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:185:LEU:HD12	9:G:185:LEU:HA	1.76	0.43
14:L:80:MET:H	14:L:80:MET:HG3	1.66	0.43
20:R:71:ILE:O	20:R:75:GLU:HG2	2.19	0.43
28:Z:62:VAL:HA	28:Z:65:TYR:HD2	1.84	0.43
1:2:72:C:C4	1:2:73:C:N4	2.87	0.43
1:2:919:A:OP1	16:N:20:ARG:NE	2.52	0.43
1:2:1374:C:O2'	1:2:1464:C:O2	2.29	0.43
1:2:1598:G:OP2	1:2:1598:G:H8	2.00	0.43
7:E:189:LEU:HD12	7:E:190:GLY:N	2.34	0.43
8:F:19:LEU:HB3	8:F:23:TRP:HB2	2.00	0.43
9:G:93:LYS:HE2	9:G:93:LYS:HB2	1.72	0.43
13:K:85:LEU:HA	13:K:86:PRO:HD3	1.87	0.43
19:Q:32:ILE:HD11	19:Q:63:PHE:HD1	1.82	0.43
21:S:48:ALA:HB2	21:S:70:ILE:HD12	2.00	0.43
21:S:130:ARG:HD2	21:S:134:GLN:OE1	2.18	0.43
22:T:80:GLY:HA2	22:T:92:PHE:CE1	2.53	0.43
23:U:55:ARG:HB3	23:U:87:ARG:HH11	1.83	0.43
25:W:111:MET:HE2	25:W:111:MET:HB3	1.86	0.43
27:Y:104:ARG:NH2	27:Y:108:LYS:HE2	2.33	0.43
1:2:84:A:O3'	27:Y:119:GLY:HA2	2.18	0.43
1:2:294:U:O4	14:L:65:ASN:HB2	2.19	0.43
1:2:339:A:H2'	1:2:340:C:C5	2.54	0.43
1:2:842:C:C2'	1:2:843:C:H5'	2.49	0.43
1:2:1440:C:HO2'	1:2:1441:U:P	2.40	0.43
1:2:1831:A:O2'	1:2:1852:C:H5'	2.19	0.43
7:E:176:ASP:OD1	7:E:177:THR:N	2.52	0.43
11:I:121:LEU:HD23	11:I:121:LEU:HA	1.84	0.43
16:N:25:TRP:CD1	30:b:82:LYS:HZ2	2.35	0.43
16:N:91:LEU:HD23	16:N:91:LEU:HA	1.72	0.43
16:N:119:GLU:O	16:N:122:ILE:HB	2.18	0.43
20:R:5:ARG:HB3	20:R:9:VAL:HG11	1.99	0.43
21:S:107:LEU:O	21:S:111:LEU:HG	2.18	0.43
29:a:24:THR:HG21	29:a:71:LEU:HD22	2.00	0.43
35:g:142:VAL:HG11	35:g:177:TRP:CZ3	2.52	0.43
1:2:60:A:C2	1:2:61:A:C2	3.07	0.43
1:2:796:G:C6	1:2:797:C:C2	3.07	0.43
1:2:926:A:C8	1:2:926:A:H5'	2.54	0.43
1:2:984:C:O2'	17:O:138:ASP:HB3	2.19	0.43
1:2:1073:U:H2'	1:2:1074:C:C6	2.54	0.43
1:2:1271:C:H5'	1:2:1301:A:C2	2.52	0.43
1:2:1277:C:H5'	13:K:54:SER:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1287:A:C6	1:2:1288:U:C2	3.06	0.43
1:2:1341:C:H4'	1:2:1342:U:H5'	2.00	0.43
1:2:1398:G:C4	35:g:63:SER:HB3	2.54	0.43
1:2:1542:C:O2'	1:2:1543:U:OP1	2.30	0.43
2:3:334:C:H41	29:a:47:ALA:HB3	1.83	0.43
3:A:102:ARG:HG2	3:A:102:ARG:HH11	1.84	0.43
16:N:70:LYS:HE2	16:N:70:LYS:HB3	1.58	0.43
20:R:41:ILE:HD12	20:R:41:ILE:O	2.17	0.43
28:Z:62:VAL:HA	28:Z:65:TYR:CD2	2.54	0.43
31:c:12:ALA:O	31:c:55:VAL:HA	2.18	0.43
35:g:213:ASP:OD1	35:g:213:ASP:N	2.51	0.43
35:g:252:THR:HG22	35:g:254:PRO:HD2	2.00	0.43
1:2:986:G:N2	17:O:135:ILE:HD11	2.34	0.43
1:2:1009:A:H5'	16:N:94:LYS:HE2	2.00	0.43
1:2:1522:A:N1	18:P:131:PRO:HD3	2.34	0.43
1:2:1692:U:H2'	1:2:1693:G:H8	1.82	0.43
3:A:31:ASP:OD1	3:A:32:PHE:N	2.52	0.43
4:B:113:MET:HE2	4:B:142:PHE:HE1	1.83	0.43
7:E:9:LEU:HD12	7:E:9:LEU:HA	1.63	0.43
12:J:28:GLU:HB2	12:J:40:LYS:HZ3	1.84	0.43
15:M:51:VAL:HB	15:M:109:VAL:HB	2.00	0.43
23:U:78:ASP:OD2	32:d:44:ARG:NE	2.37	0.43
25:W:106:THR:HB	25:W:122:GLY:O	2.19	0.43
1:2:555:A:OP2	33:e:25:LYS:NZ	2.52	0.43
1:2:958:G:O2'	1:2:959:G:O4'	2.28	0.43
1:2:1118:C:H3'	1:2:1119:A:H5''	2.01	0.43
1:2:1440:C:HO2'	1:2:1441:U:C5'	2.29	0.43
1:2:1608:U:H5''	21:S:130:ARG:CD	2.49	0.43
1:2:1859:A:N6	1:2:1860:A:N6	2.67	0.43
2:3:258:G:N2	2:3:273:G:H2'	2.34	0.43
13:K:32:HIS:ND1	13:K:42:ASN:OD1	2.51	0.43
14:L:40:ILE:HD12	14:L:41:GLY:H	1.83	0.43
14:L:96:ILE:HD11	14:L:103:GLU:OE2	2.19	0.43
20:R:21:TYR:CE2	20:R:73:LEU:HD23	2.54	0.43
20:R:111:PHE:C	20:R:113:SER:H	2.27	0.43
22:T:114:GLU:HB2	22:T:124:THR:CG2	2.49	0.43
35:g:131:LEU:HD12	35:g:140:TYR:HB3	2.00	0.43
1:2:99:A:H8	1:2:99:A:O5'	2.01	0.43
1:2:221:A:H2'	1:2:222:U:C6	2.54	0.43
1:2:958:G:N1	1:2:959:G:C6	2.87	0.43
1:2:1425:G:O2'	1:2:1426:U:OP1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1566:G:H4'	1:2:1566:G:OP1	2.19	0.43
1:2:1731:A:H2'	1:2:1732:G:H8	1.82	0.43
2:3:47:G:O2'	2:3:48:U:O5'	2.34	0.43
4:B:87:ILE:O	4:B:98:THR:HA	2.19	0.43
5:C:144:SER:HB3	5:C:150:ALA:HB2	2.00	0.43
10:H:12:ASN:OD1	10:H:12:ASN:N	2.52	0.43
12:J:13:TYR:CE2	12:J:41:ARG:HD2	2.54	0.43
20:R:43:SER:HB3	20:R:44:LYS:H	1.49	0.43
21:S:3:LEU:N	28:Z:90:GLU:OE2	2.52	0.43
32:d:19:ARG:O	32:d:27:ARG:HG2	2.19	0.43
36:h:7:LYS:HE2	36:h:11:ARG:NH2	2.34	0.43
1:2:342:C:H5'	1:2:343:A:OP2	2.19	0.42
3:A:57:LYS:HD2	3:A:57:LYS:HA	1.80	0.42
4:B:137:LEU:HD22	4:B:215:VAL:HG22	2.01	0.42
10:H:138:GLU:OE2	16:N:21:SER:OG	2.35	0.42
11:I:25:ARG:HD3	11:I:25:ARG:HA	1.62	0.42
12:J:28:GLU:HB2	12:J:40:LYS:NZ	2.34	0.42
12:J:134:HIS:ND1	12:J:163:SER:HB2	2.33	0.42
14:L:18:GLN:H	14:L:18:GLN:HG2	1.50	0.42
20:R:17:ILE:HA	20:R:24:LEU:HD11	2.00	0.42
21:S:83:PHE:CE2	22:T:36:THR:HG23	2.54	0.42
23:U:28:ASN:ND2	23:U:30:LYS:HB2	2.34	0.42
29:a:73:TYR:CB	29:a:78:VAL:HG22	2.44	0.42
35:g:62:HIS:CD2	35:g:66:VAL:HG22	2.54	0.42
1:2:441:C:H2'	1:2:442:C:C6	2.55	0.42
1:2:657:U:O2'	1:2:658:U:OP2	2.27	0.42
1:2:1016:U:OP2	16:N:14:SER:HA	2.18	0.42
1:2:1478:U:H2'	1:2:1479:G:H8	1.79	0.42
1:2:1720:U:H5''	1:2:1721:U:OP2	2.19	0.42
1:2:1730:U:H2'	1:2:1731:A:O4'	2.20	0.42
3:A:16:LEU:HD23	3:A:16:LEU:HA	1.67	0.42
3:A:37:TYR:OH	3:A:57:LYS:NZ	2.39	0.42
3:A:147:LEU:HD13	3:A:161:ILE:HB	2.00	0.42
10:H:101:LEU:HD23	10:H:101:LEU:HA	1.89	0.42
10:H:169:LYS:C	10:H:172:THR:HG22	2.45	0.42
11:I:4:SER:HB3	11:I:24:LYS:HD3	2.00	0.42
12:J:124:HIS:CD2	33:e:35:ARG:CZ	3.02	0.42
17:O:119:LEU:O	17:O:124:MET:HB2	2.18	0.42
18:P:94:VAL:O	18:P:105:VAL:HB	2.19	0.42
20:R:77:GLU:HG3	20:R:81:ARG:NE	2.34	0.42
22:T:6:VAL:HB	22:T:65:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:47:MET:HB2	27:Y:48:TYR:CD1	2.54	0.42
28:Z:88:LEU:HD12	28:Z:88:LEU:HA	1.87	0.42
35:g:110:SER:OG	35:g:153:CYS:HA	2.18	0.42
1:2:71:G:H1'	1:2:79:A:H62	1.84	0.42
1:2:1348:G:C8	1:2:1349:G:C8	3.07	0.42
1:2:1453:C:N4	1:2:1455:A:H1'	2.34	0.42
1:2:1464:C:H2'	1:2:1465:A:H8	1.84	0.42
1:2:1515:G:H21	18:P:99:GLY:CA	2.32	0.42
1:2:1623:A:H5''	21:S:132:ARG:O	2.19	0.42
2:3:129:C:H2'	2:3:130:C:C6	2.54	0.42
3:A:58:LEU:HD23	3:A:58:LEU:HA	1.81	0.42
4:B:136:ARG:C	4:B:137:LEU:HD23	2.45	0.42
7:E:68:ARG:HB3	7:E:76:VAL:HG11	2.02	0.42
12:J:25:LEU:HA	12:J:40:LYS:HZ1	1.84	0.42
25:W:30:CYS:HB2	25:W:61:ILE:HD11	2.01	0.42
1:2:1271:C:H2'	1:2:1272:C:C6	2.54	0.42
1:2:1326:U:H4'	1:2:1327:G:O5'	2.20	0.42
1:2:1445:U:O4	1:2:1446:A:N6	2.52	0.42
1:2:1534:C:H5'	1:2:1536:G:O4'	2.19	0.42
1:2:1566:G:O6	22:T:97:LYS:HB2	2.19	0.42
1:2:1599:U:C4	8:F:166:ILE:HG23	2.54	0.42
4:B:86:LEU:HB3	4:B:98:THR:HG22	2.00	0.42
5:C:120:GLN:H	5:C:120:GLN:HG2	1.66	0.42
7:E:75:LYS:HB2	7:E:77:ARG:NH1	2.35	0.42
15:M:95:ASP:HB2	15:M:99:LYS:HB2	2.00	0.42
25:W:87:GLU:HG2	25:W:117:ARG:NH2	2.34	0.42
27:Y:100:LYS:NZ	27:Y:107:ARG:HD3	2.35	0.42
31:c:44:ARG:NH2	31:c:60:GLU:O	2.47	0.42
1:2:123:G:N2	1:2:342:C:C2	2.87	0.42
1:2:152:U:H4'	9:G:132:ARG:NH1	2.35	0.42
1:2:220:U:H2'	1:2:221:A:H8	1.83	0.42
1:2:638:C:O2'	1:2:639:C:P	2.77	0.42
1:2:1120:U:H3'	1:2:1121:G:H5''	2.00	0.42
1:2:1466:G:H2'	1:2:1467:C:C6	2.54	0.42
1:2:1728:U:H5'	1:2:1729:U:OP2	2.19	0.42
6:D:138:VAL:HG22	6:D:184:ILE:HG22	2.00	0.42
6:D:169:ASP:OD2	6:D:190:LEU:HD21	2.19	0.42
6:D:221:THR:O	6:D:223:ILE:HG13	2.19	0.42
17:O:106:LYS:NZ	17:O:136:PRO:HD2	2.33	0.42
19:Q:24:HIS:O	19:Q:68:ILE:HA	2.20	0.42
23:U:30:LYS:HD3	23:U:30:LYS:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:808:A:O2'	1:2:809:A:C8	2.72	0.42
1:2:1052:A:H2'	1:2:1053:C:O4'	2.18	0.42
1:2:1159:G:H2'	1:2:1160:U:O4'	2.20	0.42
1:2:1273:C:C2	1:2:1506:A:C6	3.07	0.42
1:2:1443:C:C2'	1:2:1444:U:H5'	2.50	0.42
1:2:1657:G:O2'	32:d:33:LYS:NZ	2.52	0.42
9:G:56:ASN:HB2	9:G:108:VAL:HB	2.01	0.42
12:J:102:ILE:HA	12:J:102:ILE:HD13	1.58	0.42
17:O:95:ILE:HD12	17:O:116:LEU:HD21	2.01	0.42
17:O:106:LYS:HZ3	17:O:135:ILE:HG13	1.85	0.42
17:O:142:ARG:HG2	17:O:142:ARG:NH1	2.33	0.42
20:R:74:GLN:O	20:R:78:ARG:HB2	2.19	0.42
29:a:10:ARG:HB3	29:a:34:LYS:HB2	2.01	0.42
34:f:133:ALA:O	34:f:139:HIS:HA	2.20	0.42
35:g:64:HIS:HB2	35:g:84:ASP:HB3	2.00	0.42
35:g:83:TRP:C	35:g:85:GLY:N	2.77	0.42
1:2:446:G:OP1	11:I:50:GLY:N	2.48	0.42
1:2:1568:C:OP2	22:T:98:SER:HB3	2.20	0.42
1:2:1712:A:H2'	1:2:1713:C:H6	1.85	0.42
1:2:1725:U:C2	1:2:1726:G:C8	3.07	0.42
6:D:51:LEU:HB3	6:D:91:VAL:HG22	2.02	0.42
9:G:134:GLY:HA2	38:w:82:ILE:HD13	2.02	0.42
1:2:336:A:H2'	1:2:337:C:O4'	2.20	0.42
1:2:408:A:C2'	1:2:409:C:O5'	2.67	0.42
1:2:465:A:H4'	1:2:466:G:O5'	2.20	0.42
1:2:1622:U:N3	18:P:122:THR:OG1	2.27	0.42
1:2:1660:C:OP2	32:d:19:ARG:NH2	2.53	0.42
2:3:70:A:C3'	2:3:71:G:H5'	2.44	0.42
9:G:131:ARG:HG2	38:w:80:ARG:NH1	2.35	0.42
16:N:75:LEU:HD12	16:N:75:LEU:HA	1.71	0.42
25:W:66:THR:HG22	25:W:68:ARG:HG3	2.02	0.42
32:d:8:TRP:CH2	32:d:12:ARG:NH1	2.88	0.42
35:g:18:VAL:O	35:g:287:THR:HB	2.20	0.42
35:g:149:GLU:HB3	35:g:170:TRP:HB2	2.02	0.42
1:2:1134:G:H2'	1:2:1135:C:H6	1.84	0.42
1:2:1528:G:H2'	1:2:1529:C:C6	2.54	0.42
1:2:1568:C:O2	1:2:1627:C:O2'	2.38	0.42
1:2:1660:C:P	32:d:19:ARG:HH22	2.43	0.42
3:A:126:ASP:HA	3:A:127:PRO:HD2	1.85	0.42
14:L:104:LYS:O	14:L:105:ARG:HG3	2.19	0.42
17:O:34:PHE:CD1	17:O:34:PHE:C	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:64:LYS:HA	18:P:73:PRO:HB3	2.01	0.42
22:T:42:HIS:HB3	22:T:93:SER:HB2	2.01	0.42
29:a:21:ILE:O	29:a:21:ILE:HG12	2.20	0.42
33:e:8:ARG:HH11	33:e:8:ARG:CG	2.32	0.42
1:2:60:A:C2	1:2:61:A:C4	3.07	0.42
1:2:1097:G:H4'	3:A:32:PHE:CD1	2.55	0.42
1:2:1159:G:OP2	26:X:5:ARG:NH1	2.53	0.42
1:2:1520:G:H5''	21:S:136:THR:H	1.84	0.42
1:2:1594:A:O2'	22:T:16:ARG:NH2	2.53	0.42
1:2:1606:G:O2'	1:2:1633:A:N6	2.53	0.42
1:2:1669:G:OP1	19:Q:132:PHE:N	2.53	0.42
8:F:201:LYS:O	8:F:204:ARG:HG3	2.20	0.42
9:G:48:TYR:CZ	9:G:116:LYS:HG3	2.55	0.42
11:I:172:LEU:HA	11:I:172:LEU:HD23	1.78	0.42
13:K:15:LEU:HD23	13:K:79:LEU:HD11	2.01	0.42
25:W:66:THR:C	25:W:68:ARG:H	2.27	0.42
28:Z:51:ASP:OD1	28:Z:52:LYS:N	2.53	0.42
1:2:76:U:H5'	9:G:159:ARG:NH2	2.23	0.41
1:2:1220:A:N6	1:2:1221:G:C6	2.88	0.41
1:2:1264:C:N3	1:2:1265:A:N6	2.67	0.41
1:2:1865:C:H4'	1:2:1866:A:OP2	2.20	0.41
2:3:159:G:C2	2:3:160:U:C4	3.07	0.41
12:J:161:LEU:H	12:J:161:LEU:HG	1.36	0.41
14:L:45:LYS:HD3	14:L:45:LYS:H	1.84	0.41
17:O:75:MET:HE3	17:O:75:MET:HB3	1.67	0.41
21:S:16:LEU:HD21	21:S:72:GLN:NE2	2.29	0.41
26:X:7:LEU:C	26:X:9:THR:N	2.78	0.41
27:Y:6:THR:O	27:Y:27:VAL:HA	2.20	0.41
29:a:78:VAL:HG13	29:a:83:VAL:HB	1.99	0.41
35:g:162:ASN:HD21	35:g:178:ASN:ND2	2.18	0.41
35:g:164:ILE:HG23	35:g:176:VAL:HG13	2.02	0.41
1:2:403:G:C4	1:2:404:G:C8	3.08	0.41
1:2:1401:A:N6	1:2:1441:U:O2'	2.53	0.41
1:2:1648:G:H1'	1:2:1649:U:OP2	2.19	0.41
1:2:1691:U:H2'	1:2:1692:U:O4'	2.21	0.41
3:A:74:VAL:O	3:A:96:ALA:HB1	2.20	0.41
4:B:207:LEU:HA	4:B:207:LEU:HD23	1.73	0.41
4:B:213:ARG:HD2	4:B:214:LYS:HB2	2.02	0.41
6:D:133:GLY:HA3	6:D:156:LEU:O	2.21	0.41
13:K:3:MET:HE2	13:K:44:HIS:HD2	1.85	0.41
17:O:40:THR:HG21	17:O:111:GLY:HA3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:29:HIS:CD2	27:Y:29:HIS:N	2.88	0.41
29:a:67:LEU:HD12	29:a:68:TYR:N	2.35	0.41
35:g:40:ILE:HD11	35:g:80:SER:HB3	2.01	0.41
38:w:81:ALA:HB1	38:w:86:SER:HA	2.01	0.41
1:2:3:C:H5''	5:C:224:THR:O	2.20	0.41
1:2:551:U:H5'	33:e:43:VAL:HG11	2.02	0.41
1:2:748:C:O2'	1:2:749:U:OP1	2.33	0.41
1:2:1222:G:C6	1:2:1223:A:C6	3.07	0.41
1:2:1563:G:C6	1:2:1564:C:C4	3.09	0.41
4:B:62:LEU:O	4:B:65:ARG:HD2	2.20	0.41
4:B:117:TRP:CE2	4:B:152:LYS:HE2	2.55	0.41
5:C:121:ARG:HH22	5:C:123:ARG:CZ	2.32	0.41
7:E:238:LEU:HA	7:E:238:LEU:HD12	1.76	0.41
12:J:103:GLU:O	12:J:107:GLU:HG2	2.20	0.41
14:L:2:ALA:C	14:L:4:ILE:H	2.28	0.41
20:R:60:ARG:NH1	20:R:66:VAL:HG13	2.35	0.41
22:T:39:LEU:HD21	22:T:47:PRO:HG3	2.02	0.41
22:T:130:ASP:O	22:T:134:ILE:HD12	2.20	0.41
29:a:37:LYS:HE2	29:a:37:LYS:HB2	1.82	0.41
29:a:50:VAL:O	29:a:54:SER:OG	2.37	0.41
1:2:148:U:C4	1:2:169:U:C4	3.08	0.41
1:2:452:G:O2'	1:2:453:C:H5'	2.20	0.41
1:2:868:G:H5''	1:2:869:A:OP2	2.19	0.41
1:2:929:G:H2'	1:2:930:C:O4'	2.19	0.41
1:2:1058:A:H2'	1:2:1059:G:C8	2.56	0.41
1:2:1181:A:O2'	1:2:1182:A:C8	2.69	0.41
1:2:1544:C:H5	1:2:1588:A:OP2	2.03	0.41
1:2:1668:U:C4	1:2:1669:G:N7	2.89	0.41
1:2:1845:A:H2'	1:2:1846:G:C8	2.55	0.41
4:B:52:THR:HG23	4:B:56:LYS:O	2.20	0.41
6:D:5:ILE:H	6:D:5:ILE:HG13	1.68	0.41
7:E:182:MET:HE3	7:E:228:ILE:HD11	2.01	0.41
8:F:80:GLY:O	8:F:83:ASN:HB2	2.21	0.41
8:F:200:ALA:O	8:F:204:ARG:HG2	2.20	0.41
9:G:59:GLN:HG3	9:G:72:ARG:HH21	1.81	0.41
11:I:12:ARG:HG3	11:I:16:GLY:O	2.20	0.41
13:K:15:LEU:HD22	13:K:49:MET:SD	2.60	0.41
14:L:42:LEU:HA	14:L:42:LEU:HD13	1.53	0.41
14:L:134:LEU:HD23	14:L:134:LEU:HA	1.71	0.41
28:Z:103:HIS:CD2	28:Z:103:HIS:C	2.98	0.41
1:2:527:C:O3'	12:J:121:LYS:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:973:C:N3	17:O:55:ARG:NH2	2.67	0.41
1:2:1136:U:H2'	1:2:1137:U:H6	1.84	0.41
1:2:1199:A:H5'	29:a:2:THR:HB	2.02	0.41
1:2:1305:C:H2'	1:2:1306:U:C6	2.55	0.41
1:2:1493:C:H4'	1:2:1494:U:H3'	2.03	0.41
3:A:177:MET:HE2	3:A:180:ARG:HH21	1.85	0.41
7:E:179:ASN:HD22	7:E:179:ASN:HA	1.68	0.41
10:H:129:ILE:HD13	10:H:180:LEU:HD13	2.03	0.41
11:I:178:ARG:O	11:I:182:CYS:HB3	2.21	0.41
14:L:99:TYR:O	14:L:100:ASN:HB2	2.20	0.41
21:S:40:TYR:HE1	21:S:79:ILE:HG21	1.85	0.41
26:X:51:VAL:HG13	26:X:70:VAL:CG1	2.50	0.41
1:2:71:G:H5''	1:2:72:C:OP2	2.20	0.41
1:2:1134:G:H2'	1:2:1135:C:C6	2.56	0.41
1:2:1549:U:OP1	32:d:34:TYR:OH	2.37	0.41
1:2:1724:A:H2'	1:2:1725:U:H6	1.86	0.41
5:C:192:LEU:HD22	5:C:192:LEU:HA	1.90	0.41
5:C:205:VAL:O	5:C:224:THR:HB	2.20	0.41
8:F:51:HIS:O	19:Q:50:LYS:HE3	2.21	0.41
9:G:75:LEU:HD23	9:G:75:LEU:HA	1.90	0.41
10:H:113:LYS:HA	10:H:113:LYS:HD3	1.78	0.41
21:S:31:THR:HG23	21:S:37:GLY:HA2	2.01	0.41
24:V:7:GLU:N	24:V:7:GLU:OE1	2.54	0.41
30:b:27:SER:HA	30:b:28:PRO:HD2	1.75	0.41
35:g:17:TRP:HB2	35:g:36:ARG:HB2	2.03	0.41
35:g:172:LYS:HG2	35:g:193:GLY:O	2.21	0.41
1:2:12:U:H2'	1:2:13:C:C6	2.56	0.41
1:2:553:U:H2'	1:2:554:A:O4'	2.20	0.41
1:2:1221:G:H2'	1:2:1222:G:C8	2.56	0.41
1:2:1429:G:O2'	1:2:1430:C:H6	2.03	0.41
1:2:1464:C:HO2'	1:2:1465:A:P	2.43	0.41
3:A:130:ASP:OD1	3:A:130:ASP:N	2.54	0.41
4:B:82:ARG:NH1	4:B:191:ASP:HB2	2.36	0.41
5:C:178:HIS:CE1	5:C:179:THR:HG22	2.56	0.41
6:D:7:LYS:HA	6:D:7:LYS:HD3	1.84	0.41
6:D:67:ARG:HH21	13:K:97:SER:HB3	1.86	0.41
6:D:138:VAL:HA	6:D:184:ILE:HG22	2.03	0.41
7:E:125:LYS:O	7:E:141:THR:HA	2.21	0.41
8:F:168:THR:HG21	28:Z:106:GLN:CD	2.46	0.41
10:H:100:ILE:HG21	10:H:122:LEU:HD23	2.02	0.41
13:K:60:GLU:HG2	13:K:69:TRP:NE1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:48:HIS:O	15:M:74:ILE:HG23	2.20	0.41
19:Q:76:GLY:O	19:Q:80:GLN:HG3	2.21	0.41
20:R:78:ARG:O	20:R:82:ASP:HB2	2.21	0.41
25:W:49:GLU:H	25:W:49:GLU:HG3	1.55	0.41
34:f:132:MET:HG2	34:f:141:CYS:HB2	2.01	0.41
35:g:18:VAL:HG21	35:g:307:VAL:HG22	2.01	0.41
1:2:1610:G:H2'	1:2:1611:G:O4'	2.20	0.41
4:B:62:LEU:HA	4:B:65:ARG:NE	2.34	0.41
5:C:74:LYS:HB3	5:C:269:PHE:CE1	2.55	0.41
19:Q:21:ALA:HB2	19:Q:83:ALA:HB1	2.03	0.41
19:Q:53:GLU:OE2	19:Q:115:TYR:OH	2.39	0.41
27:Y:23:MET:HE1	27:Y:75:ILE:HD12	2.03	0.41
1:2:48:C:H2'	1:2:49:C:O4'	2.21	0.41
1:2:293:C:O2	1:2:293:C:H2'	2.19	0.41
1:2:383:G:C6	1:2:384:U:N3	2.89	0.41
1:2:415:A:H2'	1:2:416:U:O4'	2.21	0.41
1:2:607:U:H6	1:2:607:U:H2'	1.65	0.41
1:2:679:A:H2'	1:2:680:G:H5'	2.03	0.41
1:2:941:C:H5''	4:B:136:ARG:HH21	1.84	0.41
1:2:967:C:H3'	1:2:968:U:H5''	2.03	0.41
1:2:1010:G:H2'	1:2:1011:A:C8	2.56	0.41
1:2:1035:A:H2'	1:2:1036:A:O4'	2.21	0.41
1:2:1368:U:O3'	20:R:2:GLY:HA3	2.21	0.41
1:2:1445:U:O2'	1:2:1446:A:OP1	2.36	0.41
1:2:1447:G:OP1	23:U:87:ARG:NH2	2.54	0.41
1:2:1518:C:H3'	1:2:1519:U:H5'	2.03	0.41
1:2:1532:C:H5''	1:2:1533:A:O4'	2.21	0.41
1:2:1545:A:N6	1:2:1546:G:O6	2.54	0.41
1:2:1724:A:H2'	1:2:1725:U:C6	2.56	0.41
1:2:1736:G:H2'	1:2:1737:G:H8	1.83	0.41
1:2:1784:G:C2'	1:2:1785:C:H5'	2.51	0.41
3:A:59:LEU:O	3:A:62:ALA:HB3	2.21	0.41
5:C:206:SER:HB3	5:C:224:THR:CB	2.50	0.41
6:D:99:ILE:O	6:D:103:GLU:HB2	2.21	0.41
7:E:11:ARG:HD3	7:E:27:PHE:O	2.21	0.41
7:E:139:LEU:HG	7:E:150:PRO:HG3	2.03	0.41
7:E:180:LEU:HD12	7:E:193:GLY:O	2.21	0.41
9:G:55:GLY:O	9:G:56:ASN:ND2	2.54	0.41
9:G:57:ASP:O	9:G:60:GLY:N	2.51	0.41
9:G:224:ARG:HA	9:G:224:ARG:HD3	1.83	0.41
11:I:3:ILE:O	11:I:30:GLY:N	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:65:PHE:HB2	11:I:109:TYR:OH	2.20	0.41
14:L:61:PRO:HA	14:L:66:VAL:HG22	2.01	0.41
14:L:68:ILE:HG13	14:L:143:LEU:HD21	2.03	0.41
20:R:100:PRO:O	20:R:103:LYS:HB3	2.21	0.41
22:T:114:GLU:HB2	22:T:124:THR:HG22	2.03	0.41
23:U:93:SER:HB2	23:U:94:PRO:HD2	2.03	0.41
28:Z:92:LEU:HD23	28:Z:92:LEU:HA	1.96	0.41
29:a:95:ARG:HH11	29:a:95:ARG:HD2	1.76	0.41
30:b:47:PHE:CD2	30:b:49:HIS:O	2.73	0.41
35:g:235:ILE:O	35:g:252:THR:HG23	2.21	0.41
1:2:219:U:H4'	11:I:182:CYS:SG	2.60	0.41
1:2:528:A:H2'	1:2:529:A:O4'	2.20	0.41
1:2:639:C:O2'	1:2:640:A:C8	2.64	0.41
1:2:969:U:OP2	1:2:970:G:H5'	2.21	0.41
1:2:1026:C:H4'	1:2:1161:U:H4'	2.03	0.41
2:3:259:U:H2'	2:3:260:A:H5'	2.02	0.41
3:A:111:GLN:CD	3:A:111:GLN:H	2.29	0.41
5:C:116:THR:HG22	5:C:117:ARG:N	2.35	0.41
5:C:195:LEU:C	5:C:196:ILE:HG12	2.46	0.41
6:D:174:HIS:HB3	6:D:181:VAL:HG11	2.03	0.41
9:G:54:GLY:HA3	9:G:110:ASN:CG	2.46	0.41
9:G:168:LYS:HA	9:G:169:PRO:HD3	1.92	0.41
12:J:25:LEU:HA	12:J:40:LYS:NZ	2.36	0.41
15:M:85:LEU:HB3	15:M:106:CYS:O	2.21	0.41
17:O:32:HIS:CD2	17:O:32:HIS:N	2.89	0.41
25:W:84:LYS:H	25:W:84:LYS:HG3	1.67	0.41
32:d:33:LYS:HG2	32:d:34:TYR:CE1	2.56	0.41
1:2:607:U:O2'	1:2:608:C:OP1	2.35	0.40
1:2:1088:U:H4'	1:2:1089:G:OP2	2.22	0.40
1:2:1325:G:H5'	1:2:1326:U:P	2.61	0.40
1:2:1428:G:N2	1:2:1585:U:H5''	2.35	0.40
1:2:1572:C:C4	1:2:1573:G:C8	3.09	0.40
1:2:1643:U:H1'	19:Q:142:GLN:HG2	2.03	0.40
1:2:1654:G:OP1	22:T:90:SER:HB2	2.21	0.40
1:2:1680:G:O2'	31:c:20:ARG:HD2	2.21	0.40
1:2:1842:C:H2'	1:2:1843:G:C8	2.56	0.40
2:3:42:C:H42	2:3:120:C:N4	2.09	0.40
2:3:230:G:HO2'	2:3:231:G:P	2.42	0.40
2:3:245:G:OP1	2:3:245:G:H8	2.03	0.40
4:B:146:ARG:HA	4:B:146:ARG:NH1	2.35	0.40
7:E:11:ARG:HA	7:E:28:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:79:ASP:OD1	7:E:82:TYR:N	2.54	0.40
7:E:216:ASN:H	7:E:216:ASN:ND2	2.19	0.40
9:G:22:ARG:O	9:G:25:ARG:HB2	2.20	0.40
9:G:76:LEU:HB2	9:G:94:ARG:NH1	2.36	0.40
10:H:162:GLN:O	10:H:165:ASN:HB3	2.21	0.40
14:L:69:ARG:HH22	14:L:132:ARG:HA	1.86	0.40
18:P:67:ALA:HA	18:P:68:PRO:HD3	1.97	0.40
22:T:6:VAL:HB	22:T:65:TYR:CZ	2.56	0.40
22:T:37:VAL:HG13	22:T:38:LYS:O	2.21	0.40
24:V:70:LEU:HD23	24:V:70:LEU:HA	1.87	0.40
26:X:130:LEU:HA	26:X:130:LEU:HD23	1.70	0.40
1:2:102:A:HO2'	1:2:103:A:P	2.44	0.40
1:2:440:G:O2'	1:2:441:C:OP1	2.36	0.40
1:2:441:C:OP2	11:I:2:GLY:HA3	2.21	0.40
1:2:1595:U:OP1	28:Z:102:LYS:NZ	2.40	0.40
1:2:1617:G:H3'	1:2:1618:C:C5'	2.51	0.40
3:A:166:LYS:HD2	3:A:166:LYS:HA	1.63	0.40
6:D:175:VAL:HG12	6:D:182:LEU:O	2.21	0.40
6:D:196:GLY:O	6:D:197:LYS:HB2	2.21	0.40
7:E:105:THR:HG21	7:E:245:ARG:HA	2.03	0.40
7:E:164:LEU:HD23	7:E:164:LEU:HA	1.79	0.40
7:E:242:LYS:HD3	7:E:242:LYS:HA	1.60	0.40
16:N:13:GLN:HG3	30:b:21:LYS:HE3	2.04	0.40
16:N:30:SER:HA	16:N:67:THR:HG22	2.03	0.40
26:X:56:GLY:N	33:e:6:LEU:HD21	2.36	0.40
27:Y:42:GLU:OE2	27:Y:52:PRO:HB3	2.21	0.40
27:Y:114:MET:O	27:Y:122:LYS:HE2	2.21	0.40
28:Z:63:PRO:O	28:Z:111:ARG:HB2	2.20	0.40
35:g:159:ASN:HB2	35:g:204:GLY:HA3	2.03	0.40
35:g:270:LEU:HD22	35:g:310:TRP:CE3	2.56	0.40
1:2:27:A:H2'	1:2:28:U:O4'	2.21	0.40
1:2:819:G:C6	1:2:820:U:C4	3.09	0.40
1:2:1580:A:H5'	23:U:57:PRO:HD2	2.03	0.40
1:2:1667:U:C4	1:2:1668:U:C4	3.09	0.40
1:2:1745:A:H2'	1:2:1746:U:C6	2.56	0.40
7:E:129:ILE:HA	7:E:138:HIS:O	2.21	0.40
8:F:165:ASN:OD1	8:F:167:LYS:HB2	2.21	0.40
9:G:54:GLY:HA3	9:G:110:ASN:ND2	2.36	0.40
11:I:79:ILE:HG13	11:I:170:LYS:HZ2	1.86	0.40
12:J:121:LYS:HE3	12:J:121:LYS:HB2	1.65	0.40
15:M:22:LEU:HD12	15:M:88:TRP:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:38:ALA:HB1	15:M:110:VAL:HG23	2.03	0.40
15:M:64:LEU:HD23	15:M:64:LEU:HA	1.93	0.40
21:S:38:ARG:O	21:S:42:HIS:ND1	2.51	0.40
33:e:28:LYS:O	33:e:33:LYS:HB2	2.20	0.40
1:2:141:A:N7	1:2:178:C:H1'	2.36	0.40
1:2:619:A:C6	26:X:114:ASP:HB2	2.56	0.40
1:2:846:G:OP2	7:E:108:ARG:NH2	2.53	0.40
1:2:905:C:H2'	1:2:906:U:O4'	2.22	0.40
1:2:910:G:OP1	37:r:173:ARG:NH1	2.55	0.40
1:2:1297:U:O2'	1:2:1301:A:N6	2.55	0.40
1:2:1623:A:N9	21:S:132:ARG:HD2	2.36	0.40
2:3:70:A:H5'	2:3:71:G:OP2	2.22	0.40
3:A:108:PHE:HD2	3:A:136:GLU:HB3	1.86	0.40
3:A:136:GLU:O	3:A:140:VAL:HG23	2.22	0.40
7:E:43:PRO:CG	7:E:46:ILE:HD13	2.50	0.40
7:E:128:LYS:O	7:E:140:VAL:HG23	2.21	0.40
7:E:160:ILE:HD12	7:E:162:ILE:HD11	2.03	0.40
16:N:101:HIS:O	16:N:101:HIS:ND1	2.55	0.40
19:Q:11:GLN:OE1	19:Q:24:HIS:HD2	2.05	0.40
30:b:73:LEU:H	30:b:73:LEU:HG	1.69	0.40
1:2:149:A:OP2	41:2:2010:HOH:O	2.22	0.40
1:2:604:A:H3'	1:2:604:A:C8	2.55	0.40
1:2:616:A:H5'	33:e:8:ARG:HB2	2.02	0.40
1:2:650:A:OP2	26:X:108:LYS:HE2	2.21	0.40
1:2:1309:C:H2'	1:2:1310:U:O4'	2.21	0.40
5:C:82:TYR:HD1	5:C:82:TYR:HA	1.74	0.40
5:C:192:LEU:HB3	5:C:227:ARG:HG3	2.04	0.40
7:E:149:TYR:CD2	9:G:205:GLU:HB3	2.56	0.40
20:R:20:TYR:CE1	20:R:38:ILE:HG23	2.55	0.40
23:U:82:MET:HB2	32:d:52:PHE:CD1	2.56	0.40
25:W:30:CYS:HB2	25:W:61:ILE:CD1	2.52	0.40
25:W:41:MET:HG2	25:W:129:PHE:CE1	2.56	0.40
27:Y:20:ARG:HD3	27:Y:76:TYR:CE1	2.56	0.40
35:g:132:TRP:CZ3	35:g:138:CYS:HB2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	
3	A	214/295 (72%)	202 (94%)	11 (5%)	1 (0%)	24	59
4	B	211/264 (80%)	200 (95%)	11 (5%)	0	100	100
5	C	216/293 (74%)	213 (99%)	3 (1%)	0	100	100
6	D	223/243 (92%)	214 (96%)	8 (4%)	1 (0%)	30	64
7	E	260/263 (99%)	252 (97%)	8 (3%)	0	100	100
8	F	187/204 (92%)	169 (90%)	16 (9%)	2 (1%)	11	43
9	G	228/249 (92%)	217 (95%)	11 (5%)	0	100	100
10	H	184/194 (95%)	172 (94%)	11 (6%)	1 (0%)	24	59
11	I	203/208 (98%)	196 (97%)	7 (3%)	0	100	100
12	J	178/194 (92%)	172 (97%)	5 (3%)	1 (1%)	21	55
13	K	93/165 (56%)	89 (96%)	4 (4%)	0	100	100
14	L	149/158 (94%)	145 (97%)	4 (3%)	0	100	100
15	M	121/132 (92%)	112 (93%)	9 (7%)	0	100	100
16	N	147/151 (97%)	143 (97%)	4 (3%)	0	100	100
17	O	133/151 (88%)	127 (96%)	6 (4%)	0	100	100
18	P	118/145 (81%)	116 (98%)	2 (2%)	0	100	100
19	Q	137/146 (94%)	131 (96%)	6 (4%)	0	100	100
20	R	130/135 (96%)	122 (94%)	8 (6%)	0	100	100
21	S	141/152 (93%)	136 (96%)	5 (4%)	0	100	100
22	T	143/146 (98%)	138 (96%)	4 (3%)	1 (1%)	18	53
23	U	99/119 (83%)	94 (95%)	5 (5%)	0	100	100
24	V	80/83 (96%)	78 (98%)	2 (2%)	0	100	100
25	W	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
26	X	139/143 (97%)	130 (94%)	8 (6%)	1 (1%)	18	53
27	Y	122/130 (94%)	118 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	Z	70/125 (56%)	66 (94%)	4 (6%)	0	100	100
29	a	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
30	b	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
31	c	59/61 (97%)	56 (95%)	3 (5%)	0	100	100
32	d	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
33	e	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
34	f	70/72 (97%)	65 (93%)	5 (7%)	0	100	100
35	g	312/315 (99%)	295 (95%)	15 (5%)	2 (1%)	21	55
36	h	22/24 (92%)	22 (100%)	0	0	100	100
37	r	11/13 (85%)	11 (100%)	0	0	100	100
38	w	47/62 (76%)	47 (100%)	0	0	100	100
All	All	4860/5459 (89%)	4641 (96%)	209 (4%)	10 (0%)	44	74

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	189	ILE
10	H	170	VAL
12	J	161	LEU
35	g	145	GLU
26	X	108	LYS
8	F	163	PHE
35	g	119	GLN
6	D	193	ASP
22	T	4	VAL
8	F	166	ILE

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	
3	A	180/243 (74%)	151 (84%)	29 (16%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B	194/231 (84%)	165 (85%)	29 (15%)	3	16
5	C	184/225 (82%)	140 (76%)	44 (24%)	1	5
6	D	189/202 (94%)	174 (92%)	15 (8%)	11	36
7	E	224/225 (100%)	185 (83%)	39 (17%)	2	12
8	F	159/170 (94%)	145 (91%)	14 (9%)	9	32
9	G	200/218 (92%)	176 (88%)	24 (12%)	5	21
10	H	167/174 (96%)	148 (89%)	19 (11%)	5	22
11	I	178/180 (99%)	153 (86%)	25 (14%)	3	17
12	J	160/168 (95%)	133 (83%)	27 (17%)	2	13
13	K	86/136 (63%)	84 (98%)	2 (2%)	44	63
14	L	135/142 (95%)	100 (74%)	35 (26%)	0	4
15	M	104/108 (96%)	95 (91%)	9 (9%)	9	33
16	N	130/131 (99%)	109 (84%)	21 (16%)	2	14
17	O	105/119 (88%)	84 (80%)	21 (20%)	1	9
18	P	107/130 (82%)	102 (95%)	5 (5%)	23	48
19	Q	115/121 (95%)	103 (90%)	12 (10%)	7	26
20	R	118/122 (97%)	100 (85%)	18 (15%)	3	15
21	S	124/132 (94%)	116 (94%)	8 (6%)	15	42
22	T	115/116 (99%)	105 (91%)	10 (9%)	9	33
23	U	93/107 (87%)	85 (91%)	8 (9%)	10	33
24	V	66/67 (98%)	49 (74%)	17 (26%)	0	4
25	W	112/113 (99%)	87 (78%)	25 (22%)	1	6
26	X	113/115 (98%)	101 (89%)	12 (11%)	6	25
27	Y	108/112 (96%)	97 (90%)	11 (10%)	7	26
28	Z	64/103 (62%)	59 (92%)	5 (8%)	11	36
29	a	89/89 (100%)	72 (81%)	17 (19%)	1	10
30	b	74/74 (100%)	63 (85%)	11 (15%)	3	16
31	c	54/54 (100%)	51 (94%)	3 (6%)	19	45
32	d	48/48 (100%)	47 (98%)	1 (2%)	47	65
33	e	45/45 (100%)	36 (80%)	9 (20%)	1	9
34	f	65/65 (100%)	63 (97%)	2 (3%)	35	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	g	272/273 (100%)	255 (94%)	17 (6%)	16	42
36	h	23/23 (100%)	21 (91%)	2 (9%)	9	33
37	r	12/12 (100%)	11 (92%)	1 (8%)	10	34
38	w	35/35 (100%)	33 (94%)	2 (6%)	18	44
All	All	4247/4628 (92%)	3698 (87%)	549 (13%)	6	20

All (549) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	5	LEU
3	A	29	ASN
3	A	38	ILE
3	A	53	ARG
3	A	59	LEU
3	A	80	ARG
3	A	94	THR
3	A	107	THR
3	A	111	GLN
3	A	112	ILE
3	A	124	VAL
3	A	130	ASP
3	A	131	HIS
3	A	136	GLU
3	A	138	SER
3	A	140	VAL
3	A	142	LEU
3	A	145	ILE
3	A	157	VAL
3	A	163	CYS
3	A	173	LEU
3	A	178	LEU
3	A	180	ARG
3	A	185	MET
3	A	186	ARG
3	A	188	THR
3	A	189	ILE
3	A	198	MET
3	A	200	ASP
4	B	25	PHE
4	B	33	VAL
4	B	38	MET

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Mol	Chain	Res	Type
4	B	47	THR
4	B	57	ILE
4	B	66	VAL
4	B	68	GLU
4	B	77	ASP
4	B	79	VAL
4	B	95	ASN
4	B	98	THR
4	B	103	MET
4	B	104	ASP
4	B	106	THR
4	B	107	ARG
4	B	125	VAL
4	B	131	ASP
4	B	136	ARG
4	B	146	ARG
4	B	163	GLN
4	B	169	MET
4	B	174	ARG
4	B	175	GLU
4	B	181	LEU
4	B	193	ILE
4	B	202	GLN
4	B	210	VAL
4	B	213	ARG
4	B	217	MET
5	C	68	ARG
5	C	73	MET
5	C	80	GLU
5	C	83	LEU
5	C	94	ILE
5	C	97	PHE
5	C	98	LEU
5	C	101	SER
5	C	112	VAL
5	C	113	GLN
5	C	120	GLN
5	C	123	ARG
5	C	132	ASP
5	C	143	CYS
5	C	147	VAL
5	C	156	ILE

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Mol	Chain	Res	Type
5	C	157	LEU
5	C	160	LEU
5	C	165	VAL
5	C	167	ARG
5	C	172	ASN
5	C	173	LYS
5	C	180	VAL
5	C	190	SER
5	C	196	ILE
5	C	204	ILE
5	C	205	VAL
5	C	212	LYS
5	C	215	MET
5	C	221	ASP
5	C	224	THR
5	C	227	ARG
5	C	230	THR
5	C	232	THR
5	C	240	THR
5	C	242	ASP
5	C	244	ILE
5	C	247	THR
5	C	249	SER
5	C	251	LEU
5	C	252	THR
5	C	260	VAL
5	C	271	ASP
5	C	276	THR
6	D	3	VAL
6	D	54	ARG
6	D	70	THR
6	D	91	VAL
6	D	103	GLU
6	D	119	CYS
6	D	126	ILE
6	D	134	CYS
6	D	146	ARG
6	D	164	VAL
6	D	176	LEU
6	D	182	LEU
6	D	195	THR
6	D	198	ILE

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Mol	Chain	Res	Type
6	D	206	ASP
7	E	11	ARG
7	E	12	VAL
7	E	19	MET
7	E	23	LEU
7	E	29	PRO
7	E	38	LEU
7	E	40	GLU
7	E	42	LEU
7	E	45	ILE
7	E	46	ILE
7	E	49	ARG
7	E	51	ARG
7	E	59	ASP
7	E	88	ASP
7	E	95	THR
7	E	102	ILE
7	E	108	ARG
7	E	111	VAL
7	E	114	ILE
7	E	140	VAL
7	E	143	ASP
7	E	145	ARG
7	E	147	ILE
7	E	151	ASP
7	E	160	ILE
7	E	169	ILE
7	E	171	ASP
7	E	181	CYS
7	E	192	ILE
7	E	197	ASN
7	E	198	ARG
7	E	200	ARG
7	E	208	VAL
7	E	225	ILE
7	E	238	LEU
7	E	240	ARG
7	E	242	LYS
7	E	247	THR
7	E	248	ILE
8	F	68	ILE
8	F	78	MET

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Mol	Chain	Res	Type
8	F	82	ASN
8	F	91	ARG
8	F	109	LEU
8	F	116	ILE
8	F	122	ARG
8	F	126	THR
8	F	130	ARG
8	F	134	VAL
8	F	140	ASP
8	F	166	ILE
8	F	176	GLU
8	F	204	ARG
9	G	16	ILE
9	G	19	ASP
9	G	22	ARG
9	G	51	ARG
9	G	52	ILE
9	G	57	ASP
9	G	67	VAL
9	G	69	THR
9	G	91	GLU
9	G	92	ARG
9	G	98	ARG
9	G	105	ASN
9	G	110	ASN
9	G	120	ASP
9	G	121	ILE
9	G	129	VAL
9	G	136	LYS
9	G	141	ILE
9	G	144	LEU
9	G	151	ASP
9	G	152	ASP
9	G	158	VAL
9	G	171	THR
9	G	181	THR
10	H	12	ASN
10	H	46	THR
10	H	51	ILE
10	H	70	LYS
10	H	75	ILE
10	H	84	GLU

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Mol	Chain	Res	Type
10	H	87	PHE
10	H	100	ILE
10	H	105	THR
10	H	121	THR
10	H	122	LEU
10	H	123	THR
10	H	125	VAL
10	H	133	LEU
10	H	134	VAL
10	H	153	LEU
10	H	180	LEU
10	H	184	ASP
10	H	188	GLU
11	I	17	LYS
11	I	18	ARG
11	I	22	HIS
11	I	29	LEU
11	I	35	ASN
11	I	38	ILE
11	I	43	ILE
11	I	49	ARG
11	I	62	VAL
11	I	72	CYS
11	I	82	VAL
11	I	95	THR
11	I	106	SER
11	I	121	LEU
11	I	128	LYS
11	I	130	THR
11	I	144	LYS
11	I	170	LYS
11	I	175	ILE
11	I	177	SER
11	I	178	ARG
11	I	184	ARG
11	I	191	GLU
11	I	194	GLU
11	I	196	GLU
12	J	3	VAL
12	J	12	THR
12	J	21	GLU
12	J	22	LYS

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Mol	Chain	Res	Type
12	J	29	LEU
12	J	42	GLU
12	J	50	LEU
12	J	61	LEU
12	J	83	ARG
12	J	88	ASP
12	J	94	LEU
12	J	95	ASP
12	J	97	ILE
12	J	102	ILE
12	J	104	ASP
12	J	108	ARG
12	J	114	VAL
12	J	117	LEU
12	J	122	SER
12	J	128	VAL
12	J	132	GLN
12	J	136	ARG
12	J	144	ILE
12	J	150	ARG
12	J	153	SER
12	J	156	HIS
12	J	161	LEU
13	K	46	MET
13	K	52	LEU
14	L	3	ASP
14	L	5	GLN
14	L	6	THR
14	L	13	GLN
14	L	15	THR
14	L	18	GLN
14	L	23	VAL
14	L	35	ARG
14	L	40	ILE
14	L	42	LEU
14	L	45	LYS
14	L	46	THR
14	L	49	GLU
14	L	51	ILE
14	L	52	GLU
14	L	60	CYS
14	L	69	ARG

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Mol	Chain	Res	Type
14	L	71	ARG
14	L	74	SER
14	L	76	VAL
14	L	78	THR
14	L	80	MET
14	L	83	GLN
14	L	85	THR
14	L	89	ARG
14	L	101	ARG
14	L	104	LYS
14	L	119	ASP
14	L	120	VAL
14	L	121	GLN
14	L	128	VAL
14	L	132	ARG
14	L	135	SER
14	L	144	LYS
14	L	146	THR
15	M	21	VAL
15	M	26	LEU
15	M	35	ILE
15	M	36	ARG
15	M	45	ARG
15	M	65	VAL
15	M	74	ILE
15	M	89	VAL
15	M	104	VAL
16	N	12	SER
16	N	14	SER
16	N	29	THR
16	N	42	LYS
16	N	70	LYS
16	N	71	ILE
16	N	75	LEU
16	N	77	SER
16	N	80	LEU
16	N	83	ASP
16	N	84	LEU
16	N	92	ILE
16	N	96	VAL
16	N	98	VAL
16	N	101	HIS

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Mol	Chain	Res	Type
16	N	106	ARG
16	N	125	LEU
16	N	127	ARG
16	N	138	ASN
16	N	143	SER
16	N	145	THR
17	O	36	SER
17	O	45	THR
17	O	52	THR
17	O	57	THR
17	O	70	SER
17	O	95	ILE
17	O	98	ARG
17	O	100	THR
17	O	103	ASN
17	O	104	ARG
17	O	105	THR
17	O	116	LEU
17	O	121	ARG
17	O	128	ARG
17	O	133	THR
17	O	137	SER
17	O	140	THR
17	O	142	ARG
17	O	146	ARG
17	O	147	ARG
17	O	150	ARG
18	P	51	ARG
18	P	75	VAL
18	P	78	THR
18	P	84	ILE
18	P	122	THR
19	Q	10	VAL
19	Q	18	THR
19	Q	42	ILE
19	Q	43	GLU
19	Q	46	THR
19	Q	52	LEU
19	Q	100	VAL
19	Q	121	VAL
19	Q	125	ARG
19	Q	130	LYS

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Mol	Chain	Res	Type
19	Q	142	GLN
19	Q	143	LYS
20	R	5	ARG
20	R	8	THR
20	R	17	ILE
20	R	34	VAL
20	R	35	CYS
20	R	41	ILE
20	R	71	ILE
20	R	78	ARG
20	R	83	ASN
20	R	85	VAL
20	R	98	VAL
20	R	101	ASP
20	R	119	VAL
20	R	124	VAL
20	R	126	MET
20	R	127	ASN
20	R	128	PHE
20	R	132	ARG
21	S	4	VAL
21	S	14	ARG
21	S	19	ASN
21	S	71	MET
21	S	98	VAL
21	S	129	LEU
21	S	131	VAL
21	S	138	THR
22	T	34	VAL
22	T	35	ASP
22	T	36	THR
22	T	56	ARG
22	T	67	ARG
22	T	78	ILE
22	T	87	VAL
22	T	99	VAL
22	T	103	VAL
22	T	131	LEU
23	U	36	CYS
23	U	55	ARG
23	U	61	LEU
23	U	68	THR

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Mol	Chain	Res	Type
23	U	74	SER
23	U	107	GLU
23	U	114	VAL
23	U	115	THR
24	V	1	MET
24	V	2	GLN
24	V	9	VAL
24	V	15	ARG
24	V	18	SER
24	V	21	ASN
24	V	31	SER
24	V	34	MET
24	V	43	THR
24	V	52	THR
24	V	62	MET
24	V	67	ASP
24	V	68	SER
24	V	69	ILE
24	V	70	LEU
24	V	72	LEU
24	V	76	ASP
25	W	4	MET
25	W	13	SER
25	W	14	ILE
25	W	23	ARG
25	W	25	VAL
25	W	27	ILE
25	W	30	CYS
25	W	39	THR
25	W	40	VAL
25	W	47	ILE
25	W	49	GLU
25	W	56	HIS
25	W	57	ARG
25	W	80	ASP
25	W	83	LEU
25	W	85	ASP
25	W	97	ARG
25	W	102	ILE
25	W	104	LEU
25	W	105	THR
25	W	106	THR

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Mol	Chain	Res	Type
25	W	107	SER
25	W	112	ASP
25	W	121	THR
25	W	125	ILE
26	X	3	LYS
26	X	5	ARG
26	X	9	THR
26	X	14	ARG
26	X	15	SER
26	X	37	LYS
26	X	45	SER
26	X	77	ASN
26	X	81	ILE
26	X	100	VAL
26	X	107	ARG
26	X	123	VAL
27	Y	5	VAL
27	Y	14	THR
27	Y	17	LEU
27	Y	23	MET
27	Y	35	VAL
27	Y	42	GLU
27	Y	46	LYS
27	Y	54	VAL
27	Y	55	ILE
27	Y	107	ARG
27	Y	117	VAL
28	Z	47	LEU
28	Z	50	PHE
28	Z	65	TYR
28	Z	88	LEU
28	Z	107	VAL
29	a	2	THR
29	a	6	ARG
29	a	7	ASN
29	a	18	VAL
29	a	21	ILE
29	a	29	CYS
29	a	30	VAL
29	a	43	ASN
29	a	45	VAL
29	a	53	ILE

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Mol	Chain	Res	Type
29	a	58	VAL
29	a	64	LEU
29	a	72	HIS
29	a	75	VAL
29	a	78	VAL
29	a	81	SER
29	a	92	ARG
30	b	3	LEU
30	b	17	ARG
30	b	20	LYS
30	b	37	CYS
30	b	43	ILE
30	b	51	GLN
30	b	53	VAL
30	b	54	VAL
30	b	63	LEU
30	b	73	LEU
30	b	83	GLN
31	c	26	GLN
31	c	37	ASP
31	c	55	VAL
32	d	28	HIS
33	e	5	SER
33	e	8	ARG
33	e	11	LYS
33	e	12	VAL
33	e	27	LYS
33	e	29	THR
33	e	34	ARG
33	e	45	VAL
33	e	58	ASN
34	f	86	THR
34	f	98	VAL
35	g	31	ILE
35	g	41	ILE
35	g	46	THR
35	g	65	PHE
35	g	74	ASP
35	g	96	THR
35	g	97	THR
35	g	102	VAL
35	g	118	ARG

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Mol	Chain	Res	Type
35	g	142	VAL
35	g	195	LEU
35	g	198	VAL
35	g	272	GLN
35	g	274	VAL
35	g	297	THR
35	g	306	LEU
35	g	309	VAL
36	h	9	ARG
36	h	14	LYS
37	r	162	ARG
38	w	91	MET
38	w	94	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	36	GLN
3	A	111	GLN
3	A	141	ASN
4	B	40	ASN
4	B	76	ASN
4	B	159	GLN
4	B	208	HIS
5	C	178	HIS
6	D	56	GLN
6	D	74	GLN
6	D	174	HIS
6	D	179	GLN
7	E	50	ASN
7	E	112	HIS
7	E	161	GLN
7	E	179	ASN
7	E	201	HIS
7	E	209	HIS
7	E	214	ASN
7	E	216	ASN
8	F	79	HIS
8	F	110	GLN
8	F	137	GLN
8	F	203	ASN
9	G	59	GLN

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Mol	Chain	Res	Type
9	G	81	HIS
9	G	105	ASN
9	G	146	ASN
9	G	186	GLN
10	H	76	GLN
10	H	112	ASN
10	H	126	HIS
10	H	157	HIS
11	I	35	ASN
11	I	84	ASN
11	I	87	ASN
11	I	138	ASN
11	I	168	GLN
12	J	125	HIS
12	J	132	GLN
13	K	39	ASN
13	K	61	GLN
14	L	11	GLN
14	L	18	GLN
14	L	65	ASN
14	L	94	HIS
14	L	121	GLN
16	N	58	HIS
16	N	62	GLN
16	N	105	ASN
17	O	43	HIS
18	P	53	GLN
18	P	79	HIS
19	Q	24	HIS
19	Q	77	HIS
19	Q	142	GLN
20	R	116	ASN
21	S	72	GLN
21	S	101	ASN
25	W	98	GLN
25	W	113	HIS
26	X	16	HIS
26	X	61	GLN
26	X	63	ASN
27	Y	15	ASN
27	Y	63	HIS
28	Z	103	HIS

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Mol	Chain	Res	Type
29	a	72	HIS
31	c	29	GLN
32	d	3	HIS
32	d	16	GLN
33	e	37	GLN
33	e	56	ASN
34	f	93	HIS
34	f	111	ASN
35	g	14	HIS
35	g	20	GLN
35	g	64	HIS
35	g	147	HIS
35	g	162	ASN
35	g	178	ASN
35	g	215	GLN
35	g	237	ASN
36	h	22	GLN
38	w	95	ASN
38	w	96	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1656/1868 (88%)	597 (36%)	83 (5%)
2	3	254/257 (98%)	148 (58%)	25 (9%)
All	All	1910/2125 (89%)	745 (39%)	108 (5%)

All (745) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	C
1	2	4	C
1	2	5	U
1	2	8	U
1	2	9	U
1	2	17	C
1	2	23	G
1	2	25	A
1	2	26	U
1	2	31	U
1	2	33	G

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Mol	Chain	Res	Type
1	2	37	C
1	2	41	G
1	2	46	A
1	2	49	C
1	2	50	A
1	2	56	G
1	2	58	C
1	2	60	A
1	2	61	A
1	2	63	U
1	2	65	C
1	2	66	G
1	2	67	C
1	2	68	A
1	2	69	C
1	2	70	G
1	2	71	G
1	2	72	C
1	2	75	G
1	2	76	U
1	2	77	A
1	2	78	C
1	2	79	A
1	2	81	U
1	2	102	A
1	2	103	A
1	2	104	A
1	2	110	U
1	2	111	A
1	2	113	G
1	2	114	G
1	2	115	U
1	2	116	U
1	2	123	G
1	2	124	U
1	2	125	C
1	2	126	G
1	2	127	C
1	2	129	C
1	2	130	G
1	2	141	A
1	2	142	C

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Mol	Chain	Res	Type
1	2	143	U
1	2	144	U
1	2	150	A
1	2	153	G
1	2	154	U
1	2	155	G
1	2	163	U
1	2	167	G
1	2	168	C
1	2	170	A
1	2	173	A
1	2	175	A
1	2	179	C
1	2	181	A
1	2	182	C
1	2	184	G
1	2	188	C
1	2	189	U
1	2	190	G
1	2	191	A
1	2	192	C
1	2	200	G
1	2	206	G
1	2	209	A
1	2	210	U
1	2	213	G
1	2	214	U
1	2	215	G
1	2	216	C
1	2	217	A
1	2	290	U
1	2	291	G
1	2	292	A
1	2	294	U
1	2	295	C
1	2	297	A
1	2	302	A
1	2	307	G
1	2	308	G
1	2	310	C
1	2	311	C
1	2	312	G

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Mol	Chain	Res	Type
1	2	315	C
1	2	317	C
1	2	319	C
1	2	320	G
1	2	321	C
1	2	332	G
1	2	333	G
1	2	334	C
1	2	335	G
1	2	336	A
1	2	338	G
1	2	339	A
1	2	342	C
1	2	347	G
1	2	351	G
1	2	360	A
1	2	362	C
1	2	364	A
1	2	368	U
1	2	369	C
1	2	370	G
1	2	377	G
1	2	381	C
1	2	382	C
1	2	383	G
1	2	384	U
1	2	385	G
1	2	386	C
1	2	398	A
1	2	400	C
1	2	407	G
1	2	408	A
1	2	409	C
1	2	417	C
1	2	418	A
1	2	421	G
1	2	425	G
1	2	426	A
1	2	427	U
1	2	434	G
1	2	437	G
1	2	438	G

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Mol	Chain	Res	Type
1	2	441	C
1	2	447	A
1	2	448	A
1	2	450	C
1	2	453	C
1	2	454	U
1	2	464	A
1	2	465	A
1	2	466	G
1	2	471	G
1	2	472	C
1	2	473	A
1	2	474	G
1	2	476	A
1	2	482	G
1	2	485	A
1	2	487	U
1	2	489	A
1	2	492	C
1	2	496	C
1	2	500	A
1	2	502	C
1	2	507	G
1	2	508	A
1	2	509	G
1	2	523	A
1	2	530	U
1	2	531	A
1	2	532	C
1	2	534	G
1	2	535	G
1	2	536	A
1	2	537	C
1	2	542	U
1	2	544	G
1	2	546	G
1	2	548	C
1	2	550	C
1	2	552	G
1	2	554	A
1	2	555	A
1	2	556	U

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Mol	Chain	Res	Type
1	2	559	G
1	2	562	U
1	2	563	G
1	2	564	A
1	2	568	C
1	2	570	C
1	2	576	A
1	2	583	A
1	2	585	C
1	2	587	A
1	2	588	G
1	2	589	G
1	2	590	A
1	2	591	U
1	2	593	C
1	2	594	A
1	2	595	U
1	2	596	U
1	2	598	G
1	2	601	G
1	2	602	G
1	2	603	C
1	2	604	A
1	2	605	A
1	2	606	G
1	2	607	U
1	2	608	C
1	2	614	C
1	2	615	C
1	2	616	A
1	2	617	G
1	2	618	C
1	2	621	C
1	2	626	G
1	2	627	U
1	2	628	A
1	2	629	A
1	2	631	U
1	2	632	C
1	2	638	C
1	2	639	C
1	2	640	A

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Mol	Chain	Res	Type
1	2	643	A
1	2	644	G
1	2	647	U
1	2	657	U
1	2	658	U
1	2	659	G
1	2	660	C
1	2	668	A
1	2	669	A
1	2	670	A
1	2	671	A
1	2	672	A
1	2	673	G
1	2	683	G
1	2	684	G
1	2	685	A
1	2	686	U
1	2	687	C
1	2	688	U
1	2	748	C
1	2	749	U
1	2	750	C
1	2	751	G
1	2	792	C
1	2	793	G
1	2	794	A
1	2	796	G
1	2	797	C
1	2	798	G
1	2	799	U
1	2	807	G
1	2	808	A
1	2	809	A
1	2	810	A
1	2	811	A
1	2	812	A
1	2	818	A
1	2	821	G
1	2	822	U
1	2	823	U
1	2	824	C
1	2	830	A

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Mol	Chain	Res	Type
1	2	834	C
1	2	842	C
1	2	843	C
1	2	845	G
1	2	847	A
1	2	852	G
1	2	856	C
1	2	861	A
1	2	869	A
1	2	870	A
1	2	871	U
1	2	872	A
1	2	873	G
1	2	877	C
1	2	878	G
1	2	880	G
1	2	881	G
1	2	882	U
1	2	887	U
1	2	888	U
1	2	890	U
1	2	898	U
1	2	903	A
1	2	909	G
1	2	913	A
1	2	914	U
1	2	917	U
1	2	918	U
1	2	919	A
1	2	920	A
1	2	922	A
1	2	926	A
1	2	931	C
1	2	933	G
1	2	934	G
1	2	938	A
1	2	943	U
1	2	954	U
1	2	959	G
1	2	962	A
1	2	968	U
1	2	969	U

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Mol	Chain	Res	Type
1	2	970	G
1	2	971	G
1	2	978	G
1	2	980	A
1	2	981	A
1	2	983	A
1	2	985	G
1	2	990	A
1	2	992	A
1	2	996	A
1	2	997	A
1	2	999	G
1	2	1001	A
1	2	1008	A
1	2	1009	A
1	2	1017	U
1	2	1023	A
1	2	1030	A
1	2	1033	G
1	2	1040	G
1	2	1041	G
1	2	1042	A
1	2	1045	U
1	2	1049	A
1	2	1053	C
1	2	1054	G
1	2	1060	A
1	2	1061	U
1	2	1067	C
1	2	1078	C
1	2	1083	A
1	2	1085	C
1	2	1087	A
1	2	1088	U
1	2	1089	G
1	2	1096	G
1	2	1099	G
1	2	1100	A
1	2	1110	G
1	2	1111	U
1	2	1112	U
1	2	1114	U

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Mol	Chain	Res	Type
1	2	1116	C
1	2	1119	A
1	2	1121	G
1	2	1122	A
1	2	1123	C
1	2	1124	C
1	2	1130	G
1	2	1131	G
1	2	1133	A
1	2	1137	U
1	2	1138	C
1	2	1139	C
1	2	1143	A
1	2	1148	A
1	2	1150	A
1	2	1153	C
1	2	1154	U
1	2	1157	G
1	2	1171	G
1	2	1180	C
1	2	1181	A
1	2	1182	A
1	2	1194	A
1	2	1195	A
1	2	1202	U
1	2	1207	G
1	2	1208	A
1	2	1211	G
1	2	1213	C
1	2	1215	C
1	2	1216	C
1	2	1217	A
1	2	1221	G
1	2	1224	G
1	2	1227	G
1	2	1232	U
1	2	1233	G
1	2	1235	G
1	2	1238	U
1	2	1242	U
1	2	1243	U
1	2	1248	U

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Mol	Chain	Res	Type
1	2	1249	C
1	2	1250	A
1	2	1251	A
1	2	1253	A
1	2	1254	C
1	2	1256	G
1	2	1257	G
1	2	1259	A
1	2	1260	A
1	2	1261	C
1	2	1266	C
1	2	1274	G
1	2	1275	G
1	2	1283	C
1	2	1284	A
1	2	1285	G
1	2	1286	G
1	2	1288	U
1	2	1298	G
1	2	1301	A
1	2	1302	G
1	2	1303	C
1	2	1308	U
1	2	1309	C
1	2	1313	A
1	2	1315	U
1	2	1317	C
1	2	1320	G
1	2	1321	G
1	2	1322	G
1	2	1326	U
1	2	1327	G
1	2	1330	G
1	2	1331	C
1	2	1343	U
1	2	1344	A
1	2	1348	G
1	2	1358	U
1	2	1364	U
1	2	1366	G
1	2	1367	U
1	2	1371	U

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Mol	Chain	Res	Type
1	2	1372	U
1	2	1373	C
1	2	1377	U
1	2	1378	A
1	2	1380	C
1	2	1381	G
1	2	1382	A
1	2	1385	G
1	2	1401	A
1	2	1404	U
1	2	1405	A
1	2	1406	G
1	2	1416	C
1	2	1426	U
1	2	1427	C
1	2	1428	G
1	2	1429	G
1	2	1430	C
1	2	1431	G
1	2	1432	U
1	2	1439	A
1	2	1441	U
1	2	1442	U
1	2	1444	U
1	2	1446	A
1	2	1448	A
1	2	1452	A
1	2	1454	A
1	2	1455	A
1	2	1462	U
1	2	1463	U
1	2	1464	C
1	2	1465	A
1	2	1466	G
1	2	1468	C
1	2	1473	G
1	2	1474	A
1	2	1477	U
1	2	1478	U
1	2	1483	A
1	2	1486	A
1	2	1487	A

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Mol	Chain	Res	Type
1	2	1489	A
1	2	1490	G
1	2	1493	C
1	2	1494	U
1	2	1495	G
1	2	1499	U
1	2	1500	G
1	2	1505	U
1	2	1507	G
1	2	1508	A
1	2	1510	G
1	2	1512	C
1	2	1515	G
1	2	1516	G
1	2	1518	C
1	2	1519	U
1	2	1520	G
1	2	1521	C
1	2	1523	C
1	2	1524	G
1	2	1526	G
1	2	1533	A
1	2	1535	U
1	2	1536	G
1	2	1543	U
1	2	1545	A
1	2	1548	G
1	2	1559	C
1	2	1560	U
1	2	1561	A
1	2	1563	G
1	2	1566	G
1	2	1567	G
1	2	1568	C
1	2	1572	C
1	2	1573	G
1	2	1574	C
1	2	1578	U
1	2	1579	A
1	2	1580	A
1	2	1581	C
1	2	1585	U

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Mol	Chain	Res	Type
1	2	1586	U
1	2	1587	G
1	2	1588	A
1	2	1598	G
1	2	1599	U
1	2	1600	G
1	2	1601	A
1	2	1602	U
1	2	1603	G
1	2	1604	G
1	2	1606	G
1	2	1610	G
1	2	1612	G
1	2	1617	G
1	2	1618	C
1	2	1621	U
1	2	1623	A
1	2	1625	U
1	2	1630	A
1	2	1632	G
1	2	1634	A
1	2	1641	A
1	2	1645	C
1	2	1648	G
1	2	1649	U
1	2	1650	A
1	2	1654	G
1	2	1660	C
1	2	1663	A
1	2	1664	A
1	2	1665	G
1	2	1671	G
1	2	1675	A
1	2	1678	A
1	2	1682	C
1	2	1683	C
1	2	1688	C
1	2	1689	C
1	2	1695	A
1	2	1699	A
1	2	1721	U
1	2	1722	G

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Mol	Chain	Res	Type
1	2	1728	U
1	2	1729	U
1	2	1737	G
1	2	1742	C
1	2	1744	G
1	2	1745	A
1	2	1746	U
1	2	1761	U
1	2	1777	G
1	2	1778	C
1	2	1779	G
1	2	1783	C
1	2	1784	G
1	2	1785	C
1	2	1786	U
1	2	1800	A
1	2	1805	G
1	2	1807	C
1	2	1815	A
1	2	1826	G
1	2	1829	G
1	2	1831	A
1	2	1835	A
1	2	1836	G
1	2	1838	U
1	2	1839	U
1	2	1841	C
1	2	1849	G
1	2	1851	A
1	2	1852	C
1	2	1855	G
1	2	1859	A
1	2	1860	A
1	2	1861	G
1	2	1862	G
1	2	1863	A
1	2	1865	C
1	2	1867	U
1	2	1868	U
1	2	1869	A
2	3	41	U
2	3	42	C

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Mol	Chain	Res	Type
2	3	43	C
2	3	44	C
2	3	45	C
2	3	46	U
2	3	47	G
2	3	48	U
2	3	49	G
2	3	52	G
2	3	55	C
2	3	57	A
2	3	58	C
2	3	59	U
2	3	61	U
2	3	62	C
2	3	63	U
2	3	65	C
2	3	66	A
2	3	68	G
2	3	70	A
2	3	71	G
2	3	72	A
2	3	73	A
2	3	74	A
2	3	75	G
2	3	78	U
2	3	83	C
2	3	84	C
2	3	85	A
2	3	86	U
2	3	87	G
2	3	92	U
2	3	93	A
2	3	95	U
2	3	96	A
2	3	97	U
2	3	99	A
2	3	100	G
2	3	101	U
2	3	102	G
2	3	106	U
2	3	107	G
2	3	108	C

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Mol	Chain	Res	Type
2	3	109	A
2	3	111	C
2	3	113	U
2	3	114	C
2	3	115	C
2	3	116	A
2	3	117	G
2	3	118	G
2	3	120	C
2	3	121	C
2	3	122	C
2	3	123	C
2	3	124	C
2	3	128	C
2	3	129	C
2	3	131	G
2	3	135	G
2	3	137	G
2	3	139	C
2	3	140	A
2	3	141	U
2	3	142	A
2	3	145	G
2	3	147	U
2	3	150	G
2	3	152	G
2	3	153	G
2	3	154	A
2	3	155	A
2	3	159	G
2	3	160	U
2	3	161	G
2	3	162	A
2	3	163	G
2	3	164	U
2	3	165	A
2	3	166	C
2	3	167	A
2	3	169	C
2	3	172	A
2	3	175	U
2	3	176	G

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Mol	Chain	Res	Type
2	3	228	U
2	3	229	G
2	3	231	G
2	3	232	C
2	3	233	G
2	3	234	U
2	3	235	G
2	3	236	C
2	3	237	C
2	3	242	C
2	3	243	A
2	3	244	A
2	3	245	G
2	3	246	A
2	3	247	C
2	3	249	G
2	3	251	U
2	3	252	A
2	3	253	G
2	3	254	C
2	3	255	C
2	3	256	G
2	3	257	A
2	3	258	G
2	3	259	U
2	3	264	U
2	3	265	U
2	3	266	G
2	3	267	G
2	3	269	U
2	3	270	C
2	3	274	A
2	3	278	G
2	3	280	C
2	3	281	U
2	3	282	U
2	3	283	G
2	3	284	U
2	3	285	G
2	3	288	A
2	3	290	U
2	3	291	G

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Mol	Chain	Res	Type
2	3	297	U
2	3	303	G
2	3	304	C
2	3	306	U
2	3	307	G
2	3	308	C
2	3	310	A
2	3	311	G
2	3	321	A
2	3	322	G
2	3	324	U
2	3	325	C
2	3	328	G
2	3	330	A
2	3	331	G
2	3	332	A
2	3	333	C
2	3	334	C
2	3	340	C
2	3	341	C

All (108) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	60	A
1	2	65	C
1	2	102	A
1	2	114	G
1	2	126	G
1	2	143	U
1	2	180	G
1	2	291	G
1	2	314	U
1	2	319	C
1	2	332	G
1	2	368	U
1	2	381	C
1	2	382	C
1	2	408	A
1	2	437	G
1	2	440	G

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Mol	Chain	Res	Type
1	2	453	C
1	2	465	A
1	2	547	G
1	2	554	A
1	2	590	A
1	2	594	A
1	2	601	G
1	2	604	A
1	2	615	C
1	2	620	G
1	2	657	U
1	2	670	A
1	2	748	C
1	2	750	C
1	2	793	G
1	2	797	C
1	2	811	A
1	2	870	A
1	2	917	U
1	2	920	A
1	2	926	A
1	2	958	G
1	2	980	A
1	2	996	A
1	2	1001	A
1	2	1060	A
1	2	1129	G
1	2	1137	U
1	2	1165	G
1	2	1180	C
1	2	1181	A
1	2	1231	C
1	2	1250	A
1	2	1253	A
1	2	1302	G
1	2	1308	U
1	2	1316	C
1	2	1321	G
1	2	1330	G
1	2	1342	U
1	2	1403	C
1	2	1404	U

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Mol	Chain	Res	Type
1	2	1425	G
1	2	1428	G
1	2	1430	C
1	2	1438	A
1	2	1440	C
1	2	1445	U
1	2	1464	C
1	2	1476	A
1	2	1493	C
1	2	1494	U
1	2	1511	U
1	2	1534	C
1	2	1542	C
1	2	1558	C
1	2	1585	U
1	2	1587	G
1	2	1601	A
1	2	1648	G
1	2	1649	U
1	2	1745	A
1	2	1783	C
1	2	1835	A
1	2	1838	U
2	3	48	U
2	3	61	U
2	3	62	C
2	3	65	C
2	3	77	G
2	3	98	G
2	3	99	A
2	3	116	A
2	3	123	C
2	3	136	A
2	3	160	U
2	3	163	G
2	3	230	G
2	3	243	A
2	3	244	A
2	3	245	G
2	3	252	A
2	3	254	C
2	3	257	A

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Mol	Chain	Res	Type
2	3	280	C
2	3	281	U
2	3	289	C
2	3	306	U
2	3	329	U
2	3	330	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 101 ligands modelled in this entry, 101 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	3	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3	177:C	O3'	222:G	P	17.37
1	3	334:C	O3'	339:A	P	15.84

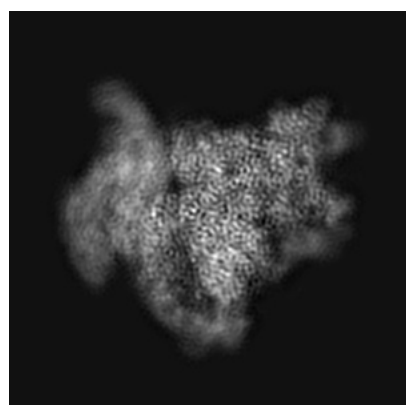
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3019. These allow visual inspection of the internal detail of the map and identification of artifacts.

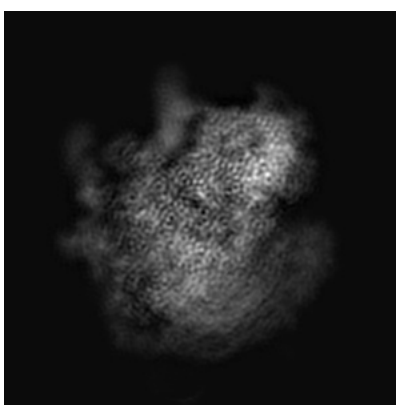
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

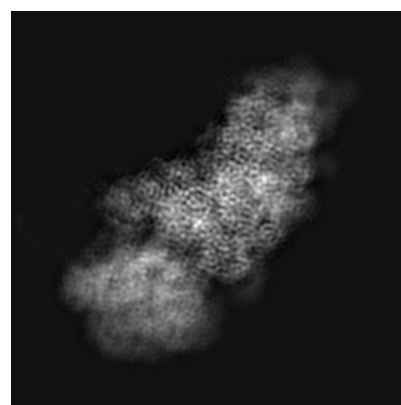
6.1.1 Primary map



X



Y

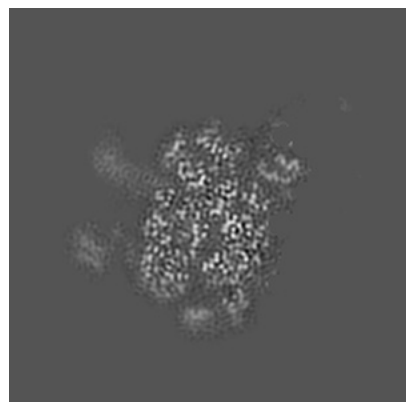


Z

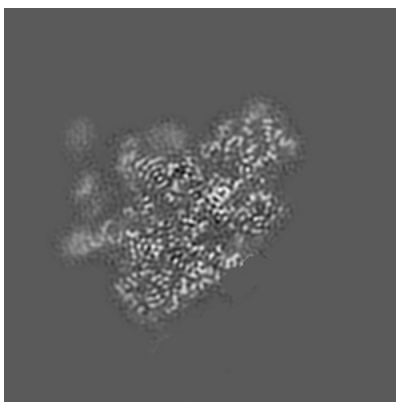
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

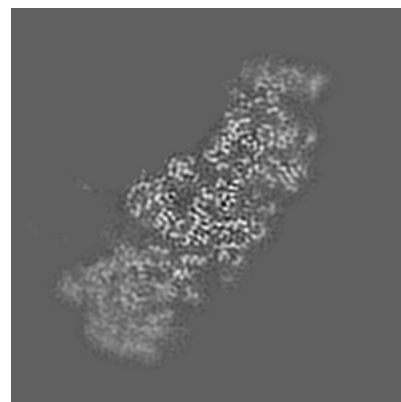
6.2.1 Primary map



X Index: 108



Y Index: 108

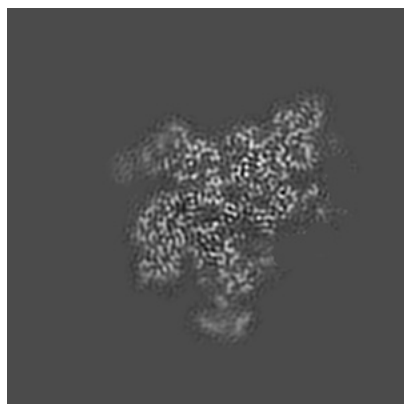


Z Index: 108

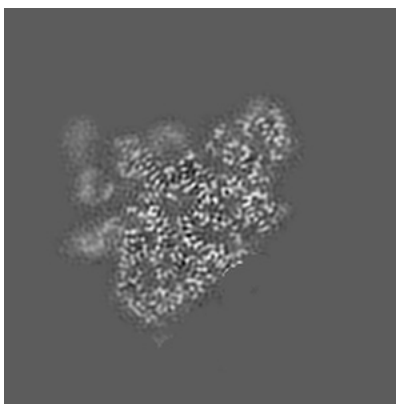
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

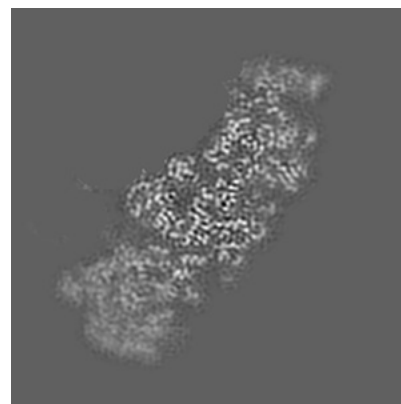
6.3.1 Primary map



X Index: 122



Y Index: 111

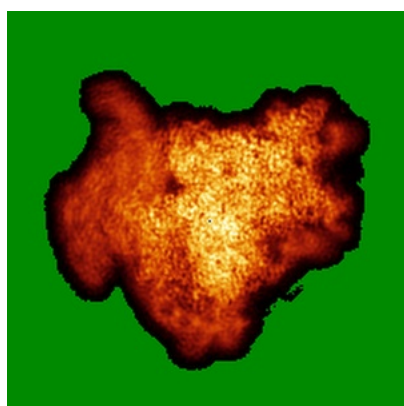


Z Index: 108

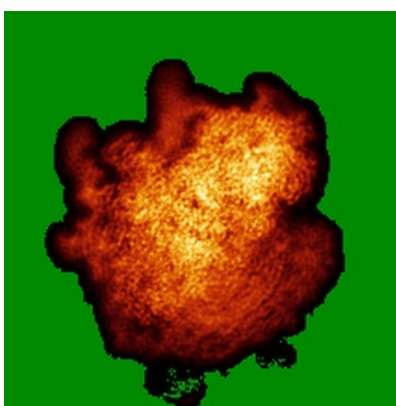
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

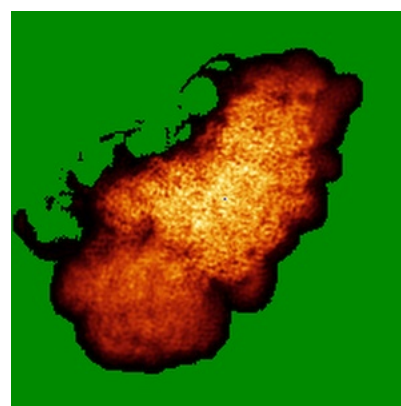
6.4.1 Primary map



X



Y

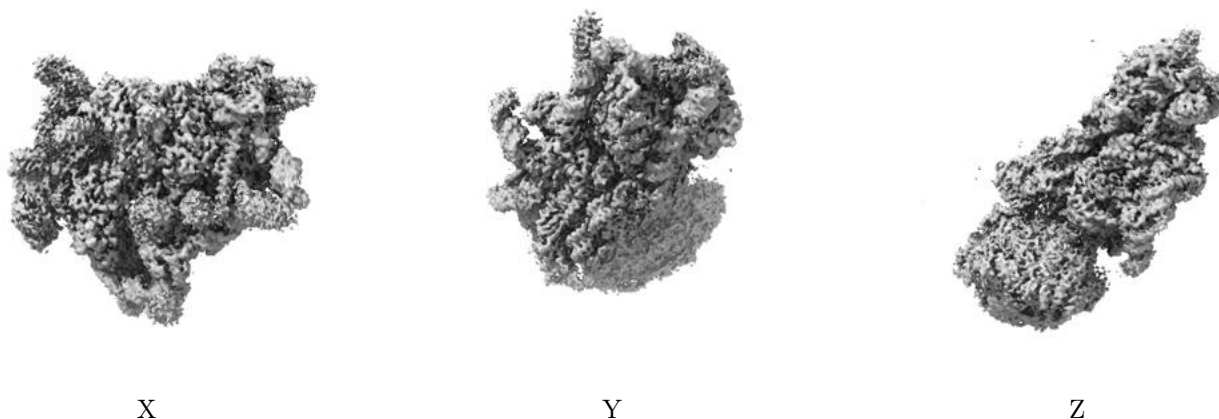


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

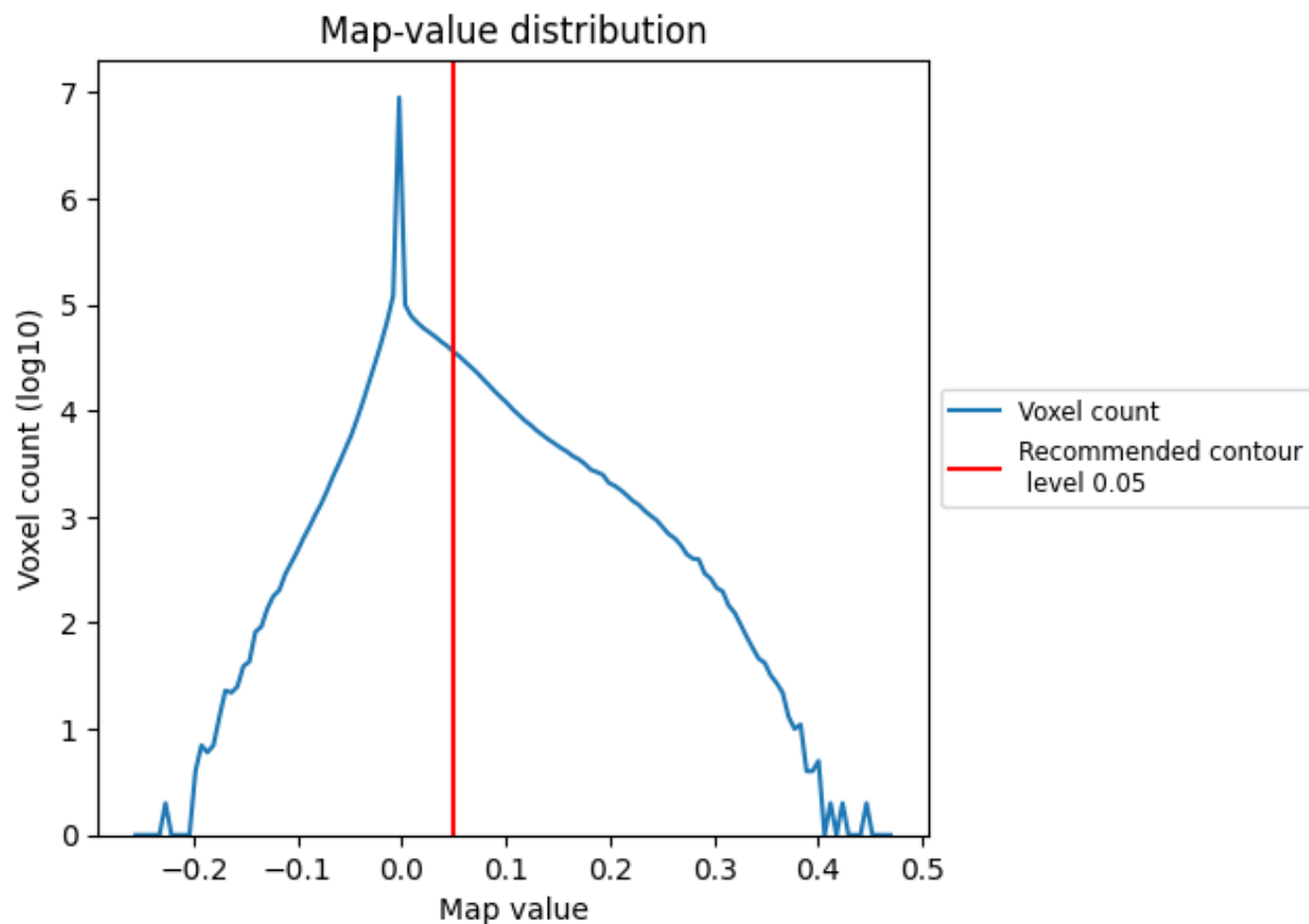
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

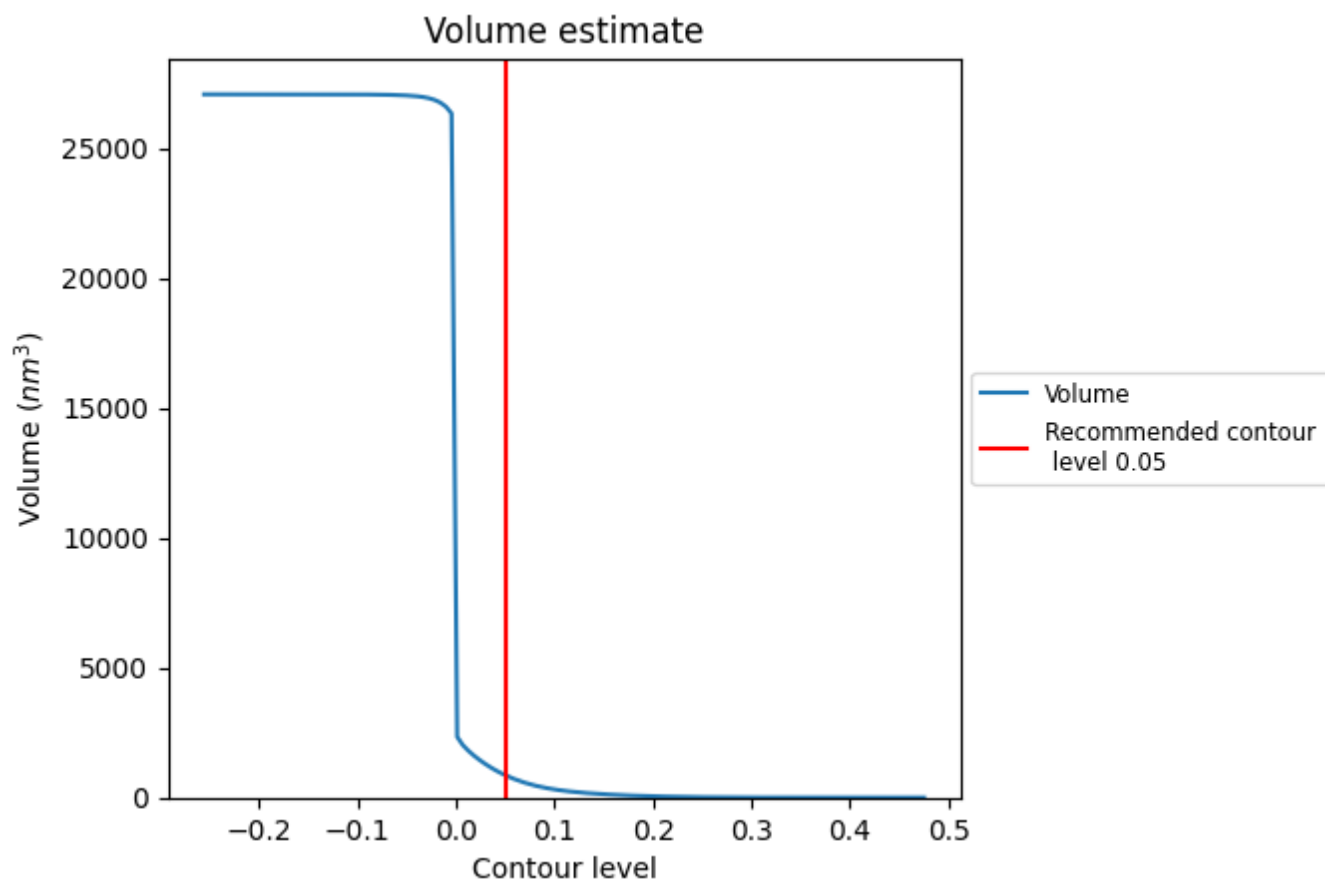
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

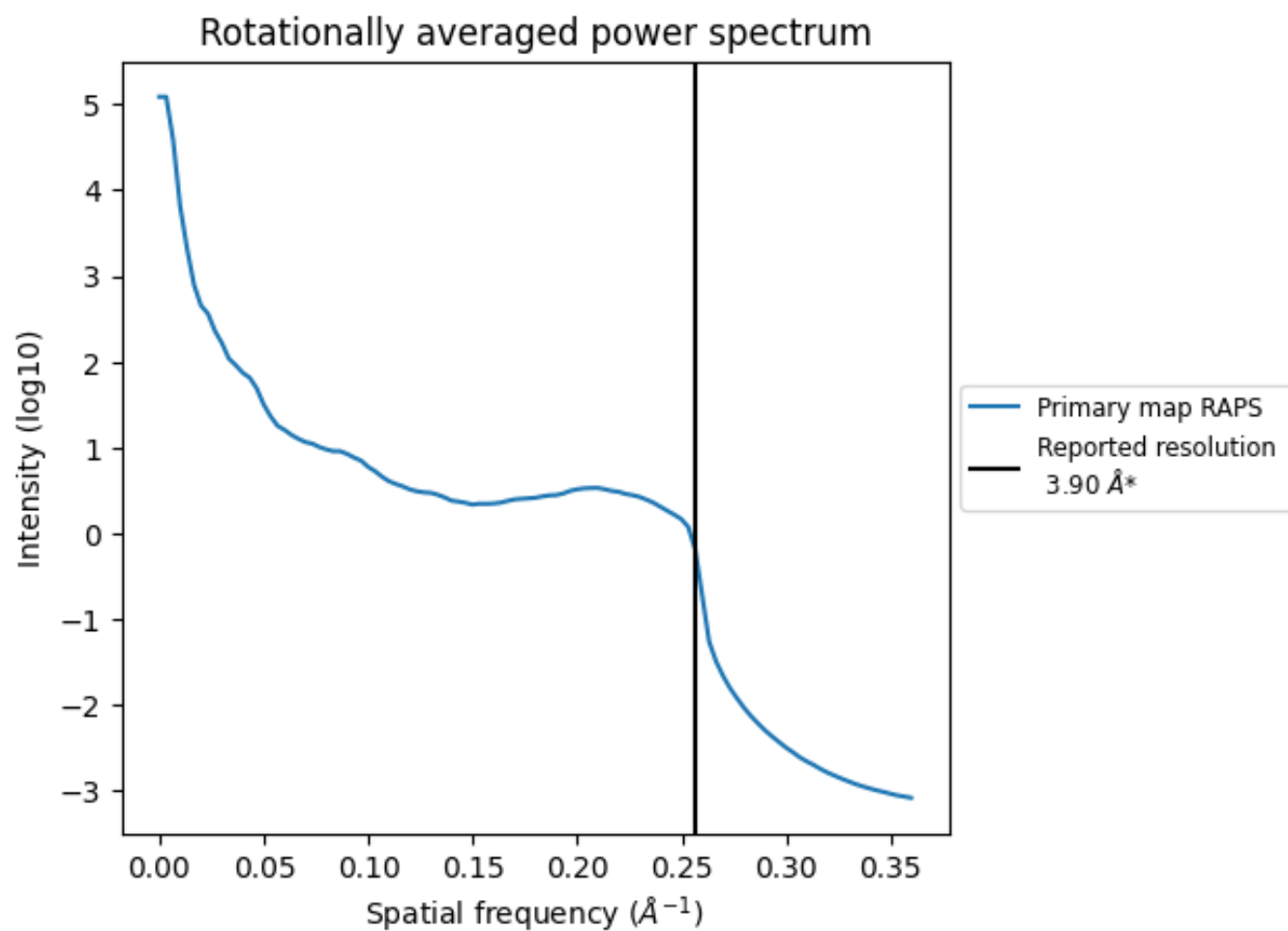
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 862 nm³; this corresponds to an approximate mass of 779 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation

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

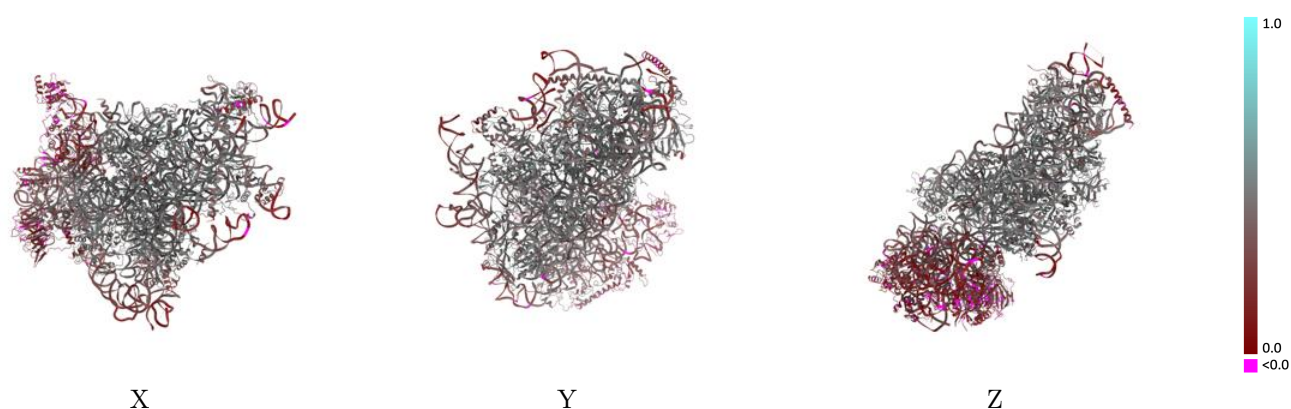
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3019 and PDB model 5A2Q. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)

This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)

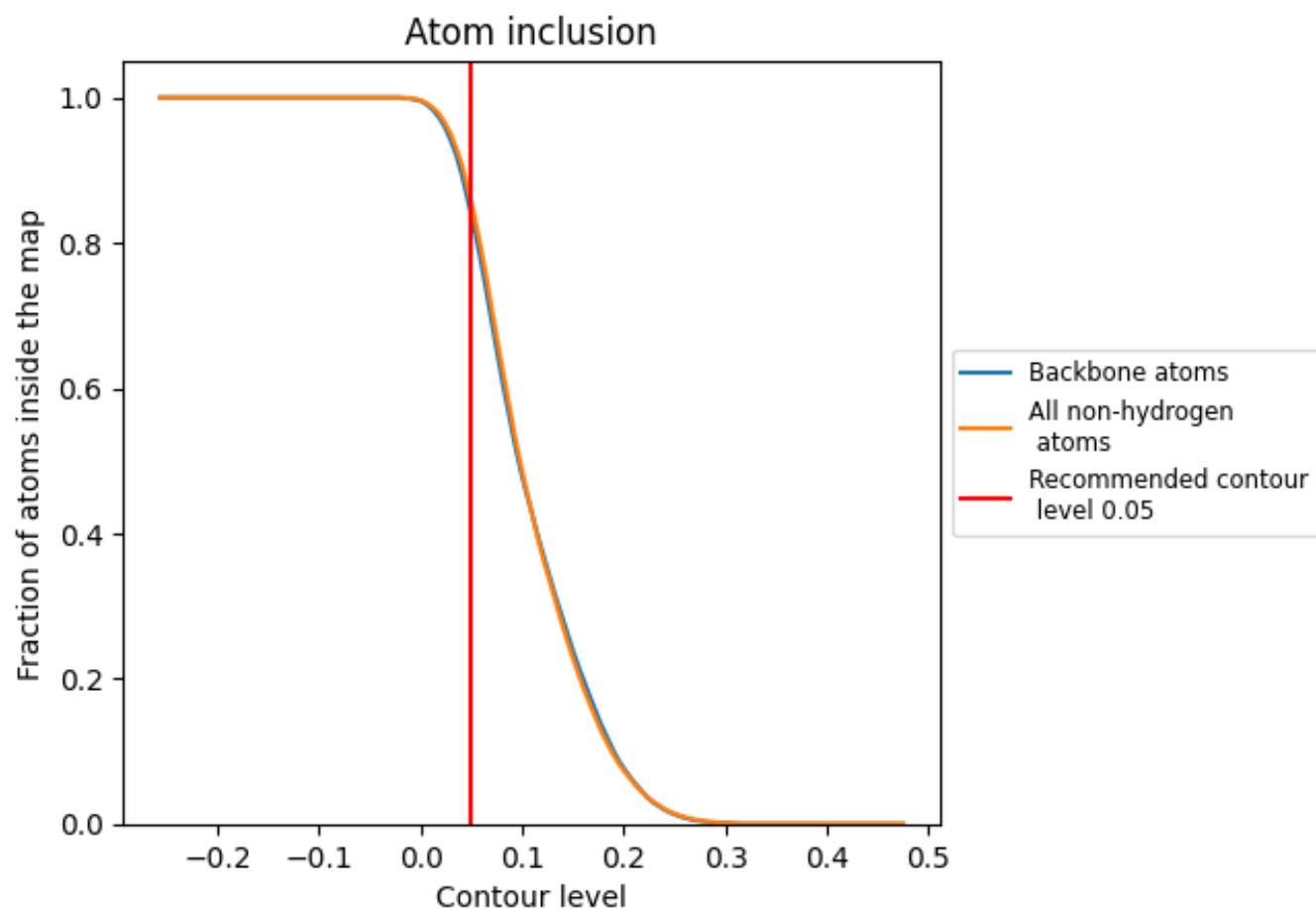


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8570	 0.3750
2	 0.9530	 0.3930
3	 0.8210	 0.2730
A	 0.8920	 0.4550
B	 0.8490	 0.4580
C	 0.8990	 0.4720
D	 0.6410	 0.2630
E	 0.9140	 0.4800
F	 0.7380	 0.3740
G	 0.8880	 0.4380
H	 0.8410	 0.4090
I	 0.8740	 0.4440
J	 0.9060	 0.4580
K	 0.6030	 0.1970
L	 0.8550	 0.4700
M	 0.3990	 0.1030
N	 0.8870	 0.4750
O	 0.8730	 0.4670
P	 0.5910	 0.1630
Q	 0.7620	 0.3140
R	 0.7320	 0.3720
S	 0.5980	 0.2170
T	 0.7000	 0.2140
U	 0.7320	 0.2800
V	 0.9020	 0.4610
W	 0.9130	 0.4870
X	 0.8900	 0.4850
Y	 0.9170	 0.4680
Z	 0.6580	 0.3220
a	 0.8570	 0.4770
b	 0.9060	 0.4710
c	 0.7420	 0.4130
d	 0.7710	 0.2390
e	 0.7750	 0.4290
f	 0.3260	 0.0900



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Chain	Atom inclusion	Q-score
g	 0.6250	 0.2040
h	 0.7520	 0.4390
r	 0.7680	 0.3440
w	 0.4070	 0.2600