



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:07 AM UTC

PDB ID : 1KQS / pdb_00001kqs
Title : The Haloarcula marismortui 50S Complexed with a Pretranslocational Intermediate in Protein Synthesis
Authors : Schmeing, T.M.; Seila, A.C.; Hansen, J.L.; Freeborn, B.; Soukup, J.K.; Scaringe, S.A.; Strobel, S.A.; Moore, P.B.; Steitz, T.A.
Deposited on : 2002-01-07
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

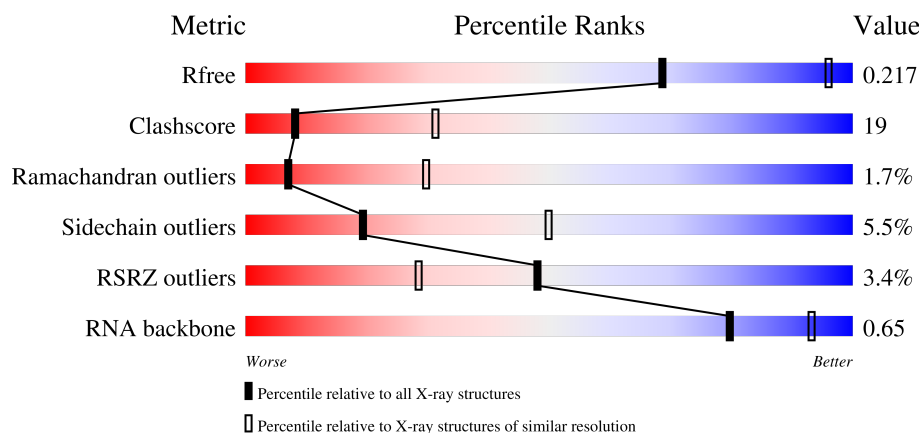
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	2922	57% 31% 5% • 6%
2	9	122	4% 52% 38% 8% •
3	3	3	100% 33% 33% 33%

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Mol	Chain	Length	Quality of chain
4	4	2	100%
5	A	239	2% 53% 40% 6%
6	B	337	50% 44% 6%
7	C	246	51% 43% 7%
8	D	176	6% 22% 49% 7% 20%
9	E	177	% 55% 40% . .
10	F	119	% 57% 40% .
11	G	348	% 5% . 92%
12	H	167	2% 29% 54% 8% . 7%
13	I	145	60% 32% 6% .
14	J	132	61% 37% .
15	K	164	3% 48% 39% . 12%
16	L	194	11% 38% 56% 6% .
17	M	186	4% 38% 53% 9% .
18	N	115	62% 36% .
19	O	148	% 69% 25% . .
20	P	95	% 71% 26% .
21	Q	154	61% 32% . .
22	R	84	63% 30% . .
23	S	119	% 49% 47% .
24	T	66	18% 36% 41% . 20%
25	U	70	4% 39% 50% . 7%
26	V	154	47% 46% 6% .
27	W	91	4% 42% 41% 8% 10%
28	X	240	39% 17% . 41%

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Mol	Chain	Length	Quality of chain
29	Y	73	49% 27% 64% 7%
30	Z	56	66% 32%
31	1	48	65% 29%
32	2	92	63% 41% 49% 9%

2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 98688 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 23S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	conflict	? 3377779

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a RNA chain called CCA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	3	Total	C	N	O	P	0	0	0
			59	28	11	18	2			

- Molecule 4 is a RNA chain called CC-Pmn-pcb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	2	Total	C	N	O	P	0	0	0
			37	18	6	12	1			

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	237	Total	C	N	O	S	0	0	0
			1754	1072	352	325	5			

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	337	Total	C	N	O	S	0	0	0
			2624	1616	493	510	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	deletion	UNP P20279
B	310	ARG	PHE	conflict	UNP P20279

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	C	246	Total	C	N	O	S	0	0	0
			1858	1131	344	382	1			

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	D	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	E	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	F	119	Total	C	N	O	S	0	0	0
			885	552	141	191	1			

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	G	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	H	156	Total	C	N	O	S	0	0	0
			1215	766	233	212	4			

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	I	142	Total	C	N	O	S	0	0	0
			1119	696	199	221	3			

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	J	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	K	145	Total	C	N	O		0	0	0
			1114	668	222	224				

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	L	194	Total	C	N	O	S	0	0	0
			1605	988	346	266	5			

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	M	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L18E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	N	115	Total	C	N	O		0	0	0
			864	529	161	174				

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L19E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	O	143	Total	C	N	O	0	0	0
			1133	680	230	223			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	71	LYS	TYR	conflict	UNP P14119

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L21E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	P	95	Total	C	N	O	0	0	0
			734	450	141	143			

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Q	150	Total	C	N	O	S	0	0	0
			1149	713	209	223	4			

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	R	81	Total	C	N	O	S	0	0	0
			641	389	111	138	3			

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	S	119	Total	C	N	O	0	0	0
			949	568	180	201			

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L24E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	T	53	Total	C	N	O	S	0	0	0
			410	244	75	86	5			

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	U	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	V	154	Total	C	N	O	S	0	0	0
			1195	737	209	243	6			

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L31E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	W	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L32E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	X	142	Total	C	N	O		0	0	0
			1130	686	228	216				

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	Y	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Z	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

- Molecule 31 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	1	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	?	-	ARG	deletion	UNP P22452

- Molecule 32 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	2	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	110	Total	Mg	0	0
			110	110		
33	9	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	J	1	Total	Mg	0	0
			1	1		
33	S	1	Total	Mg	0	0
			1	1		
33	X	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		
33	2	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	2	Total	K	0	0
			2	2		

- Molecule 35 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	73	Total	Na	0	0
			73	73		
35	9	2	Total	Na	0	0
			2	2		
35	A	1	Total	Na	0	0
			1	1		

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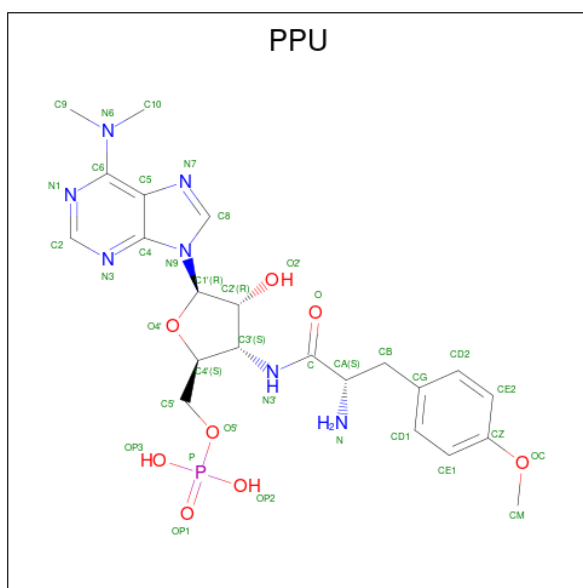
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	C	1	Total 1	Na 1	0	0
35	H	1	Total 1	Na 1	0	0
35	I	1	Total 1	Na 1	0	0
35	K	1	Total 1	Na 1	0	0
35	L	1	Total 1	Na 1	0	0
35	P	1	Total 1	Na 1	0	0
35	Q	3	Total 3	Na 3	0	0
35	R	1	Total 1	Na 1	0	0

- Molecule 36 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

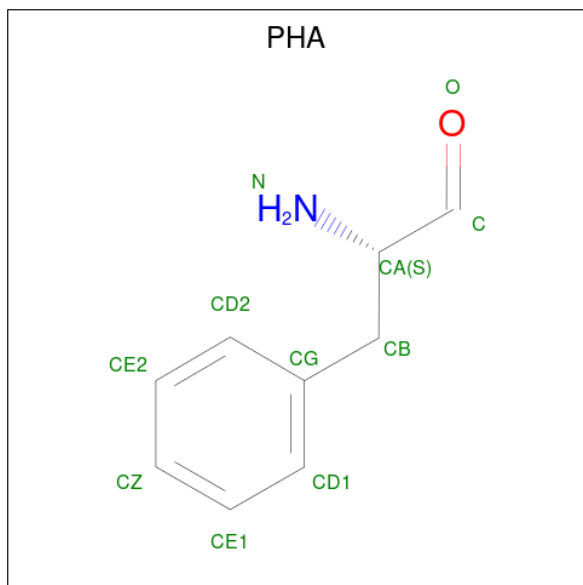
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	10	Total 10	Cl 10	0	0
36	A	1	Total 1	Cl 1	0	0
36	B	1	Total 1	Cl 1	0	0
36	I	3	Total 3	Cl 3	0	0
36	K	1	Total 1	Cl 1	0	0
36	L	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0
36	N	1	Total 1	Cl 1	0	0
36	Q	1	Total 1	Cl 1	0	0
36	X	1	Total 1	Cl 1	0	0
36	2	1	Total 1	Cl 1	0	0

- Molecule 37 is PUROMYCIN-5'-MONOPHOSPHATE (CCD ID: PPU) (formula: $C_{22}H_{30}N_7O_8P$).



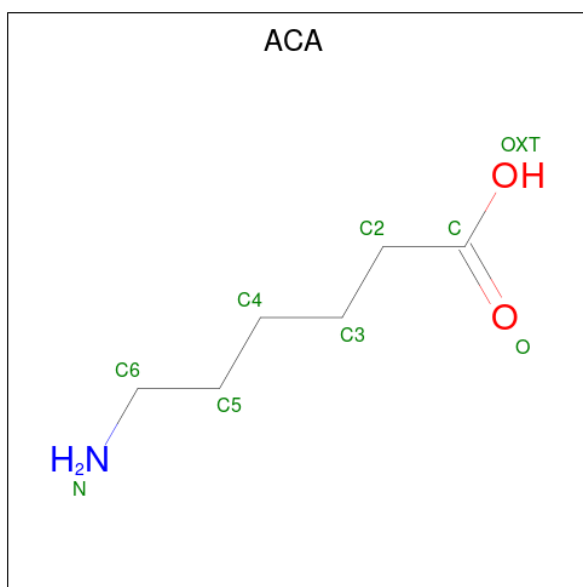
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
37	4	1	Total	C	N	O	P	0	0
			37	22	7	7	1		

- Molecule 38 is PHENYLALANINAL (CCD ID: PHA) (formula: $C_9H_{11}NO$).



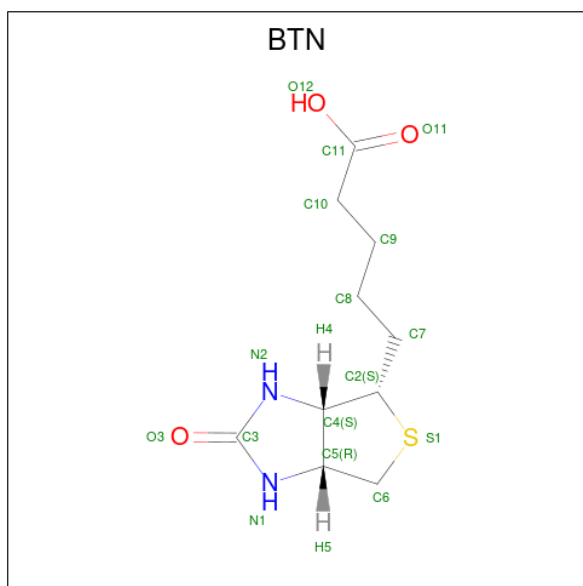
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	4	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 39 is 6-AMINOHEXANOIC ACID (CCD ID: ACA) (formula: $C_6H_{13}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
39	4	1	Total	C	N	O	0	0
			8	6	1	1		

- Molecule 40 is BIOTIN (CCD ID: BTN) (formula: $C_{10}H_{16}N_2O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
40	4	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

- Molecule 41 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	N	1	Total Cd 1 1	0	0
41	T	1	Total Cd 1 1	0	0
41	Y	1	Total Cd 1 1	0	0
41	Z	1	Total Cd 1 1	0	0
41	2	1	Total Cd 1 1	0	0

- Molecule 42 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	0	5873	Total O 5873 5873	0	0
42	9	140	Total O 140 140	0	0
42	3	4	Total O 4 4	0	0
42	4	4	Total O 4 4	0	0
42	A	132	Total O 132 132	0	0
42	B	143	Total O 143 143	0	0
42	C	176	Total O 176 176	0	0
42	D	51	Total O 51 51	0	0
42	E	44	Total O 44 44	0	0
42	F	29	Total O 29 29	0	0
42	G	22	Total O 22 22	0	0
42	H	78	Total O 78 78	0	0
42	I	57	Total O 57 57	0	0
42	J	61	Total O 61 61	0	0
42	K	84	Total O 84 84	0	0

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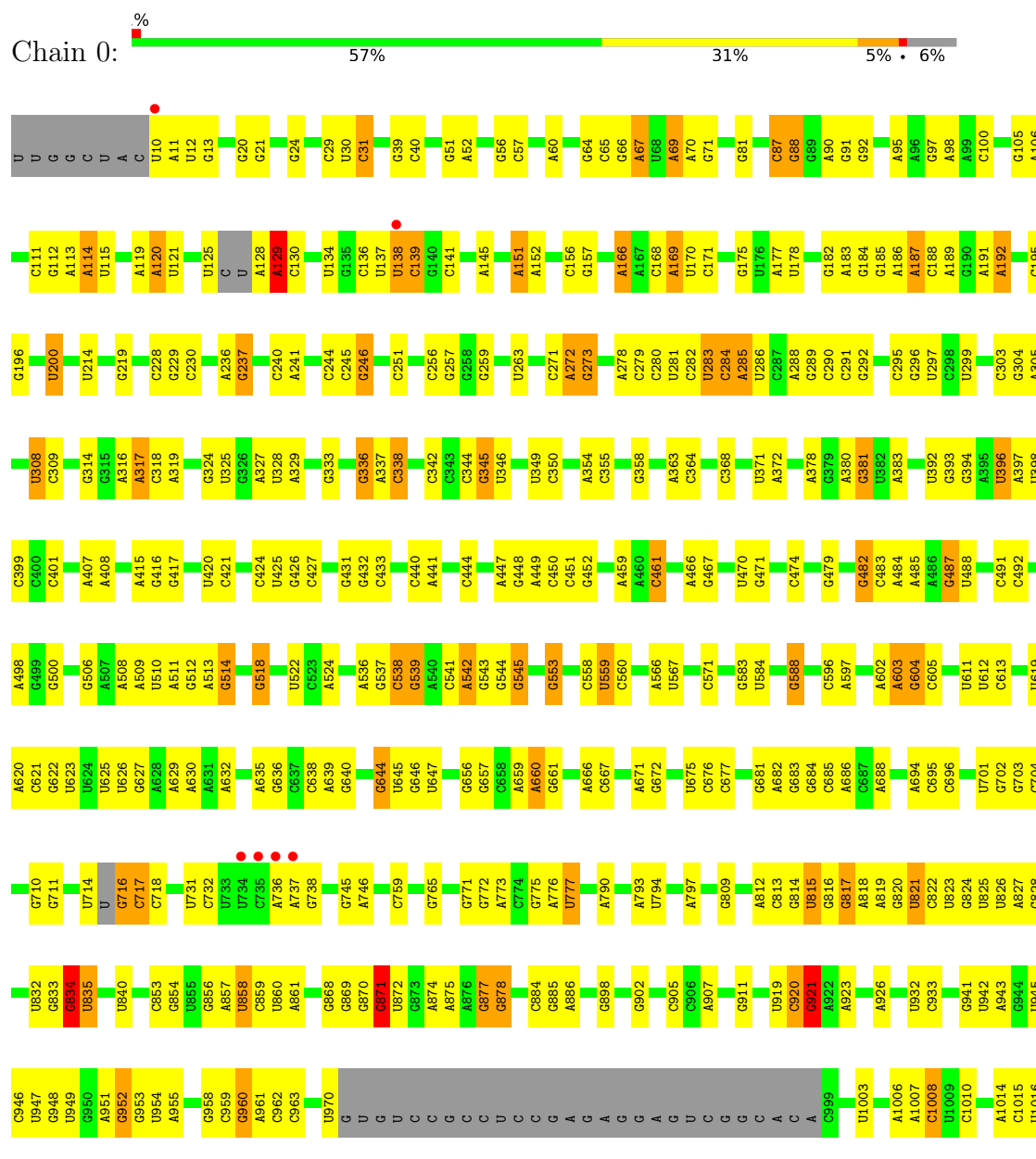
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	L	138	Total 138	O 138	0	0
42	M	70	Total 70	O 70	0	0
42	N	42	Total 42	O 42	0	0
42	O	67	Total 67	O 67	0	0
42	P	56	Total 56	O 56	0	0
42	Q	87	Total 87	O 87	0	0
42	R	36	Total 36	O 36	0	0
42	S	37	Total 37	O 37	0	0
42	T	26	Total 26	O 26	0	0
42	U	16	Total 16	O 16	0	0
42	V	66	Total 66	O 66	0	0
42	W	30	Total 30	O 30	0	0
42	X	96	Total 96	O 96	0	0
42	Y	33	Total 33	O 33	0	0
42	Z	55	Total 55	O 55	0	0
42	1	42	Total 42	O 42	0	0
42	2	76	Total 76	O 76	0	0

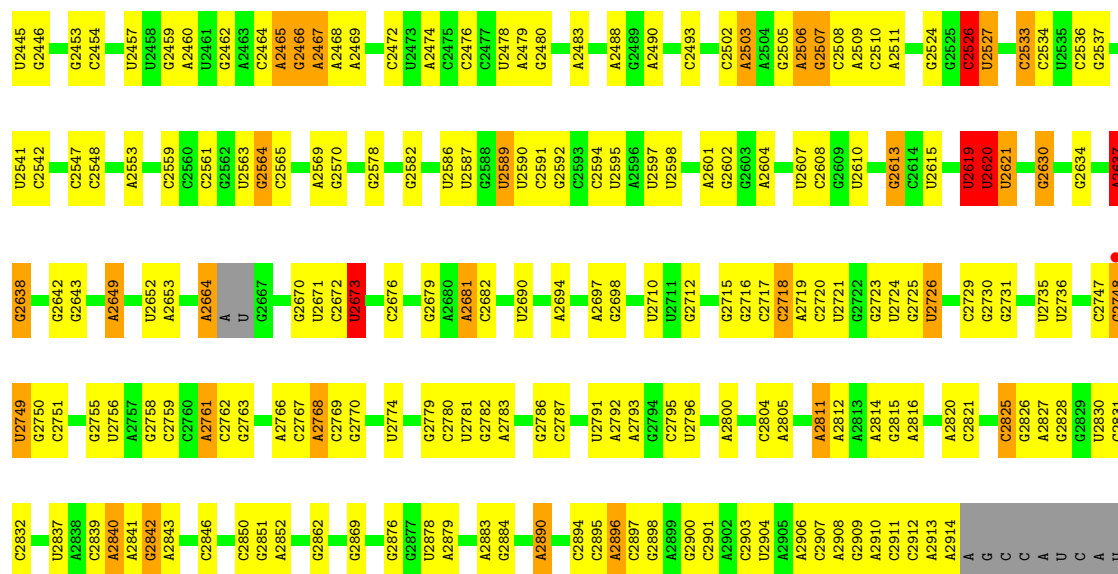
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 23S rRNA



A2353	G2256	G	A2123	G2033	A1924	A1783	C1880	A1573	A1463	U1333	G1216	G1134	C1025
A2354	G2257	C	G2128	U2034	G1925	U1784	G1881	A1580	U1464	C1334	G1224	G1136	U1029
A2355	A2258	A	U2129	A2039	G1926		A1883	G1589	A1470	G1340	G1225	G1137	
G2357	U2265	C	U2133	G2044	A1930	U1788	A1884	G1588	A1471	A1341	G1229	G1151	G1039
G2358	A2266	G	G2134	G2045	A1931		A1885	G1589	A1472	C1342	U1234	G1158	G1044
G2359	G2267	G	A2135	G2046	U1939	U1798	C1886	G1582	U1473	C1343	U1235	G1159	G1045
C2360	C2268	G	G2136	C2047	C1940		C1887	G1593	A1474	G1344	U1236	G1160	
A2361	C2269	C	A	G2050	A1941	A1804	C1692	G1594	U1477	A1345	U1237	A1161	G1050
A2362	G2270	C	C	G	A1942	G1805	C1699	G1595	U1478	U1346	U1238	G1162	G1051
G2363	G2271	C	G	G	C1943	G1806	C1700	U1596	C1483	G1351	G1239	G1163	G1052
A2364	G2272	C	U	A2054			C1701	A1597	G1484	A1352	U1240	U1164	G1053
G2365	C2273	C	G		G1951	C1810	A1702	A1598	A1485	C1353	A1242	G1165	G1054
A2369	A2274	C	U	U2064	U		U1702	A1603		C1360	C1243	G1166	G1055
U2276	G2275	G	G	G2068	A	A1815	A1710	G1604	A1494	C1366	U1244	G1167	U1056
U2277	U2277	U	C		A	U1816	A1711	G1605	A1495	C1245	U1245	U1057	
U2281		G	G	C2071	C	U1817	A1712	G1609	G1496	A1246	U1249	U1169	A1058
U2282		C	C	G2072	U	G1818		G1610	G1497	A1372	U1250	U1170	G1059
G2285		A	G	G2073	U	G1819	A1717	G1613	U1498	C1377	G1251	A1171	
A2291		A	U	A2074	G	G1820	U1722	G1614	U1499	G1378	C1252	A1172	U1066
A2300		C	U	G2075	C	G1828	U1723	G1615	U1500	A1379	A1253	A1173	A1067
A2301		C	G	U2078	C	A1829	U1724	A1616	U1503	U1380	C1253	A1174	
A2302		C	U	G2079	C	G1830	C1725	C1617	A1504			G1175	G1072
A2303		C	A	G2080	U1984	C1834	G1730	A1624	U1506	U1266		C1176	
A2401		A	C	A2081		U1835	C1731	U1624	U1505	C1267	U1078	A1177	
A2402		U	G	C2084	A1969	A1840	A1732	U1625	A1515	C1268	A1079	U1180	
A2403		U	C	A2085	G1970	U1841	A1733	A1626	C1516	G1269	C1080	U1181	
A2408		C	A	U2088	U1972	C1856	C1734	G1627	U1517		A1081	C1182	
C2409		C	U	A2089	A1973	G1868	C1735	C1633	G1523	C1273		C1183	
C2410		C	G	G2090	G1974	U1874	U1741	U1634	U1524	U1279	A1086	C1184	
C2411		C	G	G2091	C	U1878	A1742	U1635	G1525	A1287	G1087	U1185	
C2412		C	U	G2092	G1979	G1878	G1743	U1636	A1526	U1288	A1088	U1186	
C2413		C	G	G2093	U1980	C1879		A1637	A1527	C1289	U1095	U1187	
C2414		C	G	G2094	U1981	U1879	G1751	A1641	A1528	U1290	U1096	U1188	
C2415		C	G	A2095	U1982	C1880	G1752	A1642	G1529	U1291	A1097	U1189	
C2416		C	G	A2096	C1993	C1881	C1753	A1653	G1535	G1304	A1098	U1190	
C2417		C	G	A2097	A1994	C1882	U1759	U1654	G1536	C1305	G1110	U1191	
C2418		C	C	G2099	G1995	U1883	A1759	G1655	C1545	U1306	A1114	U1192	
C2419		C	C	A2100	U1996	A1884	G1760	G1656	G1546	A1307	U1115	C1201	
C2420		C	U	G2102	U2004	A1885	U1761	A1657	G1557	A1308	U1116	U1117	
C2421		C	U	A2103	G2005	U1887	C1762	A1658	C1558	G1311	U1118	U1119	
C2422		C	C		U2008	G1902	C1763	A1659	U	G1312	U1205	G1119	
C2423		C	C	G2110	U2009	U1903	U1765	G1660	U1561	U1206	U1120	U1207	
C2424		C	C	G2111	A2010	A1904	A1767	C1666	C1562	G1316	C1208	G1121	
C2425		C	C	G2112	A2011		C1768	A1667	G1563	G1325	U1209	U1122	
C2426		C	C	G2113	U2012	A1909	C1769	U1668	C1564	A1328	G1210	A1123	
C2427		C	C	G2114	G2013	A1910	U1770	A1669	C1450	A1329	C1212	U1130	
C2428		C	C	U2115	G2014		U1771	G1670	U1451	A1330	G1213	G1131	
C2429		C	C	U2116	A2015	G1916	C1772	G1671	G1568	A1331	G1214	A1132	
C2430		C	C	U2117	U2016		G1773	A1677	U1569	C1332	C1215	A1133	
C2431		C	C	U2118	U2017	A1919	A1778	G1678					
C2432		C	C	U2119	U2018	G1923	A1779	C1679					
C2433		C	C	U2120	A2019								
C2434		C	C	U2121									
C2435		C	C	U2122									
C2436		C	C										
C2437		C	C										
C2438		C	C										
C2439		C	C										
C2440		C	C										
C2441		C	C										
C2442		C	C										
C2443		C	C										
C2444		C	C										



• Molecule 2: 5S RRNA



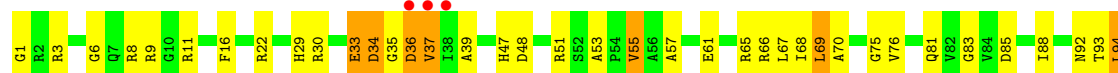
• Molecule 3: CCA

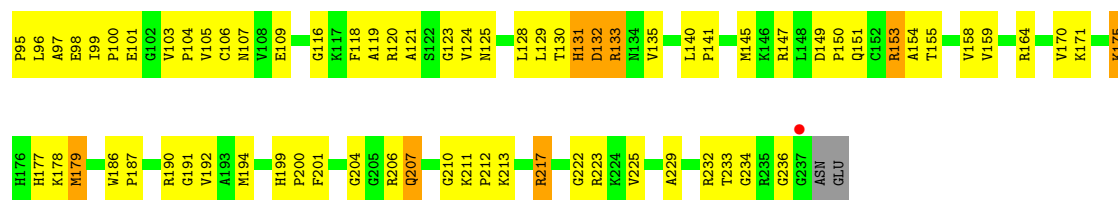


• Molecule 4: CC-Pmn-pcb



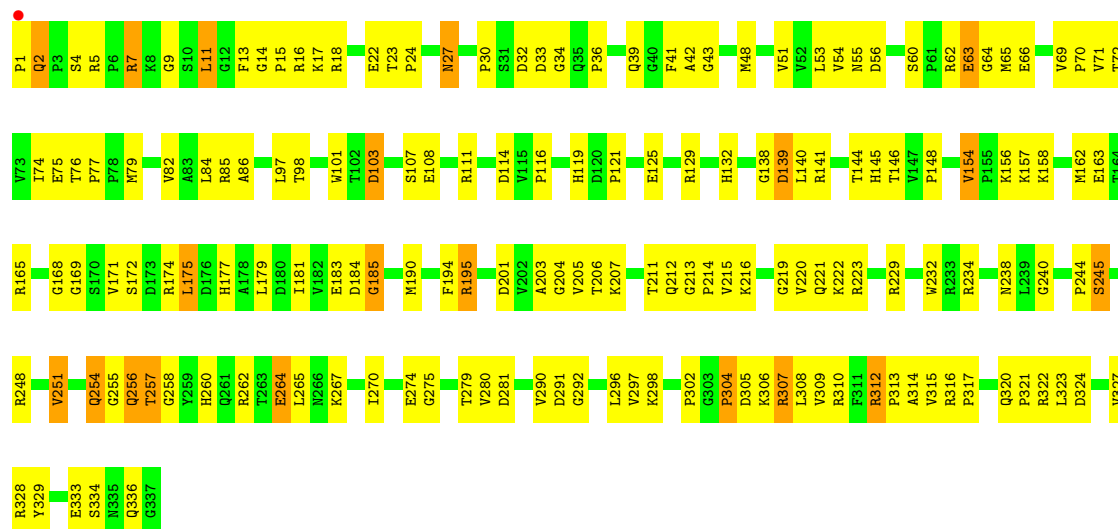
• Molecule 5: RIBOSOMAL PROTEIN L2





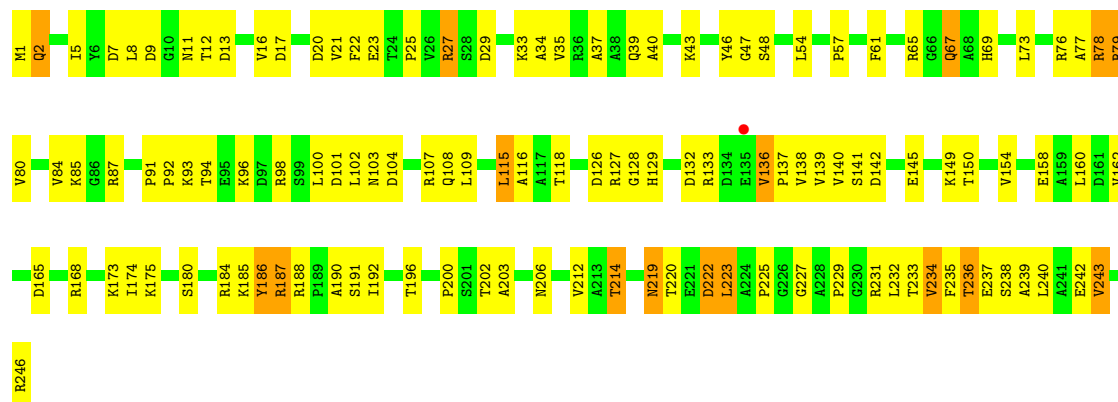
• Molecule 6: RIBOSOMAL PROTEIN L3

Chain B: 50% 44% 6%



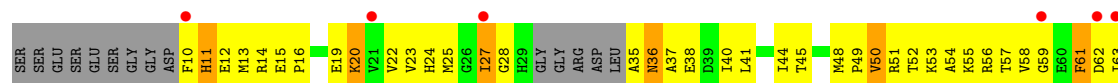
• Molecule 7: RIBOSOMAL PROTEIN L4

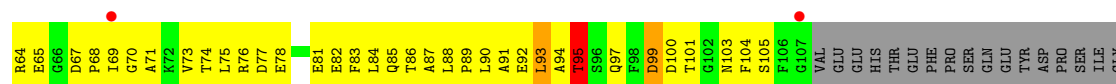
Chain C: 51% 43% 7%



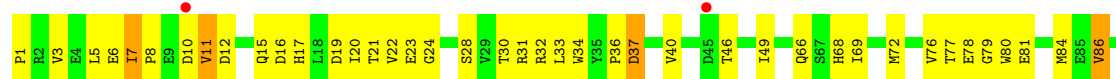
• Molecule 8: RIBOSOMAL PROTEIN L5

Chain D: 6% 22% 49% 7% 20%

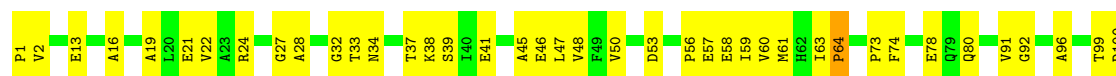




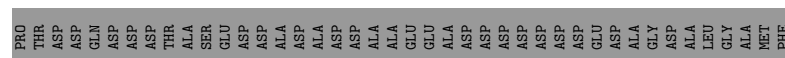
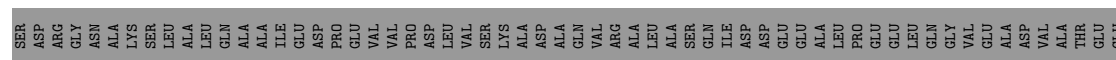
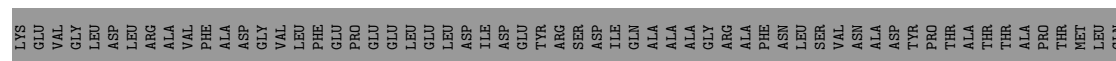
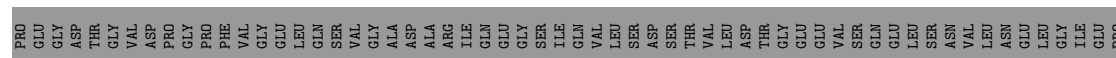
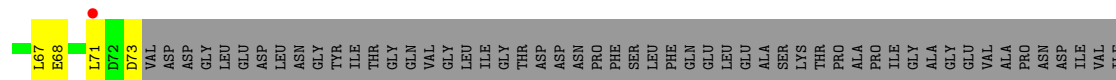
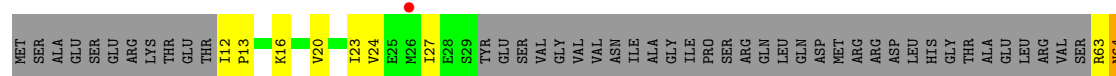
● Molecule 9: RIBOSOMAL PROTEIN L6



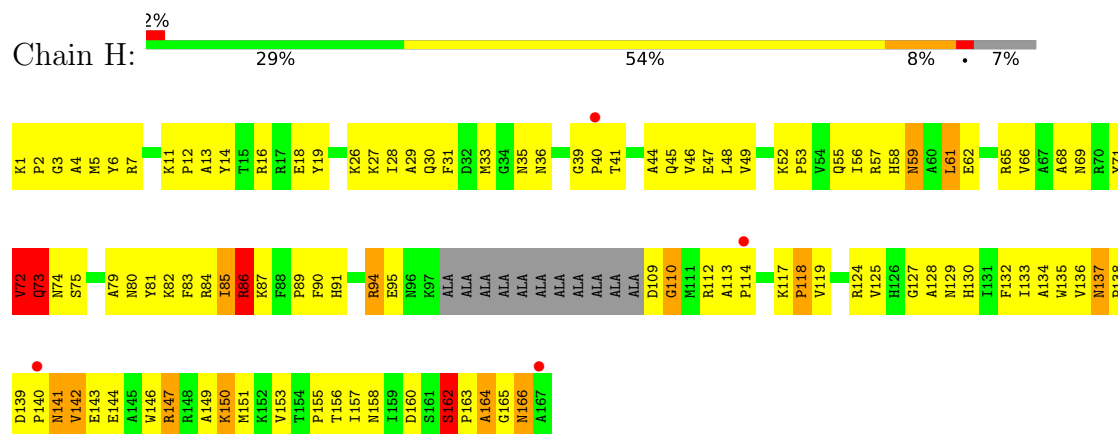
● Molecule 10: RIBOSOMAL PROTEIN L7AE



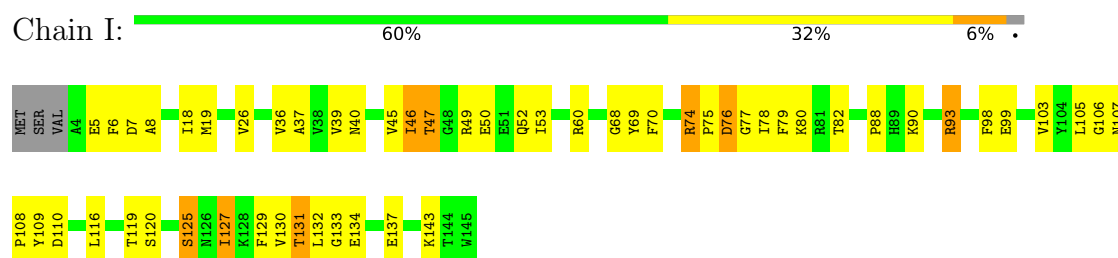
● Molecule 11: RIBOSOMAL PROTEIN L10



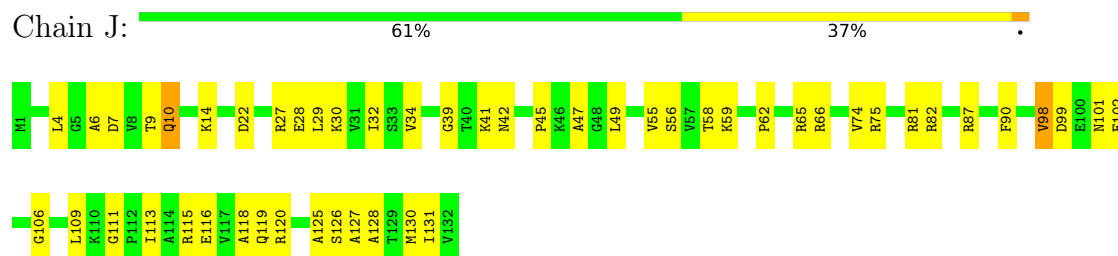
• Molecule 12: RIBOSOMAL PROTEIN L10E



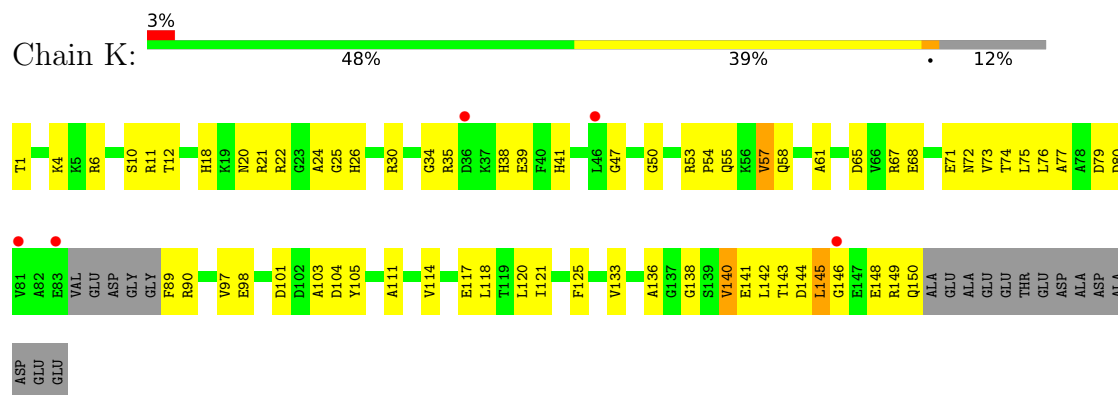
• Molecule 13: RIBOSOMAL PROTEIN L13



• Molecule 14: RIBOSOMAL PROTEIN L14

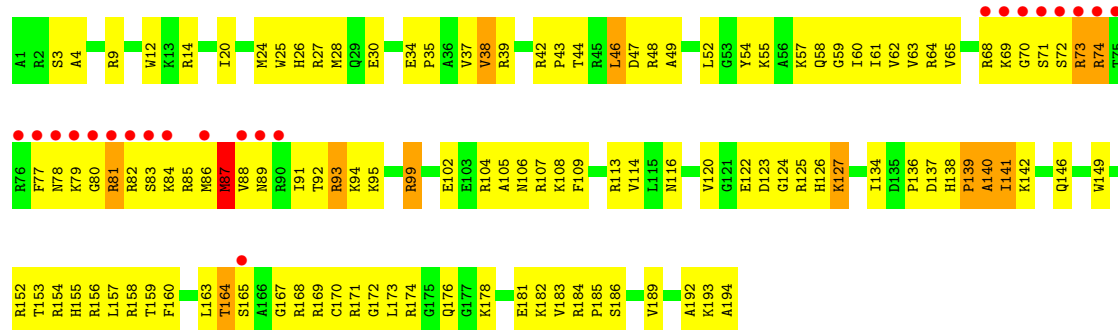


• Molecule 15: RIBOSOMAL PROTEIN L15

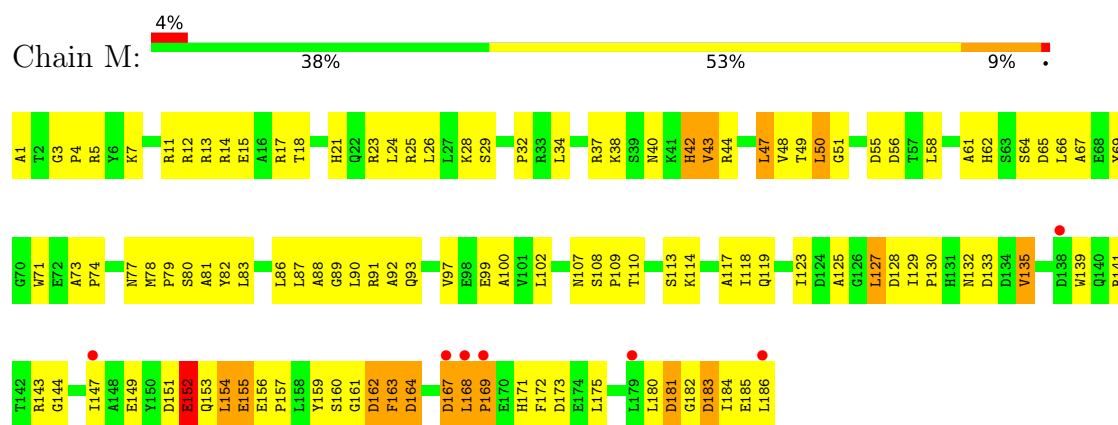


• Molecule 16: RIBOSOMAL PROTEIN L15E

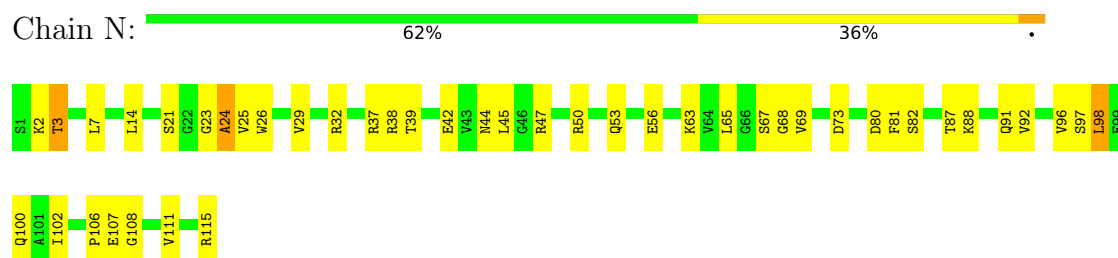




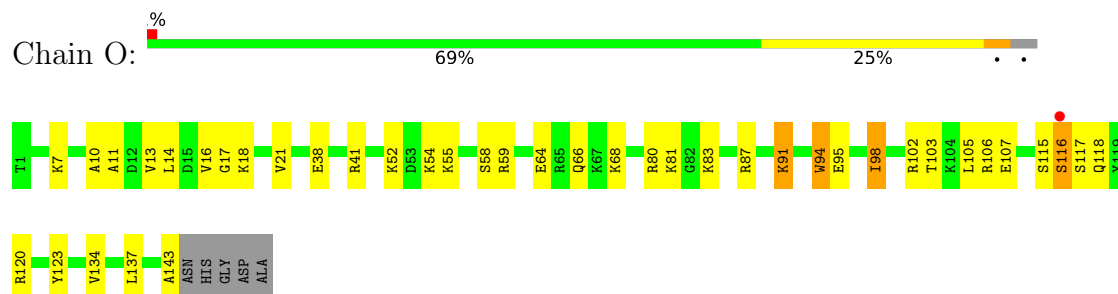
• Molecule 17: RIBOSOMAL PROTEIN L18



• Molecule 18: RIBOSOMAL PROTEIN L18E



• Molecule 19: RIBOSOMAL PROTEIN L19E

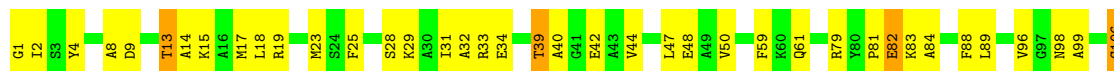


• Molecule 20: RIBOSOMAL PROTEIN L21E

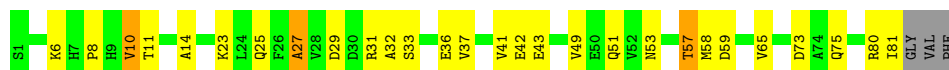




• Molecule 21: RIBOSOMAL PROTEIN L22



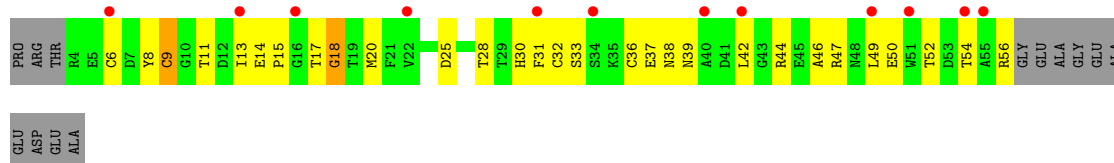
• Molecule 22: RIBOSOMAL PROTEIN L23



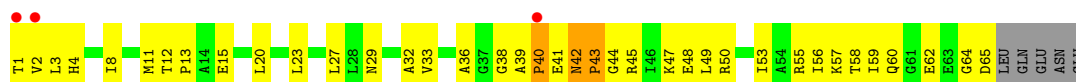
• Molecule 23: RIBOSOMAL PROTEIN L24



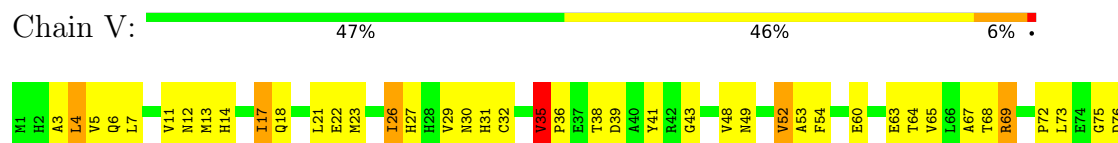
• Molecule 24: RIBOSOMAL PROTEIN L24E



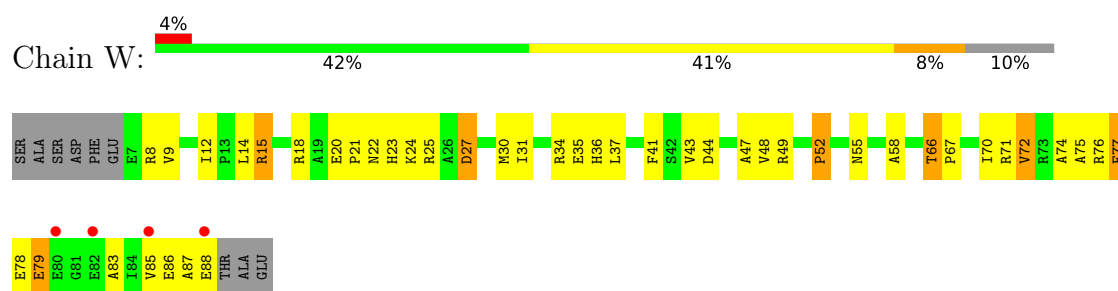
• Molecule 25: RIBOSOMAL PROTEIN L29



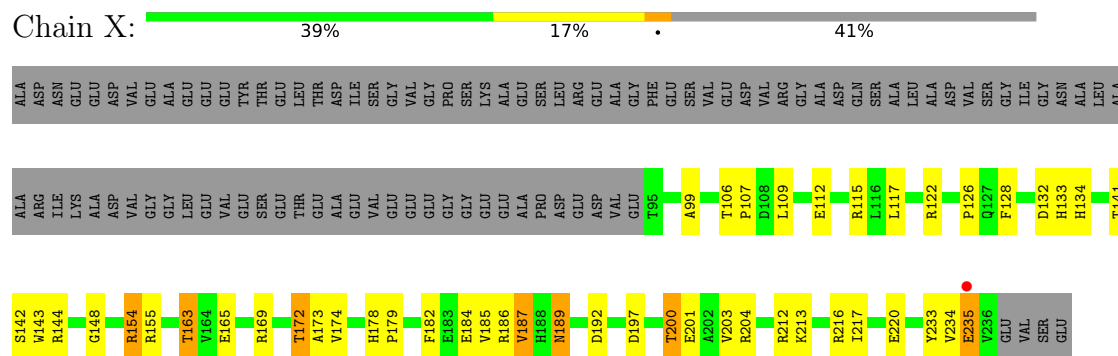
• Molecule 26: RIBOSOMAL PROTEIN L30



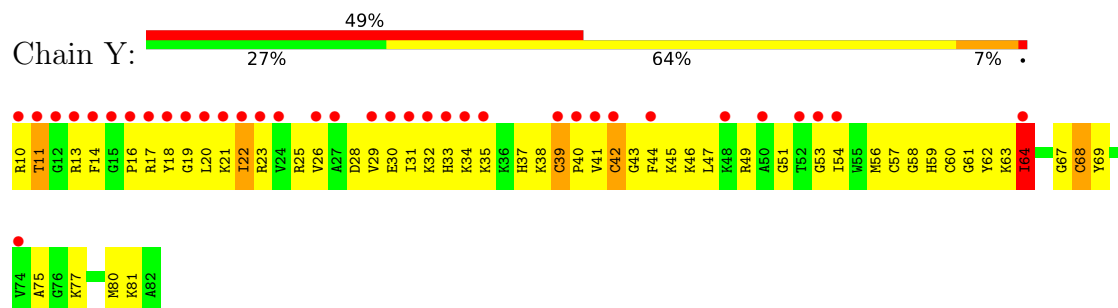
• Molecule 27: RIBOSOMAL PROTEIN L31E



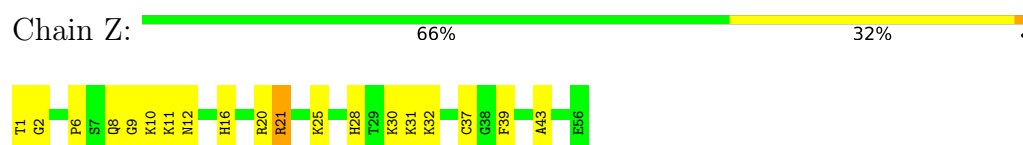
• Molecule 28: RIBOSOMAL PROTEIN L32E



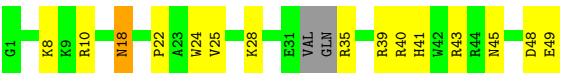
• Molecule 29: RIBOSOMAL PROTEIN L37Ae



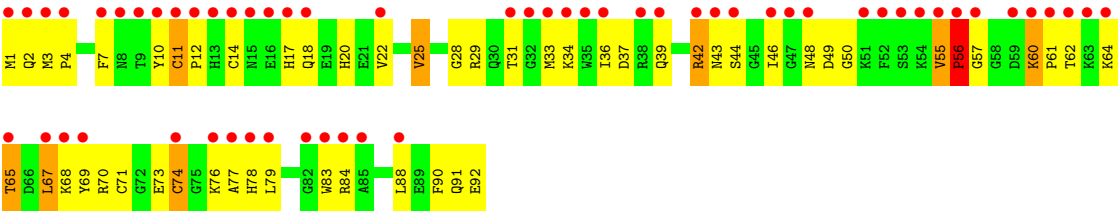
• Molecule 30: RIBOSOMAL PROTEIN L37E



• Molecule 31: RIBOSOMAL PROTEIN L39E



● Molecule 32: RIBOSOMAL PROTEIN L44E



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.78Å 300.35Å 574.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 20.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.10) 95.9 (20.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 3.06Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.173 , 0.220 0.172 , 0.217	Depositor DCC
R_{free} test set	3329 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	98688	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PPU, CD, CL, K, MG, ACA, BTN, PHA

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	0	0.40	2/66076 (0.0%)	0.63	37/103052 (0.0%)
2	9	0.41	0/2905	0.67	4/4528 (0.1%)
3	3	0.68	0/65	1.13	0/99
4	4	0.36	0/40	0.64	0/60
5	A	0.45	0/1787	1.01	9/2409 (0.4%)
6	B	0.45	0/2689	1.02	9/3652 (0.2%)
7	C	0.51	0/1883	0.99	8/2551 (0.3%)
8	D	0.38	0/1111	0.94	7/1498 (0.5%)
9	E	0.43	0/1382	0.89	2/1880 (0.1%)
10	F	0.40	0/896	0.88	2/1219 (0.2%)
11	G	0.40	0/241	0.79	0/324
12	H	0.49	0/1246	1.24	14/1686 (0.8%)
13	I	0.46	0/1135	0.96	3/1530 (0.2%)
14	J	0.42	0/1003	1.01	2/1351 (0.1%)
15	K	0.39	0/1126	1.01	5/1504 (0.3%)
16	L	0.52	0/1633	1.07	8/2180 (0.4%)
17	M	0.38	0/1473	1.10	16/1999 (0.8%)
18	N	0.47	0/873	0.97	5/1181 (0.4%)
19	O	0.45	0/1143	0.86	0/1521
20	P	0.44	0/748	1.03	5/1005 (0.5%)
21	Q	0.47	0/1172	0.97	5/1578 (0.3%)
22	R	0.41	0/648	0.90	2/875 (0.2%)
23	S	0.43	0/957	0.97	3/1289 (0.2%)
24	T	0.37	0/417	0.88	1/562 (0.2%)
25	U	0.40	0/502	0.99	2/675 (0.3%)
26	V	0.51	0/1218	1.03	8/1655 (0.5%)
27	W	0.46	0/664	0.99	2/895 (0.2%)
28	X	0.49	0/1146	0.97	2/1536 (0.1%)
29	Y	0.40	0/575	1.01	3/763 (0.4%)
30	Z	0.48	0/437	0.97	2/578 (0.3%)
31	1	0.40	0/398	0.76	0/527
32	2	0.42	0/771	0.95	7/1024 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.41	2/98360 (0.0%)	0.75	173/147186 (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
1	0	1	37
2	9	0	1
26	V	0	1
All	All	1	39

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	U	O5'-C5'	-7.30	1.31	1.42
1	0	2620	U	C2'-O2'	5.77	1.50	1.41

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	13.73	130.09	109.50
16	L	141	ILE	N-CA-C	-13.57	100.91	111.90
12	H	141	ASN	N-CA-C	-13.49	96.91	113.50
1	0	1979	G	C2'-C3'-O3'	12.99	128.98	109.50
12	H	74	ASN	N-CA-C	-11.86	95.15	113.89
17	M	135	VAL	N-CA-C	-11.40	101.95	113.47
1	0	2619	U	C5'-C4'-C3'	-9.84	101.24	116.00
1	0	1164	U	OP1-P-O3'	-9.79	78.64	108.00
16	L	74	ARG	N-CA-C	9.69	124.31	108.52
1	0	1563	G	C4'-C3'-O3'	8.86	122.68	109.40
1	0	1164	U	OP2-P-O3'	-8.81	81.56	108.00
6	B	154	VAL	CA-C-N	8.68	128.26	119.24
6	B	154	VAL	C-N-CA	8.68	128.26	119.24
1	0	1942	A	C5'-C4'-C3'	8.65	128.97	116.00
8	D	136	ARG	CA-C-N	8.64	130.64	119.84
8	D	136	ARG	C-N-CA	8.64	130.64	119.84
12	H	137	ASN	N-CA-C	-8.57	98.88	110.36
1	0	2620	U	C4'-C3'-O3'	-8.56	96.56	109.40
1	0	2619	U	C4'-C3'-O3'	-8.22	100.67	113.00
12	H	156	THR	N-CA-C	-8.21	98.32	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	157	LYS	N-CA-C	-7.99	104.14	114.04
23	S	52	ARG	N-CA-C	7.86	123.63	113.18
9	E	11	VAL	N-CA-C	7.81	121.30	109.20
12	H	147	ARG	N-CA-C	-7.66	102.93	111.82
15	K	57	VAL	N-CA-C	-7.58	105.45	112.43
5	A	222	GLY	N-CA-C	-7.40	105.04	114.37
8	D	100	ASP	N-CA-C	-7.40	104.25	113.28
32	2	11	CYS	CA-C-N	7.34	127.04	119.56
32	2	11	CYS	C-N-CA	7.34	127.04	119.56
27	W	22	ASN	N-CA-C	7.31	119.88	111.11
20	P	17	LYS	N-CA-C	-7.28	100.58	109.83
17	M	169	PRO	N-CA-C	-7.25	104.49	114.27
26	V	35	VAL	N-CA-C	7.16	116.13	107.61
16	L	87	MET	N-CA-C	7.14	120.57	110.50
2	9	3039	U	N1-C1'-C2'	7.12	122.69	112.00
17	M	133	ASP	N-CA-C	7.10	119.92	111.33
16	L	70	GLY	N-CA-C	6.97	123.25	112.45
6	B	265	LEU	N-CA-C	6.86	120.63	110.48
18	N	82	SER	N-CA-C	-6.86	101.98	110.41
17	M	153	GLN	N-CA-C	-6.82	103.92	113.20
1	0	1120	U	C5'-C4'-C3'	-6.78	105.82	116.00
16	L	139	PRO	N-CA-C	-6.78	100.83	111.34
23	S	54	ASP	N-CA-C	-6.76	105.00	113.18
15	K	145	LEU	N-CA-C	-6.72	104.03	111.36
1	0	834	G	C2'-C3'-O3'	-6.63	103.75	113.70
32	2	55	VAL	CA-C-N	6.60	128.09	119.84
32	2	55	VAL	C-N-CA	6.60	128.09	119.84
6	B	222	LYS	N-CA-C	-6.60	100.19	110.42
13	I	88	PRO	N-CA-C	-6.57	103.61	112.48
8	D	48	MET	N-CA-C	6.55	117.14	109.60
30	Z	43	ALA	N-CA-C	-6.52	104.25	111.36
29	Y	64	ILE	N-CA-C	6.38	118.94	108.99
21	Q	34	GLU	N-CA-C	6.37	118.23	111.28
14	J	111	GLY	CA-C-N	6.34	126.30	120.21
14	J	111	GLY	C-N-CA	6.34	126.30	120.21
1	0	2726	U	N1-C1'-C2'	6.30	121.45	112.00
5	A	70	ALA	N-CA-C	6.29	118.72	109.42
5	A	213	LYS	N-CA-C	6.28	120.20	112.54
26	V	69	ARG	N-CA-C	6.21	120.49	112.41
18	N	2	LYS	N-CA-C	-6.21	101.29	110.48
22	R	57	THR	N-CA-C	6.19	118.91	110.55
21	Q	122	GLN	N-CA-C	-6.18	99.09	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1819	G	C5'-C4'-C3'	6.17	125.26	116.00
2	9	3039	U	C4'-C3'-O3'	-6.17	103.75	113.00
12	H	162	SER	CA-C-N	-6.16	112.14	119.84
12	H	162	SER	C-N-CA	-6.16	112.14	119.84
25	U	42	ASN	CA-C-N	6.15	127.53	119.84
25	U	42	ASN	C-N-CA	6.15	127.53	119.84
12	H	1	LYS	CA-C-N	6.13	126.04	119.85
12	H	1	LYS	C-N-CA	6.13	126.04	119.85
5	A	118	PHE	N-CA-C	6.12	119.54	110.48
7	C	80	VAL	CA-C-N	6.06	126.50	119.47
7	C	80	VAL	C-N-CA	6.06	126.50	119.47
5	A	133	ARG	N-CA-C	-6.04	105.74	113.23
6	B	213	GLY	CA-C-N	6.03	125.51	119.24
6	B	213	GLY	C-N-CA	6.03	125.51	119.24
30	Z	21	ARG	N-CA-C	6.02	118.74	111.40
5	A	207	GLN	N-CA-C	5.99	118.05	108.41
12	H	155	PRO	N-CA-C	5.98	120.38	111.41
18	N	24	ALA	N-CA-C	-5.97	106.97	114.56
28	X	143	TRP	N-CA-C	5.96	118.98	110.10
26	V	75	GLY	N-CA-C	5.95	119.53	112.33
20	P	47	VAL	CA-C-N	5.95	127.27	119.84
20	P	47	VAL	C-N-CA	5.95	127.27	119.84
1	0	1504	A	N9-C1'-C2'	5.93	120.89	112.00
1	0	920	C	C2'-C3'-O3'	-5.89	104.86	113.70
7	C	175	LYS	N-CA-C	5.88	117.88	110.24
1	0	1592	G	N9-C1'-C2'	5.84	120.77	112.00
17	M	108	SER	CA-C-N	5.84	127.15	119.84
17	M	108	SER	C-N-CA	5.84	127.15	119.84
17	M	51	GLY	CA-C-N	5.84	125.98	119.32
17	M	51	GLY	C-N-CA	5.84	125.98	119.32
24	T	18	GLY	N-CA-C	5.79	119.34	112.33
22	R	27	ALA	N-CA-C	-5.79	99.29	108.73
17	M	117	ALA	N-CA-C	-5.78	104.89	111.07
18	N	69	VAL	N-CA-C	5.78	116.80	108.48
5	A	48	ASP	CA-C-N	5.76	125.43	119.56
5	A	48	ASP	C-N-CA	5.76	125.43	119.56
2	9	3103	A	C5'-C4'-O4'	5.75	118.43	109.80
8	D	15	GLU	CA-C-N	5.75	127.03	119.84
8	D	15	GLU	C-N-CA	5.75	127.03	119.84
16	L	73	ARG	N-CA-C	-5.70	98.64	108.56
7	C	186	TYR	N-CA-C	5.65	118.83	110.46
21	Q	137	ASN	N-CA-C	5.65	118.82	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	I	110	ASP	N-CA-C	-5.64	106.06	113.12
16	L	127	LYS	N-CA-C	-5.64	98.33	108.48
32	2	60	LYS	N-CA-C	-5.63	102.98	110.07
26	V	17	ILE	N-CA-C	-5.62	106.22	111.45
1	0	2301	A	N9-C1'-C2'	5.61	120.41	112.00
18	N	50	ARG	N-CA-C	5.60	117.46	111.36
32	2	43	ASN	N-CA-C	5.60	119.95	113.18
7	C	219	ASN	N-CA-C	5.59	117.74	109.69
20	P	84	ILE	N-CA-C	5.59	115.90	107.80
17	M	168	LEU	N-CA-C	5.58	120.80	108.64
1	0	871	G	C5'-C4'-O4'	-5.57	101.44	109.80
1	0	2620	U	C5'-C4'-C3'	-5.57	106.84	115.20
1	0	129	A	C2'-C3'-O3'	5.54	122.01	113.70
1	0	2664	A	N9-C1'-C2'	5.53	120.29	112.00
26	V	143	THR	N-CA-C	-5.53	105.35	111.71
27	W	79	GLU	N-CA-C	5.53	119.87	113.18
20	P	49	ASN	N-CA-C	5.50	117.63	110.53
1	0	138	U	C2'-C3'-O3'	-5.49	105.46	113.70
17	M	102	LEU	N-CA-C	5.49	117.64	109.25
1	0	2313	C	C5'-C4'-C3'	5.47	124.21	116.00
6	B	175	LEU	N-CA-C	-5.47	105.22	111.07
12	H	86	ARG	N-CA-C	5.47	119.95	113.28
26	V	35	VAL	CA-C-N	5.43	125.37	119.78
26	V	35	VAL	C-N-CA	5.43	125.37	119.78
15	K	12	THR	N-CA-C	5.41	119.86	113.16
1	0	2291	A	N9-C1'-C2'	5.40	120.09	112.00
7	C	78	ARG	N-CA-C	5.37	116.43	108.60
1	0	2637	A	C4'-C3'-O3'	5.35	117.43	109.40
29	Y	39	CYS	CA-C-N	5.33	124.66	118.85
29	Y	39	CYS	C-N-CA	5.33	124.66	118.85
17	M	3	GLY	CA-C-N	5.32	125.13	119.28
17	M	3	GLY	C-N-CA	5.32	125.13	119.28
12	H	7	ARG	N-CA-C	5.30	119.37	113.01
17	M	152	GLU	N-CA-C	-5.30	105.67	111.82
12	H	110	GLY	N-CA-C	-5.30	100.63	113.18
7	C	191	SER	CA-C-O	5.26	120.99	117.94
8	D	137	PRO	N-CA-C	5.26	123.30	112.47
5	A	175	LYS	N-CA-C	-5.25	105.45	111.07
23	S	78	THR	N-CA-C	5.25	117.39	109.41
1	0	874	A	C4'-C3'-O3'	-5.24	105.14	113.00
17	M	42	HIS	N-CA-C	5.23	116.61	109.18
1	0	921	G	N9-C1'-C2'	5.21	119.82	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2620	U	C3'-C2'-O2'	5.21	122.42	114.60
1	0	2526	C	N1-C1'-C2'	5.21	119.81	112.00
1	0	1165	G	N9-C1'-C2'	5.21	119.81	112.00
1	0	2673	U	N1-C1'-C2'	5.19	119.78	112.00
1	0	1504	A	C1'-O4'-C4'	-5.17	104.72	109.90
1	0	2071	C	N1-C1'-C2'	5.17	119.76	112.00
1	0	1450	C	C2'-C3'-O3'	-5.12	106.02	113.70
28	X	187	VAL	N-CA-C	5.11	115.26	108.11
7	C	20	ASP	N-CA-C	5.10	117.50	111.33
26	V	118	LEU	N-CA-C	5.10	116.52	110.19
10	F	111	ILE	N-CA-C	-5.09	105.57	110.72
10	F	118	LEU	N-CA-C	-5.09	107.13	113.19
1	0	2615	U	N1-C1'-C2'	5.08	119.62	112.00
21	Q	50	VAL	N-CA-C	-5.08	105.37	110.30
15	K	47	GLY	N-CA-C	5.07	117.23	111.85
17	M	13	ARG	N-CA-C	-5.06	105.42	112.45
1	0	1504	A	C4'-C3'-O3'	-5.04	105.44	113.00
12	H	73	GLN	N-CA-C	-5.04	104.30	110.65
16	L	126	HIS	CB-CA-C	-5.03	101.41	110.36
9	E	37	ASP	N-CA-C	5.03	119.36	113.23
2	9	3002	U	C2'-C3'-O3'	5.02	117.03	109.50
13	I	68	GLY	N-CA-C	5.02	118.55	112.48
6	B	114	ASP	N-CA-C	-5.01	99.16	108.24
21	Q	141	VAL	N-CA-C	5.01	116.51	108.89
32	2	67	LEU	N-CA-C	5.01	117.48	109.81
15	K	20	ASN	N-CA-C	5.01	120.28	110.56
1	0	1819	G	C4'-C3'-C2'	-5.00	97.59	102.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1039	G	Sidechain
1	0	1078	A	Sidechain
1	0	1342	C	Sidechain
1	0	1524	U	Sidechain
1	0	1614	G	Sidechain
1	0	1653	A	Sidechain

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Mol	Chain	Res	Type	Group
1	0	171	C	Sidechain
1	0	1878	G	Sidechain
1	0	1972	U	Sidechain
1	0	1979	G	Sidechain
1	0	2308	U	Sidechain
1	0	246	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2526	C	Sidechain
1	0	2564	G	Sidechain
1	0	2607	U	Sidechain
1	0	2619	U	Sidechain
1	0	2620	U	Sidechain
1	0	2630	G	Sidechain
1	0	2673	U	Sidechain
1	0	2774	U	Sidechain
1	0	2793	A	Sidechain
1	0	2811	A	Sidechain
1	0	2842	G	Sidechain
1	0	333	G	Sidechain
1	0	393	G	Sidechain
1	0	396	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	815	U	Sidechain
1	0	817	G	Sidechain
1	0	952	G	Sidechain
2	9	3039	U	Sidechain
26	V	90	TYR	Sidechain

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	0	59017	0	29805	988	0
2	9	2600	0	1326	69	0
3	3	59	0	35	4	0
4	4	37	0	23	5	0
5	A	1754	0	1763	134	0
6	B	2624	0	2533	173	0
7	C	1858	0	1816	135	0
8	D	1094	0	1085	136	0
9	E	1357	0	1266	85	0
10	F	885	0	854	66	0
11	G	240	0	231	21	0
12	H	1215	0	1215	166	0
13	I	1119	0	1098	64	0
14	J	993	0	1027	62	0
15	K	1114	0	1072	64	0
16	L	1605	0	1676	174	0
17	M	1444	0	1401	143	0
18	N	864	0	873	35	0
19	O	1133	0	1127	43	0
20	P	734	0	729	23	0
21	Q	1149	0	1122	59	0
22	R	641	0	605	28	0
23	S	949	0	923	57	0
24	T	410	0	366	36	0
25	U	499	0	511	38	0
26	V	1195	0	1137	108	0
27	W	654	0	653	51	0
28	X	1130	0	1133	60	0
29	Y	563	0	601	72	0
30	Z	430	0	426	24	0
31	1	393	0	406	20	0
32	2	755	0	731	63	0
33	0	110	0	0	0	0
33	2	1	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	J	1	0	0	0	0
33	S	1	0	0	0	0
33	X	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	73	0	0	0	0
35	9	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	I	1	0	0	0	0
35	K	1	0	0	0	0
35	L	1	0	0	0	0
35	P	1	0	0	0	0
35	Q	3	0	0	0	0
35	R	1	0	0	0	0
36	0	10	0	0	0	0
36	2	1	0	0	0	0
36	A	1	0	0	1	0
36	B	1	0	0	0	0
36	I	3	0	0	1	0
36	K	1	0	0	0	0
36	L	1	0	0	1	0
36	M	1	0	0	1	0
36	N	1	0	0	0	0
36	Q	1	0	0	0	0
36	X	1	0	0	0	0
37	4	37	0	26	2	0
38	4	11	0	8	1	0
39	4	8	0	6	0	0
40	4	15	0	15	2	0
41	2	1	0	0	0	0
41	N	1	0	0	0	0
41	T	1	0	0	0	0
41	Y	1	0	0	0	0
41	Z	1	0	0	0	0
42	0	5873	0	0	208	0
42	1	42	0	0	4	0
42	2	76	0	0	6	0
42	3	4	0	0	3	0
42	4	4	0	0	0	0
42	9	140	0	0	11	0
42	A	132	0	0	17	0
42	B	143	0	0	24	0
42	C	176	0	0	36	0
42	D	51	0	0	19	0
42	E	44	0	0	11	0
42	F	29	0	0	12	0
42	G	22	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	H	78	0	0	22	0
42	I	57	0	0	4	0
42	J	61	0	0	10	0
42	K	84	0	0	19	0
42	L	138	0	0	22	0
42	M	70	0	0	15	0
42	N	42	0	0	8	0
42	O	67	0	0	6	0
42	P	56	0	0	3	0
42	Q	87	0	0	9	0
42	R	36	0	0	6	0
42	S	37	0	0	10	0
42	T	26	0	0	3	0
42	U	16	0	0	3	0
42	V	66	0	0	11	0
42	W	30	0	0	5	0
42	X	96	0	0	17	0
42	Y	33	0	0	12	0
42	Z	55	0	0	3	0
All	All	98688	0	59624	2903	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 19.

All (2903) 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)
12:H:86:ARG:NH1	12:H:133:ILE:HG13	1.61	1.16
6:B:162:MET:HE1	6:B:308:LEU:HD21	1.34	1.09
25:U:12:THR:HG22	25:U:15:GLU:HG3	1.34	1.09
8:D:25:MET:HE2	8:D:41:LEU:HG	1.30	1.08
7:C:236:THR:HG22	7:C:239:ALA:H	0.97	1.07
21:Q:99:ALA:HB1	21:Q:109:MET:HE1	1.29	1.06
1:O:156:C:H5''	16:L:171:ARG:HD3	1.38	1.05
12:H:45:GLN:HB3	12:H:163:PRO:HD2	1.40	1.04
1:O:1134:G:H4'	12:H:151:MET:HE1	1.35	1.04
17:M:47:LEU:HD11	17:M:127:LEU:HD21	1.40	1.02
16:L:87:MET:HG2	32:2:46:ILE:HG21	1.40	1.02
1:O:871:G:H5'	1:O:871:G:H8	1.21	1.02
13:I:19:MET:HE3	13:I:132:LEU:HD11	1.37	1.01
1:O:871:G:H5'	1:O:871:G:C8	1.95	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:86:ARG:HH11	12:H:133:ILE:CG1	1.74	1.00
14:J:10:GLN:NE2	14:J:10:GLN:H	1.60	1.00
29:Y:46:LYS:HD3	29:Y:59:HIS:HB2	1.41	1.00
7:C:5:ILE:HD11	7:C:16:VAL:HG23	1.43	0.99
23:S:71:VAL:HG11	23:S:90:PRO:HB3	1.39	0.99
12:H:165:GLY:HA3	42:H:8399:HOH:O	1.61	0.99
1:O:1160:G:H5'	1:O:1161:A:H5'	1.40	0.99
1:O:870:G:H2'	1:O:871:G:H5''	1.42	0.98
8:D:134:LEU:HD11	8:D:166:ILE:HD11	1.44	0.98
2:9:3056:A:H2'	2:9:3057:A:H5''	1.45	0.98
16:L:52:LEU:HD11	42:L:8618:HOH:O	1.61	0.98
5:A:211:LYS:HB3	5:A:212:PRO:HD2	1.44	0.98
6:B:264:GLU:HG2	6:B:267:LYS:HE2	1.45	0.97
7:C:115:LEU:HD13	7:C:223:LEU:HD21	1.45	0.97
5:A:191:GLY:HA2	5:A:194:MET:HE2	1.48	0.96
7:C:2:GLN:HB3	42:C:8337:HOH:O	1.62	0.96
27:W:37:LEU:HD13	27:W:85:VAL:HG21	1.47	0.96
1:O:1242:A:H5'	13:I:82:THR:HG23	1.44	0.95
1:O:1751:G:H2'	1:O:1752:G:H5''	1.47	0.95
1:O:856:G:H2'	42:O:4905:HOH:O	1.67	0.95
14:J:10:GLN:H	14:J:10:GLN:HE21	0.99	0.95
1:O:960:G:H4'	42:O:6897:HOH:O	1.66	0.95
7:C:127:ARG:NH2	7:C:225:PRO:HG2	1.81	0.95
28:X:200:THR:HG22	28:X:201:GLU:HG3	1.47	0.94
7:C:236:THR:HG22	7:C:239:ALA:N	1.82	0.94
1:O:2717:C:H2'	1:O:2718:C:H5''	1.49	0.94
2:9:3006:C:H5''	17:M:37:ARG:NH1	1.81	0.94
6:B:238:ASN:HD22	6:B:240:GLY:H	1.09	0.94
31:1:41:HIS:H	31:1:45:ASN:HD22	1.14	0.94
6:B:86:ALA:HA	42:B:8579:HOH:O	1.68	0.94
26:V:149:LEU:HG	26:V:153:MET:HE2	1.46	0.94
12:H:27:LYS:H	12:H:58:HIS:HD2	1.13	0.93
32:2:70:ARG:HG2	32:2:77:ALA:HB2	1.51	0.93
12:H:29:ALA:HB3	12:H:65:ARG:HH12	1.33	0.93
1:O:21:G:H5'	21:Q:2:ILE:HA	1.50	0.93
8:D:105:SER:HB2	8:D:131:THR:HG23	1.50	0.93
19:O:115:SER:H	19:O:118:GLN:HE21	1.00	0.93
1:O:1166:A:H1'	1:O:1192:A:C2	2.03	0.93
1:O:2533:C:H5'	1:O:2533:C:H6	1.34	0.93
17:M:87:LEU:HD12	17:M:186:LEU:HD21	1.49	0.93
26:V:88:THR:HB	42:V:6679:HOH:O	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:O:4697:HOH:O	14:J:39:GLY:HA2	1.67	0.92
1:O:1835:U:H5	1:O:1840:A:N7	1.66	0.92
10:F:91:VAL:HG12	10:F:92:GLY:H	1.35	0.92
42:O:3938:HOH:O	16:L:146:GLN:HG2	1.69	0.91
12:H:55:GLN:HE21	12:H:124:ARG:HE	1.16	0.91
16:L:102:GLU:OE1	16:L:164:THR:HG21	1.69	0.91
21:Q:17:MET:HE1	21:Q:19:ARG:NH2	1.85	0.91
14:J:81:ARG:HB2	14:J:87:ARG:HH11	1.35	0.90
2:9:3076:G:H3'	2:9:3077:A:H5''	1.54	0.90
1:O:545:G:H5'	1:O:545:G:H8	1.37	0.90
12:H:150:LYS:HB2	12:H:157:ILE:HD12	1.54	0.89
13:I:76:ASP:HA	42:I:5907:HOH:O	1.70	0.89
16:L:106:ASN:ND2	36:L:8518:CL:CL	2.42	0.89
12:H:162:SER:HB2	12:H:163:PRO:HD3	1.52	0.89
1:O:962:C:H1'	17:M:5:ARG:NH1	1.88	0.89
12:H:139:ASP:HA	42:H:8370:HOH:O	1.70	0.89
6:B:140:LEU:HA	42:B:8579:HOH:O	1.73	0.89
6:B:62:ARG:HA	6:B:65:MET:HE3	1.54	0.88
12:H:86:ARG:HH11	12:H:133:ILE:HG13	0.79	0.88
12:H:26:LYS:HD2	12:H:28:ILE:HD12	1.53	0.88
26:V:6:GLN:HB2	26:V:26:ILE:HD12	1.55	0.88
14:J:10:GLN:HE21	14:J:10:GLN:N	1.72	0.88
10:F:96:ALA:HA	42:F:3111:HOH:O	1.74	0.87
26:V:88:THR:HG22	26:V:89:ASP:H	1.38	0.87
2:9:3023:U:H5''	2:9:3024:U:OP2	1.73	0.87
29:Y:40:PRO:HD3	29:Y:47:LEU:HD11	1.54	0.87
16:L:35:PRO:CG	16:L:38:VAL:HG23	2.04	0.87
1:O:381:G:H5''	42:O:3798:HOH:O	1.74	0.87
1:O:1701:A:H5'	42:O:5760:HOH:O	1.75	0.86
8:D:154:LYS:H	8:D:154:LYS:HD2	1.37	0.86
19:O:115:SER:H	19:O:118:GLN:NE2	1.73	0.86
20:P:25:PRO:HB2	42:P:4350:HOH:O	1.75	0.86
1:O:1771:U:H4'	29:Y:20:LEU:HD21	1.57	0.86
8:D:27:ILE:HG22	8:D:28:GLY:H	1.40	0.86
6:B:212:GLN:HB2	6:B:257:THR:HG21	1.56	0.86
1:O:1116:U:O2'	1:O:1118:A:H2	1.59	0.86
1:O:1164:U:C4'	1:O:1165:G:OP1	2.22	0.85
6:B:201:ASP:HB2	6:B:312:ARG:HD2	1.58	0.85
6:B:18:ARG:HG3	6:B:256:GLN:HG3	1.57	0.85
7:C:242:GLU:HG3	42:C:8388:HOH:O	1.74	0.85
15:K:79:ASP:HB3	42:K:8565:HOH:O	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:192:VAL:HB	42:A:8602:HOH:O	1.76	0.85
14:J:29:LEU:HB3	14:J:55:VAL:HG11	1.58	0.85
13:I:131:THR:HG22	13:I:134:GLU:H	1.41	0.85
16:L:89:ASN:HA	42:L:8556:HOH:O	1.75	0.85
1:O:1603:A:H5'	1:O:1605:G:O4'	1.77	0.85
14:J:14:LYS:HB2	14:J:45:PRO:HG2	1.57	0.85
6:B:162:MET:HE2	6:B:310:ARG:HD3	1.59	0.85
23:S:9:LYS:HE3	23:S:13:ARG:NH1	1.91	0.85
1:O:506:G:H22	1:O:509:A:H5'	1.40	0.84
1:O:2717:C:C2'	1:O:2718:C:H5''	2.07	0.84
16:L:35:PRO:HG2	16:L:38:VAL:HG23	1.57	0.84
5:A:35:GLY:O	5:A:36:ASP:HB3	1.78	0.84
1:O:870:G:C2'	1:O:871:G:H5''	2.06	0.84
17:M:144:GLY:O	17:M:147:ILE:HG22	1.76	0.84
42:O:4333:HOH:O	16:L:14:ARG:HG2	1.78	0.83
18:N:42:GLU:HB2	42:N:2176:HOH:O	1.77	0.83
1:O:542:A:H5'	1:O:542:A:H8	1.43	0.83
1:O:289:G:H22	1:O:363:A:H2	1.27	0.83
9:E:97:VAL:HG12	42:E:4191:HOH:O	1.77	0.83
1:O:1165:G:H4'	1:O:1174:A:O2'	1.78	0.83
1:O:2506:A:O2'	1:O:2507:G:H8	1.59	0.83
28:X:187:VAL:HG23	28:X:192:ASP:HB2	1.60	0.83
42:9:5071:HOH:O	17:M:23:ARG:HD3	1.78	0.83
22:R:51:GLN:HE21	22:R:53:ASN:HD21	1.27	0.83
1:O:2586:U:H3	1:O:2592:G:H22	1.23	0.83
13:I:74:ARG:HB3	13:I:74:ARG:HH11	1.43	0.82
21:Q:9:ASP:O	21:Q:13:THR:HB	1.79	0.82
6:B:190:MET:HE2	6:B:194:PHE:CD1	2.14	0.82
12:H:26:LYS:HG2	12:H:28:ILE:H	1.44	0.82
12:H:59:ASN:HD22	12:H:59:ASN:N	1.78	0.82
12:H:59:ASN:HD22	12:H:59:ASN:H	1.26	0.82
16:L:164:THR:HG22	16:L:167:GLY:H	1.42	0.82
16:L:164:THR:HG23	16:L:165:SER:N	1.94	0.82
7:C:132:ASP:HB3	42:C:8368:HOH:O	1.78	0.82
17:M:7:LYS:HE3	20:P:21:ARG:O	1.78	0.82
19:O:115:SER:OG	19:O:118:GLN:HG3	1.79	0.82
29:Y:39:CYS:HA	29:Y:47:LEU:HD11	1.61	0.82
1:O:2435:U:OP1	32:2:28:GLY:HA3	1.80	0.81
42:O:5772:HOH:O	8:D:99:ASP:HA	1.80	0.81
42:O:4423:HOH:O	2:9:3103:A:H4'	1.80	0.81
1:O:2716:G:H5''	6:B:206:THR:HG21	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:223:ARG:HG3	42:A:8609:HOH:O	1.77	0.81
12:H:162:SER:HB2	12:H:163:PRO:CD	2.10	0.81
16:L:24:MET:HE3	16:L:28:MET:HE3	1.61	0.81
26:V:137:GLN:HE21	26:V:141:HIS:HE1	1.24	0.81
27:W:78:GLU:HG2	27:W:79:GLU:H	1.46	0.81
1:O:21:G:C5'	21:Q:2:ILE:HA	2.10	0.81
1:O:1116:U:HO2'	1:O:1118:A:H2	0.81	0.81
10:F:63:ILE:HB	10:F:64:PRO:HD3	1.61	0.81
12:H:139:ASP:N	12:H:140:PRO:HD3	1.95	0.81
6:B:321:PRO:HA	42:B:8654:HOH:O	1.81	0.81
7:C:104:ASP:HA	7:C:107:ARG:HH12	1.44	0.81
17:M:83:LEU:HD13	17:M:175:LEU:HD23	1.64	0.80
1:O:1165:G:OP1	1:O:1165:G:H3'	1.81	0.80
1:O:2578:G:H5'	1:O:2578:G:H8	1.45	0.80
14:J:81:ARG:HB2	14:J:87:ARG:NH1	1.97	0.80
29:Y:38:LYS:HG2	29:Y:45:LYS:HG2	1.63	0.80
21:Q:8:ALA:HB1	21:Q:13:THR:HG21	1.64	0.80
8:D:20:LYS:HA	8:D:75:LEU:O	1.82	0.80
9:E:37:ASP:OD1	13:I:125:SER:HB3	1.82	0.79
26:V:4:LEU:HD22	26:V:52:VAL:HG21	1.64	0.79
6:B:179:LEU:O	6:B:183:GLU:HG2	1.83	0.79
1:O:1372:A:H3'	42:O:6659:HOH:O	1.81	0.79
42:O:5268:HOH:O	16:L:170:CYS:SG	2.39	0.79
26:V:72:PRO:HG2	26:V:77:ALA:HB3	1.63	0.79
1:O:1116:U:H3	1:O:1246:A:H62	1.30	0.79
13:I:19:MET:HE2	13:I:79:PHE:HA	1.64	0.79
28:X:187:VAL:HG23	28:X:192:ASP:CB	2.13	0.79
42:O:3217:HOH:O	16:L:157:LEU:HD11	1.83	0.79
10:F:91:VAL:HG12	10:F:92:GLY:N	1.96	0.79
12:H:14:TYR:H	12:H:91:HIS:CE1	2.01	0.79
32:2:25:VAL:HG22	32:2:68:LYS:HG3	1.65	0.79
1:O:506:G:H22	1:O:509:A:C5'	1.94	0.79
15:K:68:GLU:HA	42:K:8549:HOH:O	1.82	0.79
1:O:2506:A:HO2'	1:O:2507:G:H8	0.81	0.78
1:O:338:C:H5''	42:C:8427:HOH:O	1.82	0.78
1:O:1667:A:H8	1:O:1667:A:H5'	1.47	0.78
10:F:53:ASP:OD1	10:F:80:GLN:HB2	1.83	0.78
12:H:142:VAL:HG13	42:H:8381:HOH:O	1.81	0.78
1:O:1134:G:C4'	12:H:151:MET:HE1	2.12	0.78
1:O:1450:C:H4'	1:O:1451:C:OP2	1.83	0.78
7:C:78:ARG:HH11	7:C:78:ARG:HG3	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:O:6246:HOH:O	17:M:4:PRO:HD2	1.83	0.78
16:L:169:ARG:HD2	42:L:8591:HOH:O	1.83	0.78
1:O:2748:G:H2'	42:O:7009:HOH:O	1.84	0.77
12:H:4:ALA:HB3	42:H:8365:HOH:O	1.83	0.77
1:O:1118:A:H8	1:O:1118:A:H3'	1.49	0.77
2:9:3056:A:C2'	2:9:3057:A:H5''	2.14	0.77
1:O:1184:C:H1'	42:O:6934:HOH:O	1.83	0.77
1:O:558:C:H5'	42:O:4735:HOH:O	1.84	0.77
2:9:3048:C:H4'	17:M:141:ARG:HH21	1.50	0.77
12:H:41:THR:HA	42:H:8396:HOH:O	1.85	0.77
16:L:172:GLY:O	16:L:183:VAL:HG11	1.85	0.77
1:O:2502:C:H2'	1:O:2503:A:H5'	1.67	0.77
12:H:137:ASN:O	12:H:139:ASP:N	2.18	0.77
26:V:122:ARG:HG2	26:V:122:ARG:HH11	1.48	0.77
27:W:71:ARG:HB3	27:W:88:GLU:OE1	1.84	0.77
7:C:236:THR:HG21	42:C:8380:HOH:O	1.83	0.77
16:L:87:MET:CG	32:2:46:ILE:HG21	2.14	0.77
17:M:113:SER:HB2	42:M:8561:HOH:O	1.84	0.77
1:O:541:C:H2'	1:O:542:A:H5''	1.65	0.77
15:K:133:VAL:HA	42:K:8578:HOH:O	1.83	0.77
16:L:69:LYS:O	16:L:73:ARG:NH2	2.18	0.77
29:Y:39:CYS:SG	29:Y:47:LEU:HD21	2.24	0.77
12:H:55:GLN:NE2	12:H:124:ARG:HE	1.83	0.77
25:U:12:THR:HG22	25:U:15:GLU:CG	2.12	0.77
1:O:2099:G:H1	40:4:79:BTN:H92	1.49	0.76
27:W:30:MET:HE1	27:W:58:ALA:HB3	1.66	0.76
1:O:1701:A:H4'	1:O:1702:U:H5''	1.66	0.76
5:A:69:LEU:HD21	5:A:120:ARG:HB3	1.67	0.76
5:A:194:MET:HE3	5:A:199:HIS:HB2	1.66	0.76
29:Y:38:LYS:HE2	29:Y:45:LYS:HE2	1.68	0.76
1:O:272:A:H3'	42:O:6997:HOH:O	1.84	0.76
1:O:1684:A:H1'	31:1:43:ARG:HH22	1.50	0.76
1:O:2526:C:O2'	1:O:2527:U:H5'	1.86	0.76
4:4:74:C:H2'	4:4:75:C:H5'	1.66	0.76
9:E:100:ASP:HB2	42:E:2789:HOH:O	1.86	0.76
21:Q:39:THR:HB	21:Q:42:GLU:HG3	1.67	0.76
1:O:1118:A:H3'	1:O:1118:A:C8	2.20	0.76
12:H:47:GLU:HB3	12:H:133:ILE:HD13	1.67	0.76
1:O:1164:U:H3	1:O:1192:A:H2	1.31	0.76
12:H:5:MET:HG3	42:H:8365:HOH:O	1.85	0.76
2:9:3006:C:H5''	17:M:37:ARG:HH12	1.48	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:877:G:H5'	1:0:878:G:OP1	1.85	0.76
10:F:2:VAL:HG22	10:F:57:GLU:OE1	1.86	0.76
14:J:74:VAL:HG13	14:J:113:ILE:HG23	1.68	0.76
1:0:2421:G:H3'	1:0:2422:U:H5''	1.67	0.76
17:M:49:THR:HG22	17:M:56:ASP:HB2	1.68	0.76
18:N:14:LEU:HD23	18:N:102:ILE:HD11	1.67	0.75
28:X:220:GLU:HG2	42:X:8551:HOH:O	1.86	0.75
1:0:282:C:H1'	1:0:368:C:N4	2.01	0.75
1:0:1164:U:H4'	1:0:1165:G:OP1	1.86	0.75
1:0:2420:G:O2'	1:0:2421:G:H5'	1.87	0.75
6:B:41:PHE:CD1	6:B:79:MET:HE2	2.20	0.75
1:0:1160:G:C5'	1:0:1161:A:H5'	2.16	0.75
1:0:2812:A:H2	1:0:2814:A:H62	1.34	0.75
7:C:139:VAL:HG13	42:C:8452:HOH:O	1.84	0.75
5:A:88:ILE:HD13	5:A:100:PRO:HD3	1.69	0.75
29:Y:30:GLU:HA	29:Y:33:HIS:HB3	1.68	0.75
1:0:541:C:C2'	1:0:542:A:H5''	2.17	0.75
1:0:346:U:H4'	42:0:6317:HOH:O	1.87	0.74
1:0:2533:C:H5'	1:0:2533:C:C6	2.22	0.74
13:I:107:ASN:ND2	13:I:109:TYR:H	1.84	0.74
13:I:74:ARG:HH11	13:I:74:ARG:CB	2.00	0.74
13:I:99:GLU:HA	42:I:7377:HOH:O	1.85	0.74
26:V:88:THR:HG23	26:V:110:GLN:NE2	2.02	0.74
1:0:2502:C:C2'	1:0:2503:A:H5'	2.18	0.74
12:H:75:SER:O	12:H:79:ALA:HB2	1.87	0.74
23:S:61:GLU:HG3	42:S:3851:HOH:O	1.86	0.74
27:W:72:VAL:HG22	27:W:85:VAL:HG12	1.69	0.74
1:0:553:G:P	28:X:204:ARG:HH22	2.11	0.74
1:0:2094:G:H4'	6:B:245:SER:HB3	1.70	0.74
2:9:3069:U:OP1	17:M:4:PRO:HG3	1.88	0.74
7:C:5:ILE:HD11	7:C:16:VAL:CG2	2.16	0.74
21:Q:106:GLY:HA2	21:Q:109:MET:HE3	1.69	0.74
5:A:153:ARG:HB2	5:A:153:ARG:HH11	1.52	0.74
1:0:871:G:H8	1:0:871:G:C5'	1.97	0.74
6:B:258:GLY:H	6:B:260:HIS:CE1	2.05	0.74
1:0:2421:G:H3'	1:0:2422:U:C5'	2.18	0.74
18:N:32:ARG:O	18:N:32:ARG:HD3	1.86	0.74
1:0:288:A:H61	1:0:364:C:H42	1.34	0.74
17:M:48:VAL:CG1	17:M:55:ASP:HB3	2.17	0.74
17:M:164:ASP:CG	17:M:167:ASP:HA	2.13	0.74
20:P:64:GLU:HG3	20:P:74:ASP:OD2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:140:VAL:HB	42:C:8455:HOH:O	1.88	0.73
12:H:47:GLU:HB3	12:H:133:ILE:CD1	2.18	0.73
18:N:47:ARG:HG3	18:N:47:ARG:HH11	1.52	0.73
19:O:59:ARG:NH2	19:O:66:GLN:HE22	1.85	0.73
42:O:3277:HOH:O	16:L:189:VAL:HG21	1.87	0.73
5:A:121:ALA:O	5:A:124:VAL:HG22	1.88	0.73
19:O:115:SER:N	19:O:118:GLN:HE21	1.82	0.73
23:S:9:LYS:HB2	42:S:7242:HOH:O	1.88	0.73
1:O:560:C:H42	1:O:597:A:H61	1.36	0.73
1:O:1878:G:H1'	42:O:5597:HOH:O	1.88	0.73
9:E:11:VAL:HG12	9:E:12:ASP:N	2.03	0.73
16:L:186:SER:O	16:L:189:VAL:HG12	1.88	0.73
1:O:711:G:H1'	42:O:6565:HOH:O	1.88	0.73
29:Y:37:HIS:HB2	29:Y:47:LEU:HB2	1.70	0.73
12:H:2:PRO:HB2	42:H:8365:HOH:O	1.89	0.73
22:R:57:THR:HG22	22:R:59:ASP:H	1.53	0.73
1:O:1835:U:C5	1:O:1840:A:N7	2.55	0.73
1:O:1919:A:H4'	42:O:4320:HOH:O	1.87	0.73
8:D:64:ARG:HG2	8:D:67:ASP:HB3	1.71	0.73
31:1:41:HIS:N	31:1:45:ASN:HD22	1.84	0.72
25:U:1:THR:HG23	25:U:2:VAL:H	1.54	0.72
25:U:39:ALA:N	25:U:40:PRO:HD2	2.04	0.72
1:O:111:C:O2'	30:Z:20:ARG:HG2	1.89	0.72
8:D:88:LEU:HB2	8:D:89:PRO:HD3	1.72	0.72
21:Q:39:THR:HG23	21:Q:107:GLU:O	1.89	0.72
26:V:22:GLU:HG2	26:V:27:HIS:CD2	2.23	0.72
1:O:1474:C:H6	1:O:1474:C:H5'	1.53	0.72
1:O:1909:A:N1	1:O:2128:G:H1'	2.04	0.72
12:H:140:PRO:HB3	42:H:8381:HOH:O	1.90	0.72
28:X:200:THR:HG22	28:X:201:GLU:CG	2.19	0.72
31:1:41:HIS:H	31:1:45:ASN:ND2	1.88	0.72
1:O:450:C:OP1	7:C:184:ARG:NH2	2.19	0.72
42:9:4707:HOH:O	17:M:147:ILE:HD12	1.88	0.72
8:D:19:GLU:O	8:D:20:LYS:HG2	1.89	0.72
16:L:139:PRO:O	16:L:140:ALA:HB3	1.89	0.72
1:O:2004:U:H4'	42:O:4785:HOH:O	1.88	0.72
6:B:71:VAL:HG11	6:B:296:LEU:HB3	1.71	0.72
11:G:12:ILE:HA	42:G:4499:HOH:O	1.88	0.72
1:O:2637:A:H4'	1:O:2638:G:O5'	1.89	0.71
1:O:2780:C:H1'	9:E:143:GLN:HE21	1.55	0.71
42:O:4058:HOH:O	16:L:87:MET:HE1	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:O:6403:HOH:O	28:X:212:ARG:HD2	1.89	0.71
9:E:84:MET:HE1	9:E:148:ILE:CD1	2.19	0.71
27:W:76:ARG:HH11	27:W:76:ARG:HG3	1.54	0.71
14:J:22:ASP:HB2	42:J:5264:HOH:O	1.89	0.71
1:O:1666:C:O2'	1:O:1667:A:H5''	1.91	0.71
17:M:61:ALA:HB3	17:M:88:ALA:HB2	1.70	0.71
24:T:9:CYS:SG	24:T:11:THR:HG23	2.31	0.71
1:O:1187:U:H2'	42:O:6368:HOH:O	1.91	0.71
1:O:1191:A:H3'	1:O:1192:A:H5''	1.72	0.71
27:W:25:ARG:HD2	42:W:3861:HOH:O	1.90	0.71
1:O:236:A:H4'	1:O:237:G:H5'	1.73	0.71
2:9:3014:G:H5'	2:9:3014:G:H8	1.54	0.71
5:A:36:ASP:OD2	5:A:85:ASP:HB2	1.90	0.71
1:O:1666:C:H2'	1:O:1667:A:H5'	1.72	0.71
6:B:145:HIS:HD2	6:B:146:THR:O	1.73	0.71
15:K:143:THR:HG22	15:K:144:ASP:N	2.06	0.71
26:V:6:GLN:HB2	26:V:26:ILE:CD1	2.20	0.71
1:O:2466:G:OP1	42:O:3138:HOH:O	2.08	0.71
1:O:1209:C:H4'	42:O:4758:HOH:O	1.90	0.71
26:V:5:VAL:HG11	26:V:153:MET:HE1	1.72	0.71
42:O:3048:HOH:O	16:L:152:ARG:HG3	1.91	0.71
5:A:33:GLU:O	5:A:34:ASP:HB2	1.90	0.71
1:O:182:G:H5'	42:O:4630:HOH:O	1.90	0.70
1:O:1209:C:H2'	1:O:1210:G:H8	1.55	0.70
42:O:4017:HOH:O	12:H:151:MET:HE2	1.90	0.70
6:B:162:MET:HE2	6:B:310:ARG:CD	2.21	0.70
9:E:6:GLU:HA	9:E:46:THR:HG22	1.72	0.70
23:S:69:LYS:O	23:S:71:VAL:HG23	1.91	0.70
26:V:21:LEU:HD22	26:V:26:ILE:CD1	2.21	0.70
1:O:2508:C:H2'	42:O:6228:HOH:O	1.91	0.70
1:O:541:C:H2'	1:O:542:A:C5'	2.20	0.70
7:C:47:GLY:HA2	7:C:92:PRO:HB2	1.72	0.70
25:U:12:THR:CG2	25:U:15:GLU:HG3	2.19	0.70
26:V:21:LEU:HD22	26:V:26:ILE:HD11	1.72	0.70
26:V:122:ARG:HH21	26:V:154:ARG:HD2	1.56	0.70
31:1:35:ARG:HB2	42:1:2691:HOH:O	1.92	0.70
1:O:284:C:H4'	1:O:285:A:O5'	1.89	0.70
1:O:545:G:H5'	1:O:545:G:C8	2.25	0.70
1:O:2604:A:H5'	42:O:5266:HOH:O	1.90	0.70
2:9:3029:C:H2'	2:9:3030:C:H5'	1.73	0.70
16:L:139:PRO:O	16:L:140:ALA:CB	2.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:107:ARG:NH1	7:C:107:ARG:HB3	2.07	0.70
1:O:396:U:H1'	42:O:7100:HOH:O	1.89	0.70
1:O:2748:G:H5'	42:O:7009:HOH:O	1.92	0.70
1:O:544:G:H2'	1:O:545:G:H5''	1.73	0.70
1:O:1206:U:H5'	1:O:1206:U:H6	1.56	0.70
9:E:107:PHE:CE2	9:E:108:LEU:HD13	2.26	0.70
19:O:103:THR:HA	19:O:106:ARG:NH1	2.06	0.69
24:T:9:CYS:HA	24:T:52:THR:HG23	1.73	0.69
1:O:2419:U:H5''	1:O:2420:G:H5'	1.72	0.69
12:H:27:LYS:H	12:H:58:HIS:CD2	2.04	0.69
12:H:162:SER:CB	12:H:163:PRO:HD3	2.21	0.69
13:I:19:MET:HE1	13:I:78:ILE:HG22	1.74	0.69
13:I:75:PRO:HG2	13:I:105:LEU:HD21	1.72	0.69
15:K:67:ARG:O	15:K:71:GLU:HG3	1.91	0.69
1:O:657:G:OP1	7:C:27:ARG:NH2	2.25	0.69
12:H:27:LYS:N	12:H:58:HIS:HD2	1.88	0.69
26:V:13:MET:HE2	26:V:18:GLN:CA	2.23	0.69
1:O:281:U:H2'	1:O:282:C:O4'	1.92	0.69
1:O:962:C:H1'	17:M:5:ARG:HH12	1.57	0.69
13:I:45:VAL:HG23	13:I:130:VAL:O	1.92	0.69
27:W:15:ARG:HB3	27:W:15:ARG:HH11	1.57	0.69
8:D:146:LYS:NZ	17:M:107:ASN:HD21	1.90	0.69
1:O:2291:A:C8	1:O:2309:C:H5'	2.28	0.69
42:O:6348:HOH:O	16:L:178:LYS:HB2	1.92	0.69
12:H:49:VAL:O	12:H:157:ILE:HG23	1.93	0.69
1:O:559:U:H6	1:O:559:U:H5'	1.57	0.69
1:O:2426:G:H1'	42:O:5568:HOH:O	1.91	0.69
9:E:84:MET:HE2	9:E:133:VAL:CG2	2.23	0.69
12:H:45:GLN:HE21	12:H:135:TRP:HE1	1.38	0.69
1:O:56:G:H5''	25:U:50:ARG:HH12	1.57	0.69
1:O:1185:U:H2'	1:O:1186:C:C6	2.28	0.69
6:B:162:MET:CE	6:B:308:LEU:HD21	2.18	0.69
10:F:99:THR:HA	42:F:3461:HOH:O	1.93	0.69
14:J:82:ARG:NH2	14:J:115:ARG:HG2	2.08	0.69
16:L:122:GLU:OE2	16:L:127:LYS:HE2	1.93	0.69
26:V:88:THR:HG22	26:V:89:ASP:N	2.08	0.69
1:O:2890:A:H1'	24:T:56:ARG:NH2	2.07	0.69
6:B:74:ILE:HD13	6:B:309:VAL:HG21	1.75	0.69
7:C:162:VAL:HG12	7:C:192:ILE:HD11	1.74	0.69
1:O:1625:U:H4'	42:O:4142:HOH:O	1.91	0.68
24:T:13:ILE:HG12	24:T:32:CYS:HB3	1.72	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:238:ASN:ND2	6:B:240:GLY:H	1.88	0.68
14:J:74:VAL:HG11	14:J:113:ILE:HG12	1.74	0.68
16:L:106:ASN:HD22	16:L:114:VAL:HG23	1.57	0.68
25:U:42:ASN:HB3	42:U:7247:HOH:O	1.92	0.68
29:Y:42:CYS:SG	29:Y:44:PHE:HB2	2.33	0.68
1:O:1160:G:H5'	1:O:1161:A:C5'	2.19	0.68
1:O:1741:U:H5'	1:O:1742:A:OP1	1.93	0.68
26:V:68:THR:HG23	26:V:69:ARG:HG2	1.76	0.68
1:O:2768:A:H2'	1:O:2769:C:O4'	1.92	0.68
8:D:55:LYS:HA	42:D:6752:HOH:O	1.94	0.68
14:J:28:GLU:OE2	14:J:58:THR:HG21	1.94	0.68
1:O:214:U:H5'	42:O:5617:HOH:O	1.92	0.68
7:C:236:THR:H	7:C:239:ALA:HB3	1.58	0.68
17:M:159:TYR:HB3	17:M:162:ASP:HB2	1.76	0.68
1:O:2241:C:O2'	1:O:2242:U:H5'	1.93	0.68
6:B:175:LEU:C	6:B:175:LEU:HD23	2.19	0.68
26:V:4:LEU:HD22	26:V:52:VAL:CG2	2.24	0.68
1:O:1751:G:C2'	1:O:1752:G:H5''	2.22	0.68
31:I:39:ARG:HG2	42:I:3143:HOH:O	1.93	0.68
1:O:1679:C:H5'	42:O:8828:HOH:O	1.94	0.68
1:O:738:G:H3'	42:O:6518:HOH:O	1.93	0.68
8:D:57:THR:HG23	8:D:63:ILE:HG22	1.76	0.68
2:9:3092:G:H2'	2:9:3093:A:C8	2.29	0.67
1:O:1130:U:H2'	1:O:1131:G:O4'	1.94	0.67
1:O:2346:C:O2'	8:D:52:THR:HG21	1.93	0.67
1:O:1119:G:H2'	13:I:52:GLN:NE2	2.09	0.67
11:G:12:ILE:N	11:G:13:PRO:HD3	2.10	0.67
12:H:130:HIS:CD2	12:H:133:ILE:HD11	2.29	0.67
24:T:46:ALA:HB1	24:T:52:THR:HG21	1.76	0.67
26:V:4:LEU:HD23	26:V:54:PHE:HB3	1.76	0.67
7:C:1:MET:HG2	7:C:2:GLN:H	1.58	0.67
28:X:186:ARG:HH11	28:X:186:ARG:HG2	1.57	0.67
13:I:103:VAL:HG12	42:I:5907:HOH:O	1.94	0.67
26:V:13:MET:HE2	26:V:18:GLN:HA	1.77	0.67
21:Q:39:THR:HG22	21:Q:42:GLU:H	1.60	0.67
29:Y:49:ARG:HD2	42:Y:8424:HOH:O	1.94	0.67
7:C:12:THR:HB	42:C:8445:HOH:O	1.95	0.67
26:V:122:ARG:NH2	26:V:154:ARG:HD2	2.09	0.67
1:O:56:G:H5''	25:U:50:ARG:NH1	2.08	0.67
1:O:1244:U:OP1	13:I:18:ILE:HD13	1.95	0.67
12:H:46:VAL:HG12	12:H:146:TRP:HZ3	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:104:ARG:O	16:L:108:LYS:HE2	1.94	0.67
1:O:1328:A:OP1	28:X:169:ARG:HD2	1.95	0.67
11:G:23:ILE:HD13	11:G:67:LEU:HD23	1.77	0.67
12:H:71:TYR:C	12:H:73:GLN:H	2.03	0.67
1:O:156:C:H5''	16:L:171:ARG:CD	2.22	0.67
1:O:1377:C:H5'	1:O:1377:C:H6	1.61	0.67
16:L:12:TRP:CE2	16:L:20:ILE:HD11	2.30	0.67
21:Q:18:LEU:HD12	21:Q:143:VAL:HG11	1.76	0.67
16:L:37:VAL:HG21	16:L:108:LYS:HG3	1.77	0.66
16:L:173:LEU:HD23	16:L:183:VAL:HG12	1.76	0.66
5:A:194:MET:HE3	5:A:199:HIS:CB	2.25	0.66
10:F:58:GLU:HA	10:F:61:MET:HE2	1.78	0.66
16:L:34:GLU:HB3	16:L:35:PRO:HD2	1.77	0.66
17:M:164:ASP:OD2	17:M:167:ASP:HA	1.95	0.66
25:U:56:ILE:O	25:U:60:GLN:HG3	1.95	0.66
42:O:4444:HOH:O	12:H:57:ARG:HG3	1.95	0.66
5:A:53:ALA:HB3	42:A:8614:HOH:O	1.95	0.66
7:C:78:ARG:HG3	7:C:78:ARG:NH1	2.10	0.66
19:O:103:THR:O	19:O:107:GLU:HG3	1.94	0.66
1:O:1058:A:H2'	1:O:1060:C:H5''	1.77	0.66
1:O:1080:C:H4'	1:O:1081:A:OP1	1.94	0.66
1:O:1299:G:O6	15:K:6:ARG:HD3	1.96	0.66
6:B:7:ARG:HG2	6:B:7:ARG:HH11	1.61	0.66
12:H:56:ILE:HG22	12:H:61:LEU:HD22	1.76	0.66
13:I:75:PRO:HG2	13:I:105:LEU:CD2	2.25	0.66
17:M:12:ARG:HD3	17:M:18:THR:OG1	1.96	0.66
25:U:4:HIS:HB3	42:U:6622:HOH:O	1.94	0.66
1:O:31:C:H4'	42:S:7242:HOH:O	1.94	0.66
8:D:35:ALA:N	42:D:5576:HOH:O	2.27	0.66
19:O:38:GLU:HA	19:O:41:ARG:NH1	2.11	0.66
26:V:88:THR:HG23	26:V:110:GLN:HE21	1.59	0.66
12:H:118:PRO:HD2	42:H:8339:HOH:O	1.96	0.66
13:I:107:ASN:HD21	13:I:109:TYR:HB2	1.61	0.66
21:Q:18:LEU:HB2	21:Q:143:VAL:CG1	2.26	0.66
1:O:1886:A:N3	42:O:4293:HOH:O	2.28	0.66
17:M:119:GLN:O	17:M:123:ILE:HG13	1.95	0.66
17:M:183:ASP:OD2	17:M:186:LEU:HD12	1.96	0.66
1:O:282:C:H1'	1:O:368:C:H42	1.60	0.66
24:T:14:GLU:O	24:T:17:THR:HB	1.96	0.66
1:O:282:C:O2'	1:O:283:U:H5'	1.96	0.65
1:O:603:A:H5''	1:O:604:G:OP1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:902:G:N7	15:K:18:HIS:HD2	1.93	0.65
5:A:131:HIS:O	5:A:132:ASP:HB2	1.94	0.65
7:C:214:THR:HG21	42:C:8409:HOH:O	1.95	0.65
11:G:12:ILE:HD12	42:G:692:HOH:O	1.96	0.65
17:M:71:TRP:CE3	17:M:175:LEU:HD22	2.32	0.65
2:9:3006:C:OP1	17:M:37:ARG:NH1	2.29	0.65
12:H:150:LYS:HE2	42:H:8383:HOH:O	1.96	0.65
16:L:74:ARG:HH11	16:L:74:ARG:HG3	1.61	0.65
5:A:76:VAL:HG23	29:Y:63:LYS:HB3	1.79	0.65
6:B:62:ARG:CA	6:B:65:MET:HE3	2.25	0.65
13:I:93:ARG:HB3	13:I:93:ARG:HH11	1.62	0.65
23:S:9:LYS:HE3	23:S:13:ARG:HH11	1.60	0.65
1:0:1923:G:H4'	32:2:31:THR:O	1.97	0.65
7:C:236:THR:HA	42:C:8455:HOH:O	1.97	0.65
14:J:62:PRO:HG3	14:J:65:ARG:HH21	1.61	0.65
17:M:86:LEU:HD12	17:M:125:ALA:HB2	1.79	0.65
22:R:57:THR:HG22	22:R:59:ASP:N	2.11	0.65
1:0:1329:A:H2	42:0:4159:HOH:O	1.78	0.65
6:B:62:ARG:HA	6:B:65:MET:CE	2.25	0.65
14:J:27:ARG:HD2	42:J:4747:HOH:O	1.96	0.65
14:J:62:PRO:HG3	14:J:65:ARG:NH2	2.12	0.65
1:0:2637:A:H3'	3:3:74:C:O5'	1.96	0.65
5:A:191:GLY:HA2	5:A:194:MET:CE	2.26	0.65
6:B:238:ASN:HD22	6:B:240:GLY:N	1.89	0.65
14:J:55:VAL:HG12	14:J:56:SER:N	2.12	0.65
9:E:7:ILE:HD11	9:E:11:VAL:C	2.22	0.65
8:D:23:VAL:HG23	8:D:23:VAL:O	1.96	0.65
12:H:141:ASN:HA	42:H:8366:HOH:O	1.97	0.65
14:J:115:ARG:HG3	14:J:116:GLU:N	2.12	0.65
1:0:645:U:OP2	15:K:4:LYS:HE2	1.96	0.64
1:0:1172:G:H1'	42:0:4446:HOH:O	1.96	0.64
1:0:1641:A:H2'	1:0:1642:A:H5'	1.79	0.64
9:E:166:VAL:HG12	42:E:3134:HOH:O	1.96	0.64
32:2:55:VAL:HG22	42:2:8511:HOH:O	1.97	0.64
1:0:182:G:H4'	16:L:157:LEU:HD13	1.79	0.64
1:0:2421:G:H4'	42:0:4252:HOH:O	1.97	0.64
8:D:64:ARG:CG	8:D:67:ASP:HB3	2.27	0.64
32:2:65:THR:HG23	32:2:67:LEU:HG	1.79	0.64
1:0:447:A:OP1	23:S:2:LYS:HG2	1.97	0.64
6:B:264:GLU:HG2	6:B:267:LYS:CE	2.23	0.64
19:O:58:SER:HB3	42:O:183:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Y:54:ILE:HD12	42:Y:8415:HOH:O	1.96	0.64
1:O:470:U:O2'	30:Z:16:HIS:HD2	1.79	0.64
1:O:2310:G:OP2	12:H:114:PRO:HD2	1.97	0.64
1:O:2827:A:H2'	1:O:2828:G:O4'	1.96	0.64
42:O:7025:HOH:O	32:2:60:LYS:HG3	1.97	0.64
5:A:179:MET:HA	5:A:179:MET:HE3	1.78	0.64
10:F:50:VAL:HG13	10:F:60:VAL:HG11	1.79	0.64
16:L:60:ILE:C	16:L:61:ILE:HD12	2.23	0.64
22:R:51:GLN:HE21	22:R:53:ASN:ND2	1.95	0.64
23:S:32:ARG:NH1	23:S:38:ARG:HH12	1.96	0.64
5:A:36:ASP:HA	5:A:83:GLY:HA3	1.80	0.64
5:A:100:PRO:HG2	5:A:103:VAL:HG21	1.79	0.64
8:D:69:ILE:HG22	8:D:69:ILE:O	1.96	0.64
8:D:97:GLN:HG2	8:D:97:GLN:O	1.96	0.64
1:O:1234:U:N3	6:B:244:PRO:HB3	2.13	0.64
6:B:195:ARG:HG2	6:B:323:LEU:HD22	1.80	0.64
11:G:64:ASN:HD22	11:G:64:ASN:N	1.94	0.64
24:T:20:MET:HE2	24:T:30:HIS:NE2	2.11	0.64
1:O:69:A:H5'	1:O:69:A:C8	2.33	0.64
42:O:4307:HOH:O	13:I:47:THR:HB	1.97	0.64
6:B:221:GLN:HE22	14:J:42:ASN:HD22	1.44	0.64
12:H:45:GLN:HE21	12:H:135:TRP:NE1	1.95	0.64
17:M:37:ARG:NE	42:M:8535:HOH:O	2.29	0.64
32:2:31:THR:HB	32:2:33:MET:HE3	1.80	0.64
1:O:383:A:H4'	42:O:4807:HOH:O	1.96	0.64
16:L:38:VAL:C	16:L:63:VAL:HG13	2.23	0.64
8:D:54:ALA:HB2	8:D:69:ILE:HD12	1.79	0.64
12:H:58:HIS:HA	12:H:61:LEU:HD23	1.80	0.64
12:H:75:SER:C	12:H:79:ALA:HB2	2.23	0.64
26:V:130:HIS:O	26:V:136:GLY:HA3	1.97	0.64
42:O:5006:HOH:O	16:L:58:GLN:HG3	1.97	0.64
12:H:28:ILE:HA	12:H:62:GLU:OE1	1.98	0.64
12:H:55:GLN:HE22	12:H:91:HIS:CD2	2.16	0.64
12:H:163:PRO:HG2	42:H:8338:HOH:O	1.97	0.64
13:I:133:GLY:O	13:I:137:GLU:HG3	1.98	0.64
31:1:22:PRO:HG2	31:1:25:VAL:HG23	1.79	0.64
1:O:125:U:H2'	42:O:3260:HOH:O	1.98	0.63
42:O:6612:HOH:O	30:Z:1:THR:HB	1.97	0.63
8:D:95:THR:C	8:D:97:GLN:H	2.06	0.63
6:B:36:PRO:HA	6:B:168:GLY:CA	2.28	0.63
16:L:84:LYS:HE2	42:L:8579:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:14:LEU:CD2	18:N:102:ILE:HD11	2.27	0.63
28:X:187:VAL:CG2	28:X:192:ASP:HB2	2.27	0.63
1:O:1119:G:H22	1:O:1246:A:H2	1.45	0.63
1:O:2459:G:OP1	32:2:64:LYS:N	2.18	0.63
6:B:125:GLU:O	6:B:129:ARG:HG3	1.99	0.63
9:E:15:GLN:HG3	9:E:20:ILE:HG12	1.80	0.63
12:H:26:LYS:HD2	12:H:28:ILE:CD1	2.26	0.63
15:K:148:GLU:HA	42:K:8577:HOH:O	1.97	0.63
16:L:87:MET:HG2	32:2:46:ILE:CG2	2.23	0.63
1:O:289:G:N2	1:O:363:A:H2	1.94	0.63
8:D:65:GLU:HG3	42:D:6752:HOH:O	1.99	0.63
12:H:69:ASN:O	12:H:72:VAL:HG12	1.97	0.63
12:H:83:PHE:HZ	12:H:146:TRP:HE1	1.46	0.63
15:K:120:LEU:HD12	15:K:133:VAL:HG21	1.80	0.63
17:M:154:LEU:O	17:M:155:GLU:HB3	1.98	0.63
29:Y:30:GLU:HA	29:Y:33:HIS:CB	2.28	0.63
1:O:285:A:H2'	1:O:286:U:O4'	1.98	0.63
9:E:3:VAL:HG22	9:E:49:ILE:HB	1.81	0.63
12:H:136:VAL:HG22	12:H:137:ASN:O	1.97	0.63
15:K:1:THR:HA	42:K:8529:HOH:O	1.99	0.63
21:Q:119:VAL:HG21	21:Q:142:ASP:CG	2.24	0.63
27:W:41:PHE:O	27:W:43:VAL:HG23	1.98	0.63
1:O:338:C:H4'	7:C:174:ILE:CD1	2.28	0.63
1:O:2769:C:H2'	1:O:2770:G:O4'	1.99	0.63
16:L:172:GLY:C	16:L:183:VAL:HG11	2.24	0.63
17:M:61:ALA:CB	17:M:88:ALA:HB2	2.29	0.63
1:O:371:U:H2'	1:O:372:A:H8	1.63	0.63
1:O:1118:A:H62	1:O:1244:U:H3	1.46	0.63
10:F:110:GLU:HG2	42:F:6926:HOH:O	1.98	0.63
12:H:33:MET:HB2	12:H:83:PHE:HB3	1.81	0.63
12:H:53:PRO:HG3	12:H:127:GLY:H	1.64	0.63
1:O:871:G:C8	1:O:871:G:C5'	2.75	0.63
8:D:23:VAL:HG22	8:D:73:VAL:HB	1.81	0.63
8:D:105:SER:CB	8:D:131:THR:HG23	2.27	0.63
26:V:110:GLN:NE2	26:V:110:GLN:HA	2.14	0.63
1:O:2432:C:O2'	1:O:2433:A:H5'	1.98	0.62
5:A:105:VAL:HG11	5:A:154:ALA:HB1	1.81	0.62
16:L:138:HIS:ND1	16:L:139:PRO:O	2.24	0.62
18:N:38:ARG:NH1	42:N:7674:HOH:O	2.30	0.62
26:V:13:MET:HE3	26:V:17:ILE:HG22	1.79	0.62
1:O:272:A:H5'	1:O:273:G:OP2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:95:THR:O	8:D:97:GLN:N	2.28	0.62
12:H:84:ARG:NH2	12:H:135:TRP:HH2	1.96	0.62
28:X:189:ASN:HD22	28:X:189:ASN:C	2.06	0.62
1:O:2054:A:N3	21:Q:128:ARG:NH2	2.47	0.62
6:B:307:ARG:HH11	6:B:307:ARG:HB2	1.64	0.62
7:C:115:LEU:HD21	7:C:243:VAL:HG13	1.81	0.62
13:I:107:ASN:HD22	13:I:107:ASN:C	2.06	0.62
16:L:164:THR:CG2	16:L:165:SER:N	2.62	0.62
30:Z:8:GLN:HE22	30:Z:11:LYS:NZ	1.97	0.62
1:O:2851:G:O2'	1:O:2852:A:H5'	1.98	0.62
21:Q:132:ARG:HG2	21:Q:133:ALA:N	2.14	0.62
25:U:39:ALA:C	25:U:41:GLU:H	2.08	0.62
26:V:90:TYR:N	26:V:90:TYR:CD1	2.66	0.62
6:B:141:ARG:HG2	6:B:165:ARG:HA	1.82	0.62
22:R:33:SER:O	22:R:37:VAL:HG23	2.00	0.62
42:O:3551:HOH:O	6:B:27:ASN:HB2	1.99	0.62
17:M:32:PRO:HD2	17:M:99:GLU:O	2.00	0.62
18:N:87:THR:O	18:N:91:GLN:HG3	1.98	0.62
21:Q:18:LEU:HB2	21:Q:143:VAL:HG12	1.81	0.62
1:O:2361:A:H5''	42:O:8523:HOH:O	1.99	0.62
16:L:68:ARG:O	16:L:68:ARG:HD3	1.99	0.62
17:M:151:ASP:O	17:M:154:LEU:HB2	2.00	0.62
28:X:133:HIS:HD2	42:X:8583:HOH:O	1.82	0.62
29:Y:10:ARG:HA	42:Y:8414:HOH:O	1.98	0.62
1:O:69:A:H5'	1:O:69:A:H8	1.65	0.62
6:B:140:LEU:HD23	42:B:8579:HOH:O	1.99	0.62
7:C:115:LEU:O	7:C:118:THR:HB	1.99	0.62
12:H:48:LEU:HG	12:H:157:ILE:HG21	1.82	0.62
5:A:211:LYS:HB3	5:A:212:PRO:CD	2.24	0.62
1:O:544:G:C2'	1:O:545:G:H5''	2.30	0.62
1:O:1886:A:H4'	42:Y:8405:HOH:O	1.98	0.62
1:O:1972:U:H2'	1:O:1973:A:H5'	1.82	0.62
5:A:94:LEU:HD23	5:A:94:LEU:N	2.15	0.61
29:Y:77:LYS:HA	29:Y:80:MET:HE2	1.82	0.61
9:E:20:ILE:HD11	9:E:40:VAL:HG11	1.81	0.61
1:O:2414:A:H2'	1:O:2415:A:C8	2.34	0.61
5:A:200:PRO:HG2	5:A:225:VAL:HG21	1.82	0.61
16:L:164:THR:HG22	16:L:167:GLY:N	2.13	0.61
27:W:78:GLU:CG	27:W:79:GLU:H	2.11	0.61
28:X:216:ARG:HD3	42:X:8570:HOH:O	2.01	0.61
1:O:188:C:H5''	16:L:163:LEU:HD21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1170:U:O2'	1:0:1172:G:N7	2.27	0.61
1:0:2276:U:H2'	1:0:2277:U:C6	2.35	0.61
1:0:2505:G:O2'	1:0:2506:A:H5'	2.01	0.61
17:M:73:ALA:N	42:M:8568:HOH:O	2.33	0.61
1:0:1829:A:N6	29:Y:18:TYR:HA	2.15	0.61
2:9:3006:C:C5'	17:M:37:ARG:NH1	2.59	0.61
12:H:44:ALA:HA	12:H:163:PRO:O	2.00	0.61
15:K:136:ALA:HB3	42:K:8578:HOH:O	2.00	0.61
22:R:51:GLN:NE2	22:R:53:ASN:HD21	1.96	0.61
23:S:63:ILE:HD11	23:S:75:GLU:HB2	1.82	0.61
1:0:558:C:O2'	1:0:559:U:H5''	2.00	0.61
6:B:148:PRO:HD2	42:B:8580:HOH:O	2.00	0.61
10:F:91:VAL:CG1	10:F:92:GLY:H	2.11	0.61
19:O:98:ILE:HD12	19:O:102:ARG:NE	2.16	0.61
26:V:137:GLN:HE21	26:V:141:HIS:CE1	2.13	0.61
29:Y:28:ASP:O	29:Y:31:ILE:HG22	2.01	0.61
32:2:62:THR:HB	42:2:8557:HOH:O	2.00	0.61
1:0:1116:U:O2'	1:0:1118:A:C2	2.42	0.61
1:0:1819:G:H2'	1:0:1820:G:H4'	1.81	0.61
1:0:2427:C:OP2	32:2:84:ARG:HD2	2.00	0.61
1:0:2896:A:H5''	42:0:5575:HOH:O	2.00	0.61
42:C:8360:HOH:O	18:N:3:THR:HG21	1.99	0.61
16:L:74:ARG:O	16:L:88:VAL:HG13	2.00	0.61
17:M:184:ILE:HG22	17:M:185:GLU:HG3	1.82	0.61
26:V:13:MET:CE	26:V:17:ILE:HG22	2.30	0.61
26:V:81:ASP:OD1	26:V:92:ASP:HB2	1.99	0.61
29:Y:51:GLY:HA3	42:Y:8415:HOH:O	2.01	0.61
1:0:1559:A:H1'	42:0:5338:HOH:O	2.01	0.61
1:0:2710:U:H1'	42:0:7092:HOH:O	2.00	0.61
6:B:141:ARG:HD2	6:B:163:GLU:OE2	2.01	0.61
7:C:118:THR:O	7:C:136:VAL:HG13	2.00	0.61
12:H:144:GLU:OE1	12:H:144:GLU:HA	2.00	0.61
32:2:10:TYR:HB2	32:2:17:HIS:CE1	2.36	0.61
1:0:1474:C:H5'	1:0:1474:C:C6	2.34	0.61
1:0:1766:U:O2	1:0:1778:A:H5'	2.01	0.61
2:9:3039:U:H1'	2:9:3044:A:H61	1.64	0.61
9:E:79:GLY:HA3	42:E:7046:HOH:O	2.00	0.61
9:E:84:MET:HE1	9:E:148:ILE:HD12	1.83	0.61
28:X:235:GLU:H	28:X:235:GLU:CD	2.07	0.61
32:2:70:ARG:HB3	42:2:8576:HOH:O	2.00	0.61
7:C:25:PRO:HG2	42:C:8324:HOH:O	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:91:ARG:HG3	17:M:186:LEU:HD23	1.82	0.60
21:Q:33:ARG:NH1	42:Q:8544:HOH:O	2.33	0.60
1:0:431:G:P	16:L:48:ARG:HH12	2.25	0.60
1:0:775:G:OP1	30:Z:16:HIS:HE1	1.84	0.60
21:Q:44:VAL:O	21:Q:48:GLU:HG3	2.02	0.60
28:X:144:ARG:CZ	42:X:8612:HOH:O	2.48	0.60
1:0:1120:U:H5'	1:0:1121:G:OP2	2.00	0.60
5:A:105:VAL:CG1	5:A:154:ALA:HB1	2.31	0.60
8:D:36:ASN:HA	42:D:7500:HOH:O	2.00	0.60
8:D:41:LEU:HA	8:D:44:ILE:HG22	1.84	0.60
26:V:122:ARG:HH22	26:V:154:ARG:C	2.09	0.60
1:0:299:U:H5'	42:0:6806:HOH:O	2.01	0.60
1:0:1114:A:H2'	1:0:1115:U:H6	1.66	0.60
1:0:2437:A:H2'	1:0:2438:G:C8	2.37	0.60
1:0:2587:U:H2'	1:0:2589:U:H5''	1.82	0.60
1:0:2783:A:H3'	42:0:4708:HOH:O	1.99	0.60
2:9:3014:G:H5'	2:9:3014:G:C8	2.36	0.60
9:E:84:MET:HE1	9:E:148:ILE:HD13	1.84	0.60
16:L:52:LEU:HD21	42:L:8618:HOH:O	2.00	0.60
17:M:80:SER:HB2	42:M:8537:HOH:O	1.99	0.60
1:0:263:U:O4'	10:F:59:ILE:HD13	2.01	0.60
1:0:1594:C:OP2	19:O:120:ARG:HD2	2.01	0.60
1:0:2676:C:H4'	13:I:70:PHE:CE1	2.35	0.60
7:C:104:ASP:HA	7:C:107:ARG:NH1	2.14	0.60
16:L:104:ARG:O	16:L:108:LYS:HG2	2.01	0.60
21:Q:39:THR:HB	21:Q:42:GLU:CG	2.30	0.60
1:0:20:G:H21	21:Q:117:HIS:HD2	1.49	0.60
1:0:1119:G:N2	1:0:1246:A:C2	2.63	0.60
9:E:5:LEU:HD21	9:E:66:GLN:HG3	1.82	0.60
10:F:107:VAL:O	10:F:111:ILE:HG13	2.01	0.60
12:H:46:VAL:O	12:H:146:TRP:HH2	1.84	0.60
12:H:166:ASN:HD22	12:H:166:ASN:N	1.98	0.60
16:L:61:ILE:HA	42:L:8627:HOH:O	2.01	0.60
22:R:81:ILE:HG23	42:R:8336:HOH:O	2.02	0.60
29:Y:30:GLU:HB3	29:Y:34:LYS:HE3	1.84	0.60
6:B:75:GLU:C	6:B:77:PRO:HD3	2.26	0.60
8:D:23:VAL:HG21	8:D:45:THR:HG21	1.84	0.60
19:O:38:GLU:HA	19:O:41:ARG:HH11	1.67	0.60
1:0:2908:A:H2'	1:0:2909:G:O4'	2.01	0.60
6:B:207:LYS:HG2	6:B:304:PRO:HB3	1.83	0.60
9:E:116:THR:HG22	9:E:151:LEU:HD22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:16:VAL:HG12	19:O:17:GLY:N	2.17	0.60
19:O:87:ARG:HG2	42:O:186:HOH:O	2.01	0.60
1:O:2690:U:O2'	9:E:111:LYS:HE3	2.02	0.60
6:B:51:VAL:CG2	6:B:327:VAL:HG13	2.31	0.60
13:I:74:ARG:O	13:I:78:ILE:HG12	2.01	0.60
1:O:1741:U:O2'	1:O:2723:G:H4'	2.01	0.60
17:M:169:PRO:O	17:M:172:PHE:HB3	2.02	0.60
21:Q:99:ALA:HB1	21:Q:109:MET:CE	2.19	0.60
30:Z:21:ARG:HD2	30:Z:37:CYS:SG	2.41	0.60
1:O:1197:G:N2	42:O:5710:HOH:O	2.34	0.59
13:I:39:VAL:HG12	13:I:40:ASN:ND2	2.17	0.59
19:O:59:ARG:HH22	19:O:66:GLN:HE22	1.51	0.59
1:O:31:C:H2'	42:O:7158:HOH:O	2.01	0.59
6:B:36:PRO:HA	6:B:168:GLY:HA3	1.84	0.59
12:H:59:ASN:N	12:H:59:ASN:ND2	2.50	0.59
29:Y:29:VAL:O	29:Y:33:HIS:HB2	2.02	0.59
1:O:2578:G:H5'	1:O:2578:G:C8	2.34	0.59
12:H:127:GLY:O	12:H:128:ALA:HB3	2.03	0.59
17:M:86:LEU:O	17:M:90:LEU:HG	2.02	0.59
29:Y:61:GLY:HA3	42:Y:8422:HOH:O	2.02	0.59
1:O:797:A:C4'	29:Y:10:ARG:N	2.65	0.59
1:O:1130:U:H5'	42:O:7141:HOH:O	2.02	0.59
1:O:1187:U:O2'	1:O:1189:A:H2	1.86	0.59
1:O:2756:U:H3	1:O:2896:A:H2	1.49	0.59
7:C:16:VAL:HG12	7:C:17:ASP:N	2.16	0.59
8:D:99:ASP:HB2	8:D:103:ASN:HB2	1.84	0.59
10:F:58:GLU:HG3	10:F:61:MET:HE2	1.82	0.59
10:F:58:GLU:OE1	16:L:27:ARG:NH2	2.34	0.59
12:H:35:ASN:ND2	12:H:80:ASN:HA	2.18	0.59
30:Z:25:LYS:O	30:Z:25:LYS:HG2	2.02	0.59
1:O:1667:A:H5'	1:O:1667:A:C8	2.35	0.59
1:O:2718:C:H6	1:O:2718:C:H5'	1.68	0.59
1:O:2755:G:H1'	42:O:4158:HOH:O	2.03	0.59
42:O:6498:HOH:O	5:A:211:LYS:HG2	2.02	0.59
5:A:81:GLN:HB2	5:A:92:ASN:ND2	2.17	0.59
5:A:88:ILE:HD13	5:A:100:PRO:CD	2.31	0.59
7:C:118:THR:HG23	42:C:8305:HOH:O	2.02	0.59
29:Y:47:LEU:HD23	29:Y:57:CYS:HB2	1.85	0.59
42:O:5501:HOH:O	20:P:50:GLY:HA2	2.02	0.59
8:D:25:MET:CE	8:D:37:ALA:HB1	2.32	0.59
14:J:34:VAL:HG22	14:J:47:ALA:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:106:GLY:HA3	42:J:5264:HOH:O	2.02	0.59
16:L:74:ARG:HG3	16:L:74:ARG:NH1	2.18	0.59
16:L:87:MET:CB	32:2:46:ILE:HG21	2.33	0.59
23:S:101:LEU:HD13	23:S:112:LEU:HD11	1.85	0.59
29:Y:31:ILE:O	29:Y:35:LYS:HG3	2.02	0.59
1:0:189:A:OP1	16:L:171:ARG:NH2	2.36	0.59
1:0:1053:G:OP1	12:H:12:PRO:HG3	2.02	0.59
2:9:3048:C:H4'	17:M:141:ARG:NH2	2.17	0.59
7:C:180:SER:HB2	42:C:8449:HOH:O	2.01	0.59
26:V:65:VAL:HA	26:V:68:THR:HG22	1.84	0.59
8:D:22:VAL:HG22	8:D:74:THR:HG22	1.84	0.59
8:D:91:ALA:HB1	42:D:5198:HOH:O	2.03	0.59
22:R:43:GLU:HB3	42:R:8344:HOH:O	2.03	0.59
1:0:88:G:H8	1:0:88:G:H5'	1.68	0.59
9:E:23:GLU:HG2	9:E:28:SER:CB	2.33	0.59
16:L:65:VAL:HG21	16:L:105:ALA:HB2	1.85	0.59
17:M:48:VAL:HG11	17:M:55:ASP:HB3	1.82	0.59
26:V:21:LEU:HD21	26:V:48:VAL:HG11	1.84	0.59
1:0:1003:U:HO2'	12:H:90:PHE:HE1	1.51	0.58
15:K:145:LEU:O	15:K:148:GLU:HG3	2.03	0.58
20:P:11:ARG:HD3	42:P:5620:HOH:O	2.03	0.58
26:V:108:ARG:HE	26:V:114:PRO:HG3	1.66	0.58
32:2:48:ASN:ND2	32:2:50:GLY:H	2.00	0.58
1:0:240:C:H4'	16:L:146:GLN:NE2	2.18	0.58
1:0:2676:C:H4'	13:I:70:PHE:HE1	1.68	0.58
42:0:7149:HOH:O	16:L:154:ARG:HB2	2.03	0.58
12:H:109:ASP:HB2	42:H:8345:HOH:O	2.03	0.58
42:0:9200:HOH:O	6:B:254:GLN:HG3	2.02	0.58
8:D:37:ALA:O	8:D:40:ILE:HG12	2.03	0.58
9:E:101:GLU:HB2	9:E:116:THR:O	2.03	0.58
11:G:12:ILE:N	11:G:13:PRO:CD	2.66	0.58
24:T:13:ILE:HG12	24:T:32:CYS:CB	2.32	0.58
8:D:64:ARG:CD	8:D:67:ASP:HB3	2.33	0.58
10:F:50:VAL:HG21	10:F:63:ILE:HG21	1.85	0.58
14:J:34:VAL:HB	42:J:7169:HOH:O	2.02	0.58
21:Q:111:ILE:HG23	21:Q:145:LEU:HD11	1.85	0.58
23:S:71:VAL:HG11	23:S:90:PRO:CB	2.26	0.58
32:2:3:MET:O	32:2:90:PHE:HA	2.03	0.58
1:0:558:C:H2'	1:0:559:U:H5'	1.86	0.58
1:0:2047:C:H5'	42:0:9316:HOH:O	2.04	0.58
42:0:6923:HOH:O	6:B:211:THR:HG21	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3013:A:O2'	2:9:3014:G:H5''	2.03	0.58
5:A:109:GLU:HG2	5:A:116:GLY:N	2.18	0.58
7:C:145:GLU:HG3	42:C:8380:HOH:O	2.02	0.58
8:D:54:ALA:CB	8:D:69:ILE:HD12	2.32	0.58
16:L:64:ARG:HD2	42:L:8586:HOH:O	2.03	0.58
16:L:87:MET:CB	32:2:46:ILE:HD13	2.33	0.58
17:M:141:ARG:N	42:M:8571:HOH:O	2.34	0.58
25:U:64:GLY:O	25:U:65:ASP:HB2	2.03	0.58
27:W:43:VAL:HG12	27:W:44:ASP:N	2.18	0.58
1:0:1701:A:H4'	1:0:1702:U:C5'	2.32	0.58
9:E:69:ILE:HA	9:E:72:MET:CE	2.33	0.58
26:V:11:VAL:O	26:V:12:ASN:HB2	2.04	0.58
9:E:132:THR:HB	42:E:2227:HOH:O	2.03	0.58
13:I:19:MET:CE	13:I:132:LEU:HD11	2.23	0.58
26:V:90:TYR:CE2	26:V:99:ALA:HB2	2.38	0.58
1:0:1008:C:H5''	12:H:16:ARG:HH12	1.68	0.58
1:0:2547:C:OP2	6:B:5:ARG:NH1	2.36	0.58
6:B:7:ARG:HD3	6:B:9:GLY:O	2.03	0.58
7:C:246:ARG:NE	42:C:8430:HOH:O	2.36	0.58
9:E:93:MET:HE1	9:E:165:GLY:N	2.18	0.58
25:U:39:ALA:N	25:U:40:PRO:CD	2.66	0.58
26:V:84:VAL:HG12	42:V:6679:HOH:O	2.04	0.58
1:0:1168:C:H2'	1:0:1169:U:O4'	2.03	0.58
1:0:1209:C:H2'	1:0:1210:G:C8	2.38	0.58
11:G:12:ILE:HB	42:G:4714:HOH:O	2.03	0.58
12:H:151:MET:HA	12:H:151:MET:HE3	1.86	0.58
13:I:45:VAL:HG21	13:I:129:PHE:CD1	2.39	0.58
25:U:58:THR:O	25:U:62:GLU:HG3	2.04	0.58
1:0:821:U:H5''	42:0:9545:HOH:O	2.02	0.58
5:A:88:ILE:O	5:A:88:ILE:HG22	2.02	0.58
5:A:164:ARG:NE	42:A:8596:HOH:O	2.36	0.58
6:B:30:PRO:HB2	6:B:39:GLN:NE2	2.19	0.58
6:B:145:HIS:CD2	6:B:146:THR:O	2.56	0.58
6:B:275:GLY:O	6:B:291:ASP:HA	2.04	0.58
8:D:38:GLU:HB3	8:D:49:PRO:HG2	1.86	0.58
12:H:136:VAL:HG23	42:H:8343:HOH:O	2.02	0.58
26:V:21:LEU:HD21	26:V:48:VAL:CG1	2.33	0.58
1:0:1205:U:C2'	1:0:1206:U:H5''	2.33	0.57
1:0:1477:C:O2'	1:0:1478:U:H5'	2.04	0.57
2:9:3020:G:O2'	2:9:3021:G:H5'	2.04	0.57
8:D:27:ILE:HG22	8:D:28:GLY:N	2.13	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:77:ALA:HB3	42:K:8537:HOH:O	2.02	0.57
1:0:371:U:H2'	1:0:372:A:C8	2.39	0.57
42:O:9038:HOH:O	19:O:81:LYS:HG2	2.04	0.57
7:C:76:ARG:HD3	42:C:8372:HOH:O	2.03	0.57
7:C:185:LYS:HD3	7:C:186:TYR:CE1	2.38	0.57
29:Y:11:THR:CG2	29:Y:23:ARG:HB2	2.35	0.57
29:Y:58:GLY:HA3	42:Y:8434:HOH:O	2.05	0.57
30:Z:8:GLN:HE22	30:Z:11:LYS:HZ1	1.52	0.57
1:0:2637:A:H5''	3:3:74:C:H5'	1.86	0.57
1:0:2717:C:H2'	1:0:2718:C:C5'	2.29	0.57
16:L:47:ASP:CG	16:L:48:ARG:N	2.62	0.57
17:M:152:GLU:C	17:M:154:LEU:H	2.10	0.57
26:V:38:THR:HG22	42:V:3580:HOH:O	2.03	0.57
29:Y:62:TYR:CE2	29:Y:64:ILE:HG23	2.39	0.57
1:0:65:C:O2'	1:0:66:G:H5'	2.03	0.57
1:0:818:A:O2'	29:Y:13:ARG:HD3	2.04	0.57
9:E:23:GLU:HG2	9:E:28:SER:HB3	1.87	0.57
14:J:74:VAL:CG1	14:J:113:ILE:HG12	2.35	0.57
27:W:78:GLU:HG2	27:W:79:GLU:N	2.17	0.57
30:Z:25:LYS:HE2	42:1:7213:HOH:O	2.02	0.57
1:0:121:U:OP2	31:1:10:ARG:NH2	2.36	0.57
1:0:1134:G:C5'	12:H:151:MET:HE1	2.34	0.57
1:0:1528:A:H2'	1:0:1529:G:O4'	2.04	0.57
1:0:2781:U:C2'	1:0:2782:G:H5'	2.35	0.57
6:B:63:GLU:HG3	6:B:63:GLU:O	2.04	0.57
12:H:26:LYS:HD3	12:H:89:PRO:HG3	1.86	0.57
15:K:54:PRO:HG2	15:K:57:VAL:CG2	2.34	0.57
1:0:183:A:H5'	16:L:157:LEU:HD12	1.87	0.57
1:0:558:C:H2'	1:0:559:U:C5'	2.35	0.57
1:0:2409:C:H4'	32:2:17:HIS:HB2	1.87	0.57
8:D:50:VAL:O	8:D:71:ALA:HA	2.05	0.57
13:I:39:VAL:HG11	13:I:107:ASN:HB2	1.86	0.57
1:0:157:G:H4'	16:L:95:LYS:HE3	1.85	0.57
1:0:380:A:OP2	16:L:9:ARG:HD2	2.04	0.57
1:0:567:U:H5''	42:V:5817:HOH:O	2.05	0.57
1:0:681:G:N3	1:0:681:G:H5'	2.20	0.57
6:B:168:GLY:N	6:B:174:ARG:HD3	2.20	0.57
8:D:19:GLU:HG3	42:D:6165:HOH:O	2.04	0.57
11:G:63:ARG:N	42:G:2569:HOH:O	2.37	0.57
12:H:157:ILE:HG22	12:H:158:ASN:N	2.19	0.57
1:0:485:A:N3	1:0:487:G:H5''	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2365:G:H4'	20:P:45:PRO:O	2.04	0.57
42:0:3996:HOH:O	16:L:94:LYS:HE3	2.05	0.57
15:K:138:GLY:HA3	42:K:8559:HOH:O	2.04	0.57
17:M:38:LYS:HD2	17:M:114:LYS:HE3	1.87	0.57
1:0:280:C:H2'	1:0:281:U:O4'	2.05	0.57
1:0:714:U:H3'	42:0:6416:HOH:O	2.04	0.57
1:0:1176:C:H1'	42:0:3420:HOH:O	2.04	0.57
12:H:47:GLU:CB	12:H:133:ILE:HD13	2.35	0.57
26:V:13:MET:HE3	26:V:17:ILE:CG2	2.35	0.57
1:0:1834:C:H2'	1:0:1840:A:N6	2.19	0.57
1:0:1942:A:H3'	42:0:6815:HOH:O	2.05	0.57
1:0:2781:U:H2'	1:0:2782:G:H5'	1.86	0.57
1:0:2840:A:OP1	6:B:211:THR:HG23	2.04	0.57
15:K:143:THR:HG22	15:K:144:ASP:H	1.70	0.57
16:L:30:GLU:O	16:L:34:GLU:HG3	2.04	0.57
16:L:113:ARG:NH2	16:L:156:ARG:HG2	2.19	0.57
22:R:37:VAL:O	22:R:41:VAL:HG23	2.05	0.57
29:Y:11:THR:OG1	29:Y:23:ARG:HB2	2.05	0.57
1:0:136:C:H2'	1:0:137:U:O4'	2.05	0.56
1:0:1086:A:C6	26:V:11:VAL:HG11	2.40	0.56
1:0:1634:G:H3'	42:0:3383:HOH:O	2.04	0.56
1:0:1887:U:OP1	29:Y:21:LYS:HE3	2.05	0.56
5:A:94:LEU:HG	5:A:99:ILE:HD11	1.87	0.56
1:0:2320:U:H4'	1:0:2321:A:O4'	2.05	0.56
2:9:3049:G:H5''	42:9:4707:HOH:O	2.04	0.56
6:B:56:ASP:OD1	6:B:322:ARG:HB3	2.04	0.56
7:C:162:VAL:HG13	7:C:232:LEU:HD21	1.87	0.56
8:D:86:THR:C	8:D:89:PRO:HD2	2.30	0.56
16:L:185:PRO:HG2	16:L:189:VAL:HG11	1.87	0.56
17:M:34:LEU:HA	17:M:47:LEU:HD23	1.86	0.56
17:M:89:GLY:O	17:M:92:ALA:HB3	2.05	0.56
26:V:122:ARG:NH2	42:V:4276:HOH:O	2.37	0.56
1:0:281:U:O2'	1:0:282:C:H5'	2.06	0.56
1:0:625:U:H5''	1:0:1044:C:N4	2.20	0.56
1:0:660:A:H4'	1:0:661:G:O5'	2.06	0.56
1:0:1180:U:H2'	1:0:1181:A:O4'	2.05	0.56
1:0:2285:G:H1	3:3:74:C:H42	1.51	0.56
1:0:2459:G:P	32:2:64:LYS:HB2	2.46	0.56
1:0:2878:U:H2'	1:0:2879:A:O4'	2.05	0.56
6:B:85:ARG:NH1	42:B:8632:HOH:O	2.38	0.56
6:B:103:ASP:HB2	42:B:8589:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:38:GLU:OE2	8:D:51:ARG:CZ	2.54	0.56
8:D:44:ILE:HG23	8:D:45:THR:HG23	1.88	0.56
8:D:86:THR:O	8:D:90:LEU:HG	2.05	0.56
9:E:11:VAL:HG12	9:E:12:ASP:H	1.69	0.56
15:K:149:ARG:O	15:K:150:GLN:HB2	2.06	0.56
16:L:37:VAL:HG21	16:L:108:LYS:CG	2.35	0.56
16:L:52:LEU:HD13	16:L:116:ASN:HB3	1.88	0.56
21:Q:18:LEU:HD12	21:Q:143:VAL:CG1	2.35	0.56
23:S:9:LYS:CE	23:S:13:ARG:NH1	2.64	0.56
29:Y:25:ARG:O	29:Y:29:VAL:HG23	2.05	0.56
1:O:960:G:N3	1:O:960:G:H2'	2.21	0.56
1:O:1730:G:H5'	1:O:1731:C:C5	2.41	0.56
1:O:2089:A:O2'	1:O:2090:G:H5'	2.06	0.56
1:O:2679:G:H2'	1:O:2681:A:OP2	2.05	0.56
2:9:3029:C:C2'	2:9:3030:C:H5'	2.35	0.56
7:C:246:ARG:NH2	42:C:8430:HOH:O	2.37	0.56
19:O:105:LEU:HD21	19:O:137:LEU:HD21	1.86	0.56
31:1:18:ASN:HD21	31:1:40:ARG:H	1.53	0.56
1:O:1119:G:H8	13:I:52:GLN:HE22	1.54	0.56
21:Q:39:THR:HB	21:Q:42:GLU:CD	2.30	0.56
28:X:185:VAL:HG12	42:X:8571:HOH:O	2.04	0.56
1:O:1123:A:C6	1:O:1238:C:H5'	2.41	0.56
1:O:2408:A:HO2'	32:2:10:TYR:HD1	1.51	0.56
2:9:3044:A:O4'	8:D:76:ARG:NE	2.39	0.56
8:D:99:ASP:CB	8:D:103:ASN:H	2.19	0.56
10:F:46:GLU:N	42:F:3461:HOH:O	2.39	0.56
10:F:47:LEU:HB2	10:F:108:LEU:HD11	1.88	0.56
11:G:12:ILE:O	11:G:12:ILE:HG22	2.05	0.56
16:L:55:LYS:HB2	16:L:60:ILE:CD1	2.35	0.56
24:T:9:CYS:CA	24:T:52:THR:HG23	2.35	0.56
25:U:44:GLY:O	25:U:48:GLU:HG2	2.05	0.56
1:O:1132:A:N6	1:O:1229:C:H2'	2.21	0.56
1:O:1441:G:O2'	1:O:1442:A:H5'	2.06	0.56
1:O:2329:C:O2'	1:O:2330:U:H5'	2.06	0.56
21:Q:23:MET:HE3	21:Q:28:SER:OG	2.06	0.56
1:O:2469:A:H1'	42:O:9736:HOH:O	2.06	0.56
5:A:199:HIS:CD2	5:A:201:PHE:H	2.24	0.56
7:C:133:ARG:HD2	42:C:8417:HOH:O	2.06	0.56
42:J:408:HOH:O	24:T:37:GLU:HB3	2.04	0.56
17:M:71:TRP:HE3	17:M:175:LEU:HD22	1.69	0.56
17:M:154:LEU:HG	17:M:155:GLU:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:558:C:C2'	1:0:559:U:H5''	2.36	0.56
1:0:659:A:H5''	42:0:6568:HOH:O	2.06	0.56
1:0:2781:U:H1'	9:E:139:GLU:OE2	2.06	0.56
2:9:3051:A:H5'	17:M:160:SER:HB3	1.88	0.56
9:E:7:ILE:HD11	9:E:11:VAL:O	2.06	0.56
16:L:149:TRP:O	16:L:152:ARG:HG2	2.04	0.56
23:S:9:LYS:HD2	42:S:7242:HOH:O	2.06	0.56
31:1:48:ASP:O	31:1:49:GLU:HB2	2.06	0.56
1:0:797:A:H4'	29:Y:10:ARG:N	2.21	0.56
1:0:1669:A:H2'	1:0:1670:G:C8	2.41	0.56
2:9:3039:U:H1'	2:9:3044:A:N6	2.21	0.56
5:A:95:PRO:HG2	5:A:98:GLU:HG2	1.88	0.56
8:D:174:VAL:HG13	42:D:6555:HOH:O	2.06	0.56
21:Q:106:GLY:HA2	21:Q:109:MET:CE	2.34	0.56
27:W:74:ALA:CB	27:W:85:VAL:HG22	2.36	0.56
1:0:157:G:H4'	16:L:95:LYS:CE	2.37	0.55
1:0:1118:A:C8	1:0:1118:A:C3'	2.85	0.55
1:0:1687:C:O2	30:Z:9:GLY:HA2	2.06	0.55
1:0:2081:A:H4'	13:I:69:TYR:CE1	2.41	0.55
1:0:2502:C:H4'	12:H:151:MET:HG2	1.88	0.55
9:E:126:ILE:HB	9:E:131:LEU:CD2	2.36	0.55
10:F:91:VAL:CG1	10:F:92:GLY:N	2.67	0.55
10:F:101:ALA:HA	42:F:5413:HOH:O	2.06	0.55
17:M:37:ARG:NH2	42:M:8535:HOH:O	2.38	0.55
21:Q:39:THR:CB	21:Q:42:GLU:HG3	2.36	0.55
26:V:141:HIS:HB2	26:V:146:ILE:HG12	1.87	0.55
27:W:43:VAL:CG1	27:W:47:ALA:HB3	2.36	0.55
28:X:106:THR:HG23	28:X:107:PRO:HD2	1.87	0.55
1:0:138:U:H5''	1:0:139:C:OP2	2.06	0.55
1:0:2274:A:N3	16:L:86:MET:HE1	2.21	0.55
1:0:2563:U:H2'	1:0:2565:C:O5'	2.06	0.55
1:0:2694:A:H4'	9:E:91:PHE:CE1	2.40	0.55
2:9:3054:A:O2'	2:9:3055:U:H5'	2.06	0.55
5:A:153:ARG:HH11	5:A:153:ARG:CB	2.19	0.55
7:C:77:ALA:O	7:C:78:ARG:HG3	2.06	0.55
7:C:236:THR:O	7:C:237:GLU:C	2.48	0.55
28:X:163:THR:HG23	42:X:8529:HOH:O	2.06	0.55
1:0:1733:A:H4'	6:B:212:GLN:HA	1.87	0.55
1:0:2694:A:H4'	9:E:91:PHE:HE1	1.70	0.55
1:0:2769:C:O2'	1:0:2770:G:H5'	2.06	0.55
7:C:142:ASP:OD1	7:C:237:GLU:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:115:SER:C	19:O:117:SER:H	2.14	0.55
1:O:1717:A:H5''	19:O:54:LYS:HB2	1.89	0.55
1:O:2115:U:H2'	1:O:2116:U:C6	2.41	0.55
1:O:2672:C:H1'	42:B:8632:HOH:O	2.06	0.55
6:B:51:VAL:HG23	6:B:329:TYR:O	2.06	0.55
12:H:59:ASN:H	12:H:59:ASN:ND2	1.95	0.55
13:I:39:VAL:CG1	13:I:107:ASN:HB2	2.36	0.55
27:W:72:VAL:HG22	27:W:85:VAL:CG1	2.35	0.55
32:2:11:CYS:HB2	32:2:20:HIS:CE1	2.41	0.55
1:O:2359:G:H3'	42:O:5166:HOH:O	2.05	0.55
42:O:4996:HOH:O	6:B:298:LYS:HD3	2.06	0.55
5:A:135:VAL:HG21	5:A:147:ARG:NH1	2.22	0.55
6:B:138:GLY:O	6:B:139:ASP:O	2.24	0.55
7:C:127:ARG:HG2	7:C:127:ARG:HH11	1.72	0.55
9:E:31:ARG:NH1	9:E:68:HIS:CG	2.75	0.55
12:H:85:ILE:HB	12:H:132:PHE:CE2	2.41	0.55
14:J:87:ARG:CZ	42:J:4854:HOH:O	2.54	0.55
16:L:57:LYS:HE2	16:L:140:ALA:O	2.06	0.55
17:M:37:ARG:CZ	42:M:8535:HOH:O	2.54	0.55
19:O:10:ALA:HA	19:O:13:VAL:HG12	1.88	0.55
21:Q:14:ALA:HB3	21:Q:147:LEU:HB2	1.87	0.55
30:Z:28:HIS:HD2	30:Z:30:LYS:H	1.54	0.55
1:O:542:A:H5'	1:O:542:A:C8	2.33	0.55
1:O:2316:G:H8	42:O:5129:HOH:O	1.88	0.55
16:L:71:SER:HB2	16:L:92:THR:HG22	1.88	0.55
17:M:87:LEU:CD1	17:M:186:LEU:HD21	2.31	0.55
23:S:37:GLN:OE1	23:S:118:SER:HA	2.06	0.55
29:Y:39:CYS:HA	29:Y:47:LEU:CD1	2.35	0.55
32:2:69:TYR:HB2	32:2:78:HIS:CE1	2.42	0.55
1:O:184:G:H5''	16:L:153:THR:HG22	1.88	0.55
1:O:1182:C:H1'	1:O:1192:A:H8	1.72	0.55
1:O:1773:G:C8	29:Y:16:PRO:HA	2.41	0.55
1:O:2769:C:C2'	1:O:2770:G:H5'	2.37	0.55
42:O:3173:HOH:O	16:L:79:LYS:HD3	2.06	0.55
5:A:199:HIS:HD2	5:A:201:PHE:H	1.55	0.55
6:B:304:PRO:HD2	6:B:307:ARG:HD2	1.87	0.55
8:D:11:HIS:C	8:D:13:MET:H	2.14	0.55
22:R:57:THR:HG22	22:R:58:MET:N	2.20	0.55
27:W:21:PRO:HG2	27:W:24:LYS:HD3	1.87	0.55
1:O:2094:G:C4'	6:B:245:SER:HB3	2.36	0.55
1:O:2638:G:H1'	42:O:7230:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:93:LYS:O	7:C:98:ARG:NH2	2.40	0.55
7:C:246:ARG:HB3	7:C:246:ARG:NH1	2.22	0.55
10:F:48:VAL:CG2	10:F:74:PHE:HB3	2.37	0.55
16:L:59:GLY:HA3	16:L:141:ILE:HD12	1.89	0.55
17:M:67:ALA:HA	17:M:71:TRP:H	1.71	0.55
18:N:96:VAL:HA	42:N:4258:HOH:O	2.05	0.55
4:4:74:C:C2'	4:4:75:C:H5'	2.35	0.55
10:F:21:GLU:O	10:F:24:ARG:HG3	2.05	0.55
16:L:61:ILE:HD12	16:L:61:ILE:N	2.22	0.55
27:W:76:ARG:O	27:W:77:PHE:HB3	2.06	0.55
31:1:22:PRO:HG2	31:1:25:VAL:CG2	2.36	0.55
1:0:1351:G:OP1	7:C:96:LYS:NZ	2.36	0.55
1:0:1759:A:N3	1:0:1818:C:H2'	2.21	0.55
6:B:162:MET:HE2	6:B:310:ARG:CG	2.37	0.55
8:D:10:PHE:CG	8:D:11:HIS:N	2.75	0.55
8:D:44:ILE:HG12	8:D:83:PHE:HE1	1.71	0.55
9:E:137:ASP:O	9:E:141:VAL:HG23	2.07	0.55
17:M:58:LEU:HD12	17:M:58:LEU:N	2.22	0.55
17:M:139:TRP:CE3	17:M:139:TRP:HA	2.41	0.55
21:Q:40:ALA:O	21:Q:44:VAL:HG23	2.07	0.55
27:W:9:VAL:HG13	27:W:88:GLU:OE2	2.07	0.55
28:X:185:VAL:HA	42:X:8565:HOH:O	2.06	0.55
1:0:1500:U:P	19:O:41:ARG:HH22	2.30	0.54
1:0:2594:C:O2'	1:0:2595:U:H5'	2.07	0.54
2:9:3042:C:H2'	42:9:6700:HOH:O	2.07	0.54
6:B:315:VAL:HG23	6:B:316:ARG:HG2	1.89	0.54
9:E:81:GLU:HG2	9:E:134:SER:HB3	1.89	0.54
12:H:150:LYS:CB	12:H:157:ILE:HD12	2.33	0.54
15:K:104:ASP:O	15:K:105:TYR:HB3	2.06	0.54
17:M:11:ARG:HG3	17:M:14:ARG:NH1	2.21	0.54
17:M:90:LEU:HB2	17:M:186:LEU:HD22	1.87	0.54
25:U:8:ILE:HA	25:U:11:MET:HE3	1.88	0.54
27:W:37:LEU:CD1	27:W:85:VAL:HG21	2.30	0.54
28:X:126:PRO:HG2	28:X:128:PHE:CE1	2.42	0.54
29:Y:57:CYS:SG	29:Y:59:HIS:HB3	2.47	0.54
6:B:55:ASN:HB3	6:B:63:GLU:HA	1.89	0.54
6:B:254:GLN:HG2	6:B:255:GLY:N	2.21	0.54
7:C:233:THR:HG22	7:C:234:VAL:N	2.22	0.54
15:K:30:ARG:NH2	42:K:8527:HOH:O	2.40	0.54
1:0:1189:A:H1'	1:0:1209:C:C1'	2.37	0.54
1:0:1525:G:H5'	1:0:1526:A:OP2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:48:VAL:HG23	10:F:74:PHE:CB	2.37	0.54
17:M:64:SER:C	17:M:66:LEU:H	2.16	0.54
18:N:39:THR:O	18:N:115:ARG:NH2	2.40	0.54
28:X:112:GLU:OE1	28:X:112:GLU:HA	2.08	0.54
1:O:1735:C:O2'	1:O:1736:A:H5'	2.07	0.54
12:H:3:GLY:HA2	12:H:57:ARG:NH1	2.22	0.54
28:X:141:THR:HG23	42:X:8589:HOH:O	2.08	0.54
1:O:1192:A:H3'	1:O:1193:A:H5'	1.90	0.54
1:O:1595:G:O2'	1:O:1596:U:H5'	2.08	0.54
1:O:1699:C:H4'	42:O:5916:HOH:O	2.06	0.54
1:O:2346:C:H6	1:O:2346:C:O5'	1.90	0.54
7:C:104:ASP:O	7:C:108:GLN:HG3	2.07	0.54
32:2:11:CYS:SG	32:2:71:CYS:HB2	2.48	0.54
1:O:1535:G:H2'	1:O:1536:C:C6	2.43	0.54
1:O:2073:G:OP2	1:O:2490:A:H5'	2.07	0.54
1:O:2316:G:H4'	42:O:5568:HOH:O	2.07	0.54
1:O:2559:C:H4'	42:O:6727:HOH:O	2.07	0.54
1:O:2830:U:H3'	42:O:4704:HOH:O	2.07	0.54
5:A:101:GLU:OE2	5:A:131:HIS:HB2	2.08	0.54
9:E:11:VAL:CG1	9:E:12:ASP:N	2.70	0.54
13:I:130:VAL:HG12	13:I:131:THR:N	2.21	0.54
16:L:87:MET:HB3	32:2:46:ILE:HD13	1.90	0.54
23:S:24:ARG:HH21	23:S:39:ASN:HD22	1.54	0.54
1:O:12:U:H2'	1:O:13:G:H5'	1.89	0.54
1:O:2122:C:H3'	42:O:4767:HOH:O	2.08	0.54
42:O:6473:HOH:O	20:P:9:GLY:HA2	2.07	0.54
6:B:139:ASP:HB2	6:B:165:ARG:HE	1.73	0.54
29:Y:18:TYR:HB3	29:Y:22:ILE:HG21	1.90	0.54
30:Z:1:THR:HA	42:Z:8411:HOH:O	2.07	0.54
1:O:2506:A:O2'	1:O:2507:G:O5'	2.26	0.54
7:C:61:PHE:HB3	42:C:8448:HOH:O	2.07	0.54
7:C:219:ASN:O	7:C:222:ASP:OD1	2.25	0.54
9:E:31:ARG:NH1	42:E:5919:HOH:O	2.40	0.54
10:F:19:ALA:O	10:F:22:VAL:HG22	2.08	0.54
11:G:64:ASN:O	11:G:68:GLU:HG3	2.08	0.54
13:I:74:ARG:NH1	13:I:76:ASP:HB2	2.23	0.54
15:K:54:PRO:HG2	15:K:57:VAL:HG21	1.88	0.54
16:L:72:SER:OG	16:L:74:ARG:HB2	2.07	0.54
16:L:74:ARG:NH2	42:L:8634:HOH:O	2.41	0.54
23:S:73:HIS:CD2	23:S:88:PRO:HG3	2.43	0.54
26:V:119:HIS:HD2	26:V:120:PRO:O	1.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:172:THR:HG22	28:X:173:ALA:N	2.21	0.54
29:Y:47:LEU:CD2	29:Y:57:CYS:HB2	2.37	0.54
1:O:289:G:O2'	1:O:290:C:H5'	2.08	0.54
1:O:328:U:O4'	7:C:202:THR:HG22	2.07	0.54
42:O:8591:HOH:O	6:B:214:PRO:HD2	2.06	0.54
5:A:132:ASP:OD1	5:A:133:ARG:N	2.40	0.54
8:D:51:ARG:HD3	42:D:7636:HOH:O	2.08	0.54
12:H:139:ASP:N	12:H:140:PRO:CD	2.70	0.54
19:O:80:ARG:HG2	19:O:87:ARG:CZ	2.38	0.54
1:O:1527:A:H1'	1:O:1528:A:C8	2.43	0.54
42:O:4554:HOH:O	6:B:216:LYS:HA	2.08	0.54
6:B:175:LEU:HD23	6:B:175:LEU:O	2.08	0.54
6:B:248:ARG:NH1	42:B:8612:HOH:O	2.40	0.54
9:E:137:ASP:OD1	9:E:139:GLU:HB2	2.08	0.54
26:V:125:HIS:HE1	42:V:3071:HOH:O	1.90	0.54
27:W:15:ARG:HB3	27:W:15:ARG:NH1	2.22	0.54
27:W:25:ARG:NH1	42:W:3861:HOH:O	2.41	0.54
7:C:214:THR:HG23	42:C:8441:HOH:O	2.07	0.53
8:D:140:ARG:O	8:D:144:ARG:HG2	2.08	0.53
25:U:49:LEU:O	25:U:53:ILE:HG13	2.08	0.53
26:V:6:GLN:CB	26:V:26:ILE:HD12	2.33	0.53
1:O:2779:G:H21	9:E:143:GLN:NE2	2.05	0.53
2:9:3041:C:O4'	8:D:50:VAL:HG23	2.08	0.53
17:M:154:LEU:HG	17:M:155:GLU:N	2.23	0.53
19:O:13:VAL:HG21	19:O:41:ARG:HG2	1.90	0.53
1:O:2312:G:H2'	1:O:2313:C:H5'	1.90	0.53
5:A:109:GLU:HG2	5:A:116:GLY:H	1.72	0.53
8:D:166:ILE:HD12	42:D:6326:HOH:O	2.07	0.53
12:H:3:GLY:HA2	12:H:57:ARG:HH12	1.72	0.53
13:I:26:VAL:HG13	13:I:36:VAL:HG11	1.90	0.53
15:K:114:VAL:HG11	42:K:8578:HOH:O	2.08	0.53
26:V:21:LEU:HB3	26:V:26:ILE:HG12	1.90	0.53
29:Y:53:GLY:HA2	29:Y:67:GLY:O	2.07	0.53
1:O:1829:A:H61	29:Y:18:TYR:HA	1.71	0.53
1:O:2768:A:O2'	1:O:2769:C:H5'	2.09	0.53
7:C:65:ARG:HG3	7:C:67:GLN:HB2	1.90	0.53
8:D:23:VAL:HG21	8:D:45:THR:CG2	2.37	0.53
13:I:107:ASN:HD22	13:I:109:TYR:H	1.56	0.53
14:J:125:ALA:C	14:J:127:ALA:H	2.16	0.53
22:R:57:THR:CG2	22:R:58:MET:N	2.70	0.53
26:V:4:LEU:O	26:V:32:CYS:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:120:A:H2'	1:0:120:A:N3	2.24	0.53
1:0:656:G:OP2	18:N:37:ARG:HD2	2.09	0.53
6:B:32:ASP:HA	42:B:8571:HOH:O	2.08	0.53
12:H:53:PRO:HA	12:H:125:VAL:O	2.07	0.53
14:J:109:LEU:HD13	14:J:113:ILE:HD11	1.89	0.53
15:K:143:THR:CG2	15:K:144:ASP:N	2.70	0.53
1:0:542:A:H2'	1:0:543:G:O4'	2.08	0.53
1:0:821:U:H2'	1:0:822:C:H6	1.72	0.53
1:0:1151:G:OP1	11:G:63:ARG:NH1	2.41	0.53
1:0:1353:C:P	42:0:4154:HOH:O	2.66	0.53
1:0:1422:U:H2'	1:0:1423:C:C6	2.44	0.53
1:0:1930:A:H1'	1:0:2128:G:H5'	1.89	0.53
1:0:2363:G:O3'	20:P:11:ARG:NH1	2.41	0.53
1:0:2502:C:C4'	12:H:151:MET:HG2	2.39	0.53
42:0:3675:HOH:O	28:X:186:ARG:HD2	2.08	0.53
42:0:8630:HOH:O	16:L:82:ARG:HD2	2.09	0.53
5:A:190:ARG:NH2	5:A:207:GLN:OE1	2.41	0.53
6:B:82:VAL:O	6:B:82:VAL:HG12	2.08	0.53
14:J:58:THR:HG22	14:J:59:LYS:HG3	1.91	0.53
24:T:9:CYS:HA	24:T:52:THR:CG2	2.39	0.53
26:V:38:THR:HB	42:V:5390:HOH:O	2.08	0.53
32:2:73:GLU:HB3	42:2:8567:HOH:O	2.07	0.53
1:0:119:A:H2'	1:0:120:A:H5''	1.91	0.53
1:0:283:U:H5''	1:0:284:C:P	2.48	0.53
1:0:349:U:O2'	1:0:350:C:H5'	2.09	0.53
1:0:514:G:O5'	1:0:514:G:H8	1.91	0.53
42:3:7215:HOH:O	37:4:76:PPU:HD2	2.09	0.53
8:D:94:ALA:HB3	8:D:174:VAL:HA	1.91	0.53
8:D:135:VAL:HG21	8:D:139:TYR:CD1	2.44	0.53
12:H:62:GLU:HA	42:H:8385:HOH:O	2.07	0.53
14:J:75:ARG:CZ	42:J:4172:HOH:O	2.57	0.53
15:K:21:ARG:N	42:K:8538:HOH:O	2.42	0.53
16:L:85:ARG:HA	16:L:87:MET:HE2	1.91	0.53
21:Q:82:GLU:HG3	21:Q:83:LYS:N	2.23	0.53
23:S:47:THR:HB	23:S:100:ASP:HB3	1.91	0.53
25:U:64:GLY:O	25:U:65:ASP:CB	2.56	0.53
1:0:1060:C:H6	1:0:1060:C:H5'	1.74	0.53
1:0:1242:A:OP2	13:I:60:ARG:NH2	2.41	0.53
1:0:671:A:O2'	1:0:672:G:H2'	2.09	0.53
1:0:1189:A:H1'	1:0:1209:C:O4'	2.09	0.53
1:0:2379:G:H4'	1:0:2380:A:H5''	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:46:TYR:CE2	7:C:98:ARG:NH1	2.77	0.53
11:G:12:ILE:O	11:G:13:PRO:C	2.50	0.53
14:J:30:LYS:O	14:J:55:VAL:HG13	2.09	0.53
17:M:11:ARG:O	17:M:15:GLU:HG3	2.09	0.53
17:M:157:PRO:HA	42:M:8526:HOH:O	2.08	0.53
27:W:15:ARG:HH11	27:W:15:ARG:CB	2.21	0.53
1:0:256:C:H2'	1:0:257:G:O4'	2.09	0.53
9:E:80:TRP:O	9:E:134:SER:HA	2.08	0.53
16:L:47:ASP:CG	16:L:48:ARG:H	2.17	0.53
17:M:29:SER:HA	42:M:8558:HOH:O	2.08	0.53
17:M:110:THR:HB	17:M:113:SER:OG	2.09	0.53
19:O:105:LEU:CD2	19:O:137:LEU:HD21	2.39	0.53
26:V:13:MET:HE2	26:V:18:GLN:N	2.24	0.53
1:0:316:A:H5'	23:S:54:ASP:OD2	2.10	0.52
1:0:2019:A:H5'	42:0:4012:HOH:O	2.09	0.52
5:A:199:HIS:HD2	5:A:201:PHE:HB2	1.74	0.52
6:B:333:GLU:HB2	24:T:14:GLU:OE2	2.09	0.52
7:C:35:VAL:HG21	7:C:227:GLY:HA2	1.91	0.52
9:E:10:ASP:HA	42:E:3707:HOH:O	2.09	0.52
12:H:86:ARG:HD3	12:H:130:HIS:HD2	1.73	0.52
16:L:87:MET:HB3	32:2:46:ILE:HG21	1.91	0.52
32:2:11:CYS:HB2	32:2:20:HIS:HE1	1.74	0.52
1:0:338:C:H4'	7:C:174:ILE:HD12	1.91	0.52
1:0:553:G:O4'	1:0:1325:G:H5'	2.08	0.52
1:0:951:A:C2'	1:0:952:G:H5'	2.39	0.52
1:0:1213:C:O2'	1:0:1214:G:H5'	2.09	0.52
1:0:1279:U:H5''	42:0:9091:HOH:O	2.09	0.52
1:0:2301:A:H5''	1:0:2302:A:H5'	1.90	0.52
1:0:2382:A:H5'	42:2:8538:HOH:O	2.09	0.52
6:B:27:ASN:HB3	42:B:8625:HOH:O	2.09	0.52
12:H:71:TYR:C	12:H:73:GLN:N	2.65	0.52
18:N:47:ARG:HG3	18:N:47:ARG:NH1	2.22	0.52
23:S:1:SER:N	42:S:5837:HOH:O	2.42	0.52
1:0:297:U:H1'	42:0:3425:HOH:O	2.09	0.52
1:0:1044:C:H5''	42:0:8544:HOH:O	2.08	0.52
1:0:1377:C:H5'	1:0:1377:C:C6	2.42	0.52
1:0:2717:C:O2'	1:0:2718:C:H5''	2.09	0.52
5:A:69:LEU:CD2	5:A:120:ARG:HB3	2.39	0.52
9:E:15:GLN:NE2	9:E:40:VAL:O	2.42	0.52
17:M:159:TYR:HE2	17:M:163:PHE:HE2	1.58	0.52
1:0:500:G:H21	21:Q:98:ASN:HD21	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:661:G:C5	1:0:686:A:C2	2.97	0.52
5:A:129:LEU:CD1	5:A:145:MET:HE1	2.39	0.52
7:C:57:PRO:HD2	7:C:73:LEU:HD22	1.91	0.52
15:K:143:THR:HG22	15:K:145:LEU:H	1.73	0.52
16:L:87:MET:CG	32:2:46:ILE:HD13	2.40	0.52
1:0:470:U:O2'	30:Z:16:HIS:CD2	2.62	0.52
1:0:1159:G:H21	1:0:1189:A:H8	1.57	0.52
1:0:1874:U:H2'	5:A:120:ARG:HG3	1.92	0.52
1:0:2445:U:H2'	1:0:2446:G:C8	2.45	0.52
42:0:9445:HOH:O	27:W:23:HIS:HD2	1.92	0.52
14:J:32:ILE:HD11	14:J:56:SER:HB3	1.91	0.52
15:K:57:VAL:O	15:K:57:VAL:HG12	2.10	0.52
27:W:18:ARG:NH1	42:W:4132:HOH:O	2.37	0.52
1:0:820:G:O2'	1:0:856:G:H4'	2.10	0.52
1:0:920:C:H5'	1:0:921:G:C4	2.44	0.52
5:A:8:ARG:HG2	42:A:8556:HOH:O	2.10	0.52
6:B:305:ASP:O	6:B:306:LYS:HB2	2.10	0.52
8:D:86:THR:HG23	42:D:7477:HOH:O	2.09	0.52
8:D:128:LEU:C	8:D:128:LEU:HD23	2.35	0.52
10:F:99:THR:HG23	10:F:99:THR:O	2.09	0.52
12:H:157:ILE:CG2	12:H:158:ASN:N	2.73	0.52
1:0:920:C:H5''	1:0:921:G:O5'	2.09	0.52
5:A:179:MET:HG2	5:A:186:TRP:CG	2.45	0.52
8:D:135:VAL:HG22	8:D:136:ARG:H	1.73	0.52
8:D:146:LYS:HZ3	17:M:107:ASN:HD21	1.56	0.52
9:E:126:ILE:HB	9:E:131:LEU:HD23	1.91	0.52
14:J:87:ARG:NE	42:J:4854:HOH:O	2.42	0.52
26:V:5:VAL:HG22	26:V:32:CYS:HB2	1.91	0.52
30:Z:10:LYS:HG3	42:Z:8434:HOH:O	2.10	0.52
1:0:1505:U:H6	1:0:1505:U:H5'	1.74	0.52
1:0:2748:G:H1'	42:0:7371:HOH:O	2.10	0.52
1:0:2815:G:N7	13:I:80:LYS:NZ	2.57	0.52
2:9:3023:U:C5'	2:9:3024:U:OP2	2.54	0.52
6:B:280:VAL:HG13	6:B:333:GLU:O	2.10	0.52
7:C:40:ALA:HB3	7:C:100:LEU:HD12	1.92	0.52
8:D:94:ALA:O	8:D:95:THR:O	2.28	0.52
9:E:31:ARG:HH12	9:E:68:HIS:CE1	2.28	0.52
10:F:117:GLU:C	10:F:119:ARG:H	2.18	0.52
13:I:46:ILE:HG12	13:I:53:ILE:HD13	1.92	0.52
24:T:17:THR:HG22	24:T:18:GLY:N	2.25	0.52
28:X:187:VAL:HG23	28:X:192:ASP:HB3	1.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:187:VAL:HB	42:X:8571:HOH:O	2.09	0.52
1:0:970:U:H2'	42:0:5804:HOH:O	2.10	0.52
1:0:2281:C:C2'	1:0:2282:U:H5'	2.39	0.52
1:0:2438:G:H2'	1:0:2439:C:O4'	2.10	0.52
42:0:5686:HOH:O	6:B:2:GLN:HA	2.10	0.52
2:9:3020:G:H3'	42:9:2984:HOH:O	2.10	0.52
10:F:107:VAL:HG23	42:F:6617:HOH:O	2.09	0.52
11:G:71:LEU:C	11:G:73:ASP:H	2.18	0.52
12:H:14:TYR:N	12:H:91:HIS:CE1	2.75	0.52
24:T:8:TYR:CD2	24:T:36:CYS:HB3	2.44	0.52
26:V:64:THR:O	26:V:68:THR:HG22	2.10	0.52
29:Y:46:LYS:O	29:Y:57:CYS:HA	2.09	0.52
1:0:407:A:H5'	42:0:5500:HOH:O	2.10	0.52
1:0:834:G:H4'	1:0:835:U:OP2	2.10	0.52
1:0:1398:G:H2'	1:0:1399:A:C8	2.45	0.52
1:0:1887:U:OP1	29:Y:21:LYS:HG3	2.10	0.52
1:0:2015:A:H2'	1:0:2016:U:O4'	2.09	0.52
6:B:195:ARG:HD2	6:B:324:ASP:OD1	2.10	0.52
7:C:33:LYS:HE2	42:C:8364:HOH:O	2.10	0.52
9:E:93:MET:HE1	9:E:165:GLY:H	1.74	0.52
10:F:46:GLU:O	10:F:73:PRO:HD2	2.10	0.52
16:L:134:ILE:HG23	16:L:141:ILE:HD13	1.91	0.52
17:M:171:HIS:CE1	42:M:8568:HOH:O	2.62	0.52
26:V:122:ARG:NE	42:V:5817:HOH:O	2.42	0.52
27:W:76:ARG:HG3	27:W:76:ARG:NH1	2.24	0.52
28:X:99:ALA:HB2	28:X:233:TYR:CZ	2.45	0.52
29:Y:19:GLY:O	29:Y:23:ARG:HG2	2.09	0.52
1:0:29:C:O2'	1:0:30:U:H5'	2.11	0.51
1:0:1010:C:H4'	17:M:4:PRO:HB2	1.92	0.51
1:0:1189:A:O2'	1:0:1208:C:H2'	2.10	0.51
1:0:1592:G:O2'	1:0:1593:C:O4'	2.28	0.51
1:0:2524:G:H21	1:0:2526:C:N4	2.08	0.51
16:L:37:VAL:CG1	16:L:63:VAL:HG11	2.40	0.51
23:S:71:VAL:CG1	23:S:90:PRO:HB3	2.27	0.51
26:V:106:THR:OG1	26:V:109:GLU:HG3	2.10	0.51
28:X:144:ARG:NE	42:X:8612:HOH:O	2.43	0.51
1:0:449:A:N7	7:C:43:LYS:HG2	2.24	0.51
1:0:1191:A:C3'	1:0:1192:A:H5''	2.41	0.51
1:0:1477:C:H5'	1:0:1868:G:C5'	2.40	0.51
1:0:1942:A:O2'	1:0:1943:C:H5'	2.10	0.51
1:0:2123:A:OP1	16:L:89:ASN:ND2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:99:ILE:O	5:A:131:HIS:CE1	2.62	0.51
15:K:101:ASP:C	15:K:103:ALA:H	2.16	0.51
16:L:81:ARG:O	16:L:86:MET:HE2	2.09	0.51
16:L:155:HIS:CE1	16:L:158:ARG:HE	2.29	0.51
26:V:154:ARG:C	42:V:4276:HOH:O	2.53	0.51
28:X:186:ARG:HG2	28:X:186:ARG:NH1	2.24	0.51
28:X:189:ASN:ND2	28:X:192:ASP:H	2.08	0.51
30:Z:28:HIS:O	30:Z:32:LYS:N	2.40	0.51
1:O:1829:A:H5''	42:O:9576:HOH:O	2.09	0.51
1:O:1884:G:O6	5:A:190:ARG:HD2	2.10	0.51
1:O:2548:C:OP2	6:B:5:ARG:NH2	2.43	0.51
5:A:66:ARG:HH11	5:A:66:ARG:HB2	1.73	0.51
6:B:248:ARG:O	6:B:251:VAL:CG1	2.58	0.51
9:E:20:ILE:CD1	9:E:40:VAL:HG11	2.39	0.51
17:M:154:LEU:O	17:M:155:GLU:CB	2.59	0.51
26:V:88:THR:HG23	26:V:110:GLN:HB3	1.91	0.51
29:Y:42:CYS:SG	29:Y:43:GLY:N	2.83	0.51
1:O:1667:A:H2'	1:O:1668:U:C6	2.45	0.51
25:U:11:MET:HB3	25:U:15:GLU:HB2	1.91	0.51
26:V:21:LEU:HD13	26:V:26:ILE:HD11	1.92	0.51
32:2:74:CYS:SG	32:2:76:LYS:HB2	2.50	0.51
1:O:2251:G:H2'	1:O:2252:A:C8	2.45	0.51
1:O:2670:G:O2'	1:O:2671:U:H5'	2.10	0.51
2:9:3076:G:C3'	2:9:3077:A:H5''	2.33	0.51
5:A:105:VAL:HG13	5:A:155:THR:O	2.11	0.51
7:C:107:ARG:NE	42:C:8462:HOH:O	2.29	0.51
7:C:200:PRO:HB3	7:C:212:VAL:HG23	1.92	0.51
8:D:11:HIS:O	8:D:12:GLU:HB3	2.10	0.51
12:H:162:SER:CB	12:H:163:PRO:CD	2.83	0.51
21:Q:132:ARG:CZ	42:Q:8585:HOH:O	2.58	0.51
28:X:155:ARG:NH1	42:X:8559:HOH:O	2.44	0.51
1:O:1181:A:H2'	1:O:1182:C:O4'	2.11	0.51
1:O:1753:C:O2	6:B:229:ARG:NH2	2.43	0.51
1:O:2114:C:OP1	5:A:1:GLY:HA2	2.11	0.51
2:9:3003:A:H2'	42:9:2430:HOH:O	2.10	0.51
8:D:64:ARG:O	8:D:67:ASP:OD2	2.28	0.51
12:H:83:PHE:CD1	12:H:134:ALA:HB2	2.46	0.51
15:K:104:ASP:HB3	42:K:8570:HOH:O	2.10	0.51
16:L:155:HIS:ND1	16:L:158:ARG:NE	2.54	0.51
18:N:21:SER:OG	18:N:106:PRO:HB2	2.11	0.51
1:O:710:G:OP1	18:N:24:ALA:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1189:A:H1'	1:0:1209:C:H1'	1.93	0.51
1:0:1299:G:N2	42:0:4159:HOH:O	2.43	0.51
1:0:2111:G:H1'	42:0:8565:HOH:O	2.08	0.51
5:A:93:THR:C	5:A:94:LEU:HD23	2.35	0.51
8:D:59:GLY:C	8:D:61:PHE:H	2.19	0.51
12:H:13:ALA:HA	12:H:91:HIS:CE1	2.46	0.51
29:Y:26:VAL:O	29:Y:30:GLU:HG3	2.11	0.51
1:0:694:A:H2'	1:0:695:C:H5'	1.92	0.51
1:0:1114:A:H2'	1:0:1115:U:C6	2.46	0.51
1:0:2408:A:H1'	32:2:10:TYR:CD1	2.46	0.51
6:B:204:GLY:HA3	42:B:8650:HOH:O	2.11	0.51
6:B:280:VAL:CG1	6:B:334:SER:HA	2.40	0.51
8:D:57:THR:HG23	8:D:63:ILE:CB	2.41	0.51
11:G:64:ASN:N	11:G:64:ASN:ND2	2.57	0.51
29:Y:22:ILE:O	29:Y:26:VAL:HG23	2.11	0.51
1:0:1878:G:C1'	42:0:5597:HOH:O	2.54	0.51
1:0:2460:A:OP1	32:2:60:LYS:HB3	2.10	0.51
42:0:9295:HOH:O	14:J:39:GLY:HA3	2.10	0.51
5:A:37:VAL:HG22	42:A:8604:HOH:O	2.10	0.51
6:B:24:PRO:CG	6:B:204:GLY:HA2	2.41	0.51
6:B:79:MET:HE3	6:B:144:THR:HG21	1.93	0.51
8:D:84:LEU:C	8:D:86:THR:H	2.18	0.51
26:V:122:ARG:HH11	26:V:122:ARG:CG	2.19	0.51
1:0:820:G:C6	5:A:171:LYS:HB2	2.46	0.51
1:0:1015:C:H2'	1:0:1016:U:C6	2.45	0.51
1:0:1174:A:C5	1:0:1201:C:H4'	2.45	0.51
1:0:1393:A:H2'	1:0:1394:C:C6	2.46	0.51
42:0:3499:HOH:O	6:B:48:MET:N	2.44	0.51
5:A:36:ASP:HB2	5:A:85:ASP:H	1.76	0.51
13:I:80:LYS:HE2	13:I:98:PHE:CZ	2.45	0.51
14:J:28:GLU:HG2	14:J:58:THR:HB	1.93	0.51
15:K:125:PHE:CZ	15:K:140:VAL:HG13	2.46	0.51
17:M:132:ASN:O	17:M:135:VAL:HG12	2.11	0.51
30:Z:12:ASN:HB3	42:Z:8452:HOH:O	2.10	0.51
1:0:559:U:H2'	1:0:560:C:O4'	2.12	0.50
1:0:2502:C:H2'	1:0:2503:A:C5'	2.40	0.50
6:B:190:MET:HE2	6:B:194:PHE:HD1	1.69	0.50
6:B:258:GLY:N	6:B:260:HIS:CE1	2.78	0.50
8:D:170:TYR:O	8:D:171:ASP:HB3	2.10	0.50
14:J:118:ALA:C	14:J:120:ARG:H	2.19	0.50
16:L:157:LEU:HB3	16:L:160:PHE:HD1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:251:C:H1'	16:L:58:GLN:HE22	1.76	0.50
1:0:553:G:P	28:X:204:ARG:NH2	2.82	0.50
1:0:1787:C:OP1	19:O:68:LYS:HE2	2.11	0.50
1:0:2064:U:H4'	1:0:2653:A:OP1	2.11	0.50
1:0:2910:A:H5''	42:O:3616:HOH:O	2.11	0.50
7:C:1:MET:HG2	7:C:2:GLN:N	2.24	0.50
9:E:156:ASP:OD2	9:E:157:LYS:NZ	2.35	0.50
17:M:49:THR:CG2	17:M:56:ASP:HB2	2.39	0.50
1:0:638:C:H2'	1:0:639:A:C8	2.46	0.50
1:0:1120:U:H5''	1:0:1120:U:C6	2.46	0.50
1:0:1333:U:H2'	1:0:1334:C:C6	2.46	0.50
1:0:2460:A:OP1	32:2:60:LYS:CB	2.60	0.50
6:B:7:ARG:CD	6:B:9:GLY:O	2.59	0.50
6:B:297:VAL:HB	42:B:8602:HOH:O	2.11	0.50
6:B:320:GLN:HG3	6:B:321:PRO:HD2	1.93	0.50
9:E:84:MET:HE2	9:E:133:VAL:HG23	1.92	0.50
10:F:50:VAL:CG1	10:F:60:VAL:HG11	2.40	0.50
26:V:3:ALA:O	26:V:54:PHE:HA	2.10	0.50
1:0:538:C:OP2	28:X:134:HIS:HE1	1.95	0.50
1:0:771:G:OP2	16:L:79:LYS:HD2	2.11	0.50
1:0:820:G:OP2	5:A:171:LYS:NZ	2.35	0.50
42:O:6181:HOH:O	28:X:165:GLU:HB3	2.11	0.50
2:9:3002:U:OP2	2:9:3003:A:H5'	2.11	0.50
5:A:125:ASN:ND2	42:A:8539:HOH:O	2.38	0.50
7:C:237:GLU:HB2	42:C:8436:HOH:O	2.10	0.50
8:D:62:ASP:HA	42:D:4233:HOH:O	2.11	0.50
15:K:97:VAL:HG12	15:K:98:GLU:O	2.11	0.50
22:R:23:LYS:HE2	42:R:8330:HOH:O	2.12	0.50
28:X:117:LEU:HD12	28:X:174:VAL:HG11	1.93	0.50
30:Z:25:LYS:HD2	31:1:49:GLU:H	1.76	0.50
1:0:168:C:O2'	1:0:169:A:H5'	2.12	0.50
1:0:911:G:H5'	1:0:932:U:OP1	2.12	0.50
2:9:3028:U:H5''	17:M:40:ASN:ND2	2.27	0.50
6:B:144:THR:HG22	6:B:145:HIS:N	2.25	0.50
8:D:25:MET:HE1	8:D:37:ALA:O	2.11	0.50
8:D:135:VAL:HG22	8:D:136:ARG:N	2.27	0.50
10:F:58:GLU:HA	10:F:61:MET:HG3	1.93	0.50
12:H:130:HIS:CG	12:H:133:ILE:HD11	2.45	0.50
12:H:147:ARG:HA	12:H:150:LYS:HZ2	1.76	0.50
14:J:34:VAL:CG2	14:J:47:ALA:HB2	2.42	0.50
19:O:115:SER:O	19:O:117:SER:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:V:26:ILE:HG13	26:V:26:ILE:O	2.10	0.50
27:W:9:VAL:HG13	27:W:88:GLU:OE1	2.12	0.50
1:0:1434:A:H2'	1:0:1436:C:C5	2.45	0.50
5:A:192:VAL:O	5:A:192:VAL:HG12	2.11	0.50
6:B:185:GLY:HA2	42:B:8631:HOH:O	2.12	0.50
6:B:329:TYR:CE2	24:T:15:PRO:HG2	2.46	0.50
7:C:162:VAL:HG12	7:C:162:VAL:O	2.11	0.50
8:D:57:THR:HG23	8:D:63:ILE:CG2	2.40	0.50
9:E:69:ILE:HA	9:E:72:MET:HE3	1.93	0.50
26:V:110:GLN:HE21	26:V:110:GLN:HA	1.75	0.50
1:0:797:A:O4'	29:Y:10:ARG:N	2.44	0.50
1:0:1930:A:H2'	1:0:1931:A:C8	2.46	0.50
1:0:2533:C:H6	1:0:2533:C:C5'	2.17	0.50
1:0:2766:A:O2'	1:0:2767:C:H5'	2.12	0.50
1:0:2842:G:H2'	1:0:2843:A:H5'	1.93	0.50
9:E:172:PRO:HB3	42:E:6931:HOH:O	2.11	0.50
12:H:75:SER:HB3	12:H:79:ALA:HB1	1.93	0.50
12:H:81:TYR:CD1	12:H:81:TYR:C	2.89	0.50
1:0:1119:G:H8	13:I:52:GLN:NE2	2.09	0.50
1:0:1902:G:H2'	1:0:1903:U:O4'	2.11	0.50
1:0:2064:U:H5'	1:0:2652:U:H4'	1.94	0.50
8:D:136:ARG:HD2	8:D:155:HIS:O	2.11	0.50
13:I:39:VAL:HG13	13:I:106:GLY:O	2.11	0.50
17:M:24:LEU:O	17:M:28:LYS:HG2	2.12	0.50
17:M:130:PRO:HA	42:M:8541:HOH:O	2.12	0.50
28:X:184:GLU:OE1	28:X:204:ARG:NH1	2.44	0.50
1:0:392:U:C5'	16:L:193:LYS:HB3	2.42	0.50
1:0:731:U:H2'	1:0:732:C:C6	2.47	0.50
1:0:797:A:H5'	29:Y:10:ARG:HG2	1.94	0.50
42:O:7049:HOH:O	29:Y:31:ILE:HG13	2.11	0.50
7:C:54:LEU:HD21	7:C:87:ARG:HD2	1.94	0.50
7:C:103:ASN:HB3	42:C:8309:HOH:O	2.10	0.50
13:I:45:VAL:HG22	13:I:46:ILE:N	2.26	0.50
17:M:67:ALA:C	17:M:69:TYR:N	2.70	0.50
23:S:53:GLY:HA3	42:S:6384:HOH:O	2.11	0.50
1:0:182:G:O3'	16:L:157:LEU:CD1	2.60	0.49
1:0:602:A:O2'	1:0:605:C:H4'	2.12	0.49
1:0:1119:G:H2'	13:I:52:GLN:HE22	1.75	0.49
1:0:1249:U:H2'	1:0:1250:C:C6	2.46	0.49
1:0:1810:C:OP1	24:T:44:ARG:NE	2.32	0.49
1:0:2621:U:H5	42:O:9480:HOH:O	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:O:5726:HOH:O	24:T:56:ARG:HB3	2.12	0.49
2:9:3064:C:H2'	2:9:3065:A:H5'	1.94	0.49
5:A:217:ARG:HG2	5:A:229:ALA:HB2	1.94	0.49
8:D:49:PRO:HG3	42:D:5828:HOH:O	2.12	0.49
8:D:154:LYS:H	8:D:154:LYS:CD	2.11	0.49
9:E:20:ILE:CD1	9:E:33:LEU:HD12	2.42	0.49
12:H:14:TYR:HB2	42:H:8352:HOH:O	2.12	0.49
12:H:26:LYS:HD3	12:H:89:PRO:CG	2.42	0.49
12:H:35:ASN:ND2	12:H:79:ALA:O	2.45	0.49
13:I:77:GLY:O	13:I:78:ILE:C	2.55	0.49
16:L:38:VAL:O	16:L:63:VAL:HG13	2.11	0.49
1:O:1503:U:H2'	1:O:1504:A:O4'	2.12	0.49
42:O:6874:HOH:O	23:S:2:LYS:HE2	2.13	0.49
6:B:175:LEU:C	6:B:175:LEU:CD2	2.85	0.49
7:C:107:ARG:HB3	7:C:107:ARG:HH11	1.77	0.49
9:E:31:ARG:HH12	9:E:68:HIS:CD2	2.30	0.49
17:M:100:ALA:O	17:M:129:ILE:HG23	2.12	0.49
17:M:114:LYS:O	17:M:118:ILE:HG13	2.12	0.49
1:O:1014:A:H2'	1:O:1015:C:H5'	1.93	0.49
1:O:1162:G:H2'	42:O:6056:HOH:O	2.12	0.49
1:O:1205:U:H2'	1:O:1206:U:H5''	1.93	0.49
2:9:3042:C:O2	8:D:76:ARG:NH1	2.45	0.49
2:9:3059:C:H5'	42:9:5233:HOH:O	2.11	0.49
4:4:74:C:H2'	4:4:75:C:C5'	2.41	0.49
9:E:11:VAL:HG13	9:E:23:GLU:O	2.11	0.49
1:O:777:U:O2'	30:Z:11:LYS:HG2	2.11	0.49
1:O:820:G:OP1	29:Y:17:ARG:NH2	2.44	0.49
1:O:932:U:H2'	1:O:933:C:C6	2.47	0.49
1:O:1702:U:H5'	42:O:9921:HOH:O	2.12	0.49
42:O:6018:HOH:O	29:Y:22:ILE:HG13	2.12	0.49
7:C:7:ASP:OD1	7:C:11:ASN:O	2.30	0.49
10:F:101:ALA:HB2	10:F:108:LEU:HD22	1.95	0.49
12:H:165:GLY:C	12:H:166:ASN:HD22	2.20	0.49
13:I:93:ARG:HB3	13:I:93:ARG:NH1	2.27	0.49
28:X:112:GLU:CD	28:X:115:ARG:NH1	2.70	0.49
1:O:1666:C:C2'	1:O:1667:A:C5'	2.91	0.49
1:O:2748:G:C5'	42:O:7009:HOH:O	2.55	0.49
42:O:6159:HOH:O	23:S:38:ARG:NH1	2.45	0.49
42:O:7015:HOH:O	16:L:91:ILE:HG23	2.12	0.49
6:B:132:HIS:CE1	6:B:171:VAL:HG21	2.46	0.49
7:C:150:THR:HA	7:C:203:ALA:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:86:VAL:CG1	9:E:129:GLU:HA	2.42	0.49
16:L:37:VAL:HG13	16:L:63:VAL:HG11	1.95	0.49
21:Q:39:THR:CG2	21:Q:42:GLU:HG3	2.42	0.49
24:T:31:PHE:CG	24:T:37:GLU:HG2	2.48	0.49
1:O:2256:G:H2'	1:O:2257:G:H5'	1.95	0.49
1:O:2266:A:H2'	1:O:2267:G:C8	2.47	0.49
1:O:2432:C:H4'	32:2:36:ILE:HG12	1.94	0.49
2:9:3049:G:O2'	2:9:3050:G:H5'	2.12	0.49
2:9:3088:G:OP1	26:V:130:HIS:NE2	2.42	0.49
10:F:63:ILE:HB	10:F:64:PRO:CD	2.38	0.49
12:H:26:LYS:HG2	12:H:28:ILE:N	2.20	0.49
12:H:45:GLN:HG3	12:H:135:TRP:NE1	2.27	0.49
15:K:65:ASP:CG	15:K:111:ALA:HB3	2.38	0.49
1:O:21:G:H4'	21:Q:2:ILE:HG22	1.95	0.49
1:O:907:A:H4'	1:O:1328:A:C2	2.48	0.49
5:A:211:LYS:HB2	42:A:8628:HOH:O	2.11	0.49
6:B:41:PHE:HB3	6:B:190:MET:HE1	1.95	0.49
10:F:22:VAL:HG21	10:F:104:ALA:HB2	1.95	0.49
1:O:175:G:H2'	16:L:192:ALA:HB3	1.93	0.49
1:O:2361:A:H2'	1:O:2362:A:C8	2.48	0.49
1:O:2637:A:C4'	1:O:2638:G:O5'	2.60	0.49
1:O:2724:U:H2'	1:O:2725:G:O4'	2.12	0.49
1:O:2837:U:H1'	6:B:307:ARG:HH12	1.77	0.49
2:9:3055:U:H4'	2:9:3056:A:C8	2.47	0.49
5:A:9:ARG:HG2	5:A:16:PHE:CD2	2.48	0.49
6:B:55:ASN:HB3	6:B:64:GLY:H	1.77	0.49
12:H:147:ARG:HA	12:H:150:LYS:NZ	2.28	0.49
16:L:114:VAL:HB	16:L:159:THR:HG23	1.94	0.49
17:M:182:GLY:O	17:M:183:ASP:O	2.31	0.49
27:W:75:ALA:O	27:W:83:ALA:HA	2.13	0.49
29:Y:23:ARG:NH1	42:Y:8404:HOH:O	2.46	0.49
1:O:588:G:O6	26:V:154:ARG:NH1	2.46	0.49
1:O:816:G:H5'	1:O:1598:A:H4'	1.94	0.49
1:O:902:G:N7	15:K:18:HIS:CD2	2.78	0.49
1:O:1384:C:H5'	27:W:30:MET:HG2	1.95	0.49
1:O:1886:A:O2'	29:Y:20:LEU:HB2	2.13	0.49
1:O:2911:C:H2'	1:O:2912:C:C6	2.48	0.49
10:F:56:PRO:CG	16:L:44:THR:HA	2.43	0.49
24:T:44:ARG:HB3	42:T:3805:HOH:O	2.11	0.49
1:O:919:U:H5'	1:O:2465:A:O2'	2.12	0.49
5:A:97:ALA:HB2	5:A:150:PRO:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:314:ALA:HB3	6:B:317:PRO:HG3	1.95	0.49
12:H:29:ALA:HB3	12:H:65:ARG:NH1	2.15	0.49
12:H:166:ASN:N	12:H:166:ASN:ND2	2.57	0.49
15:K:146:GLY:C	15:K:148:GLU:H	2.21	0.49
16:L:74:ARG:HD3	16:L:91:ILE:HD12	1.94	0.49
1:0:621:C:H5'	28:X:132:ASP:OD2	2.12	0.48
1:0:1783:A:O2'	1:0:1784:U:H5'	2.12	0.48
1:0:2507:G:H2'	1:0:2510:C:H42	1.78	0.48
42:9:4707:HOH:O	17:M:147:ILE:HB	2.12	0.48
6:B:119:HIS:O	6:B:121:PRO:HD3	2.12	0.48
6:B:205:VAL:O	6:B:307:ARG:NE	2.46	0.48
13:I:107:ASN:ND2	13:I:107:ASN:C	2.68	0.48
15:K:133:VAL:HB	42:K:8564:HOH:O	2.13	0.48
26:V:139:GLY:O	26:V:141:HIS:HD2	1.95	0.48
1:0:244:C:OP2	10:F:38:LYS:HE3	2.13	0.48
1:0:1183:C:N4	42:0:3874:HOH:O	2.46	0.48
42:0:9954:HOH:O	13:I:46:ILE:HD12	2.13	0.48
12:H:86:ARG:NH1	12:H:130:HIS:CD2	2.81	0.48
15:K:72:ASN:O	15:K:76:LEU:HG	2.13	0.48
15:K:73:VAL:HG23	15:K:74:THR:N	2.28	0.48
27:W:8:ARG:NH1	42:W:2479:HOH:O	2.38	0.48
27:W:9:VAL:HG13	27:W:88:GLU:CD	2.37	0.48
1:0:1268:C:O2'	1:0:1269:G:H5'	2.13	0.48
1:0:1654:U:H2'	5:A:47:HIS:CD2	2.49	0.48
1:0:1787:C:H4'	1:0:2883:A:O4'	2.13	0.48
1:0:2453:G:H4'	15:K:50:GLY:C	2.39	0.48
1:0:2672:C:O2'	1:0:2673:U:H5'	2.13	0.48
6:B:24:PRO:HG2	6:B:204:GLY:HA2	1.94	0.48
6:B:36:PRO:HA	6:B:168:GLY:HA2	1.94	0.48
6:B:248:ARG:NH2	42:B:8523:HOH:O	2.46	0.48
8:D:35:ALA:HB1	42:D:3279:HOH:O	2.12	0.48
9:E:69:ILE:HA	9:E:72:MET:HE2	1.94	0.48
14:J:29:LEU:HB3	14:J:55:VAL:CG1	2.39	0.48
14:J:99:ASP:OD1	14:J:101:ASN:N	2.45	0.48
15:K:55:GLN:HA	15:K:58:GLN:NE2	2.27	0.48
16:L:139:PRO:HA	16:L:142:LYS:HB2	1.94	0.48
16:L:182:LYS:HB2	16:L:194:ALA:HB2	1.95	0.48
18:N:44:ASN:OD1	18:N:65:LEU:HB2	2.12	0.48
27:W:70:ILE:HG23	27:W:70:ILE:O	2.13	0.48
1:0:827:A:H2'	1:0:828:G:O4'	2.13	0.48
1:0:1495:C:H1'	1:0:1573:A:H1'	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1878:G:O2'	1:0:1879:U:P	2.71	0.48
1:0:2758:G:H2'	1:0:2759:C:C6	2.49	0.48
1:0:2896:A:OP1	27:W:15:ARG:NH1	2.46	0.48
6:B:1:PRO:O	6:B:2:GLN:HB2	2.14	0.48
6:B:7:ARG:NH1	6:B:11:LEU:HD22	2.28	0.48
8:D:163:VAL:HA	42:D:6326:HOH:O	2.13	0.48
10:F:106:THR:HB	42:F:6617:HOH:O	2.13	0.48
12:H:150:LYS:NZ	42:H:8379:HOH:O	2.44	0.48
19:O:55:LYS:HA	42:O:182:HOH:O	2.13	0.48
19:O:115:SER:C	19:O:117:SER:N	2.70	0.48
23:S:50:VAL:HG12	23:S:56:ALA:HA	1.95	0.48
30:Z:28:HIS:CD2	30:Z:31:LYS:HG3	2.48	0.48
32:2:91:GLN:O	32:2:92:GLU:HB2	2.12	0.48
1:0:128:A:C8	1:0:128:A:H3'	2.47	0.48
1:0:200:U:H2'	42:0:9938:HOH:O	2.12	0.48
1:0:398:U:H2'	1:0:399:C:C6	2.48	0.48
1:0:1166:A:H1'	1:0:1192:A:N1	2.25	0.48
1:0:1342:C:O2'	1:0:1343:C:H5'	2.14	0.48
1:0:1730:G:H5'	1:0:1731:C:C6	2.49	0.48
1:0:2004:U:O2	1:0:2004:U:H2'	2.13	0.48
9:E:11:VAL:CG1	9:E:12:ASP:H	2.27	0.48
9:E:31:ARG:CZ	42:E:5919:HOH:O	2.60	0.48
9:E:32:ARG:O	9:E:33:LEU:HD23	2.12	0.48
19:O:143:ALA:HA	42:O:193:HOH:O	2.12	0.48
21:Q:113:HIS:O	21:Q:145:LEU:HD12	2.13	0.48
24:T:6:CYS:HB2	24:T:32:CYS:HB3	1.94	0.48
24:T:52:THR:HG22	24:T:54:THR:N	2.27	0.48
1:0:182:G:O3'	16:L:157:LEU:HD13	2.14	0.48
1:0:506:G:H22	1:0:509:A:H5''	1.75	0.48
1:0:1236:A:H2'	1:0:1237:U:O4'	2.14	0.48
1:0:1778:A:H2'	1:0:1779:A:H5'	1.95	0.48
1:0:2403:C:H5'	42:0:5501:HOH:O	2.14	0.48
5:A:164:ARG:CZ	42:A:8596:HOH:O	2.61	0.48
6:B:41:PHE:CZ	6:B:79:MET:HG3	2.48	0.48
6:B:72:THR:HB	42:B:8602:HOH:O	2.13	0.48
8:D:35:ALA:O	8:D:37:ALA:N	2.46	0.48
17:M:139:TRP:HA	17:M:139:TRP:HE3	1.79	0.48
21:Q:15:LYS:HE3	42:Q:8579:HOH:O	2.12	0.48
21:Q:96:VAL:HG13	21:Q:106:GLY:HA3	1.95	0.48
26:V:29:VAL:O	26:V:30:ASN:HB2	2.13	0.48
1:0:558:C:C2'	1:0:559:U:C5'	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:820:G:C5	5:A:171:LYS:HB2	2.49	0.48
1:0:1298:U:H2'	1:0:1299:G:C8	2.48	0.48
1:0:1878:G:O2'	1:0:1879:U:C6	2.64	0.48
1:0:1943:C:O4'	5:A:212:PRO:HA	2.13	0.48
1:0:2466:G:H5''	42:0:3138:HOH:O	2.13	0.48
5:A:51:ARG:HB2	42:A:8614:HOH:O	2.12	0.48
7:C:27:ARG:HG3	7:C:29:ASP:OD1	2.13	0.48
8:D:35:ALA:C	8:D:37:ALA:N	2.72	0.48
12:H:45:GLN:NE2	12:H:135:TRP:HE1	2.07	0.48
12:H:132:PHE:O	12:H:133:ILE:HD13	2.14	0.48
12:H:150:LYS:HA	12:H:153:VAL:HG22	1.94	0.48
17:M:67:ALA:HA	17:M:71:TRP:HB3	1.95	0.48
18:N:96:VAL:HG12	18:N:97:SER:O	2.14	0.48
26:V:149:LEU:CG	26:V:153:MET:HE2	2.33	0.48
28:X:197:ASP:C	28:X:197:ASP:OD1	2.56	0.48
1:0:128:A:O2'	1:0:129:A:H5'	2.14	0.48
1:0:426:G:H2'	1:0:427:C:O4'	2.14	0.48
1:0:1185:U:H5'	42:0:6934:HOH:O	2.14	0.48
1:0:1805:G:H2'	1:0:1806:G:H8	1.78	0.48
1:0:2413:A:N7	17:M:109:PRO:HB3	2.28	0.48
1:0:2472:C:O2'	1:0:2634:G:H4'	2.13	0.48
1:0:2637:A:H2'	1:0:2637:A:N3	2.28	0.48
1:0:2781:U:H2'	1:0:2782:G:C5'	2.43	0.48
1:0:2787:C:H5	42:0:4107:HOH:O	1.95	0.48
42:0:3246:HOH:O	16:L:108:LYS:HD2	2.14	0.48
6:B:17:LYS:O	6:B:260:HIS:HD2	1.96	0.48
8:D:58:VAL:HG12	8:D:59:GLY:N	2.29	0.48
8:D:95:THR:C	8:D:97:GLN:N	2.69	0.48
12:H:26:LYS:HD2	12:H:28:ILE:CG1	2.43	0.48
16:L:49:ALA:C	16:L:54:TYR:HB3	2.39	0.48
26:V:35:VAL:HG23	26:V:41:TYR:CD2	2.48	0.48
1:0:816:G:C6	1:0:817:G:N1	2.81	0.48
1:0:1299:G:N7	15:K:6:ARG:NH1	2.62	0.48
1:0:1669:A:H2'	1:0:1670:G:H8	1.79	0.48
6:B:27:ASN:HD22	6:B:27:ASN:H	1.60	0.48
7:C:127:ARG:HG2	7:C:127:ARG:NH1	2.27	0.48
9:E:36:PRO:HD3	13:I:127:ILE:HD12	1.96	0.48
14:J:130:MET:SD	24:T:25:ASP:O	2.72	0.48
15:K:143:THR:CG2	15:K:144:ASP:H	2.26	0.48
16:L:24:MET:HE1	16:L:120:VAL:O	2.14	0.48
17:M:161:GLY:O	17:M:162:ASP:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:541:C:C2'	1:0:542:A:C5'	2.88	0.48
1:0:858:U:H2'	1:0:859:C:H6	1.79	0.48
1:0:1636:G:O2'	1:0:1637:A:H5'	2.13	0.48
1:0:2119:C:O2'	1:0:2120:U:H5'	2.14	0.48
1:0:2276:U:H2'	1:0:2277:U:H6	1.76	0.48
1:0:2379:G:H4'	1:0:2380:A:C5'	2.44	0.48
5:A:99:ILE:O	5:A:131:HIS:HE1	1.96	0.48
6:B:310:ARG:HD2	42:B:8645:HOH:O	2.13	0.48
7:C:235:PHE:HE2	7:C:243:VAL:HG21	1.79	0.48
8:D:23:VAL:O	8:D:23:VAL:CG2	2.62	0.48
12:H:139:ASP:H	12:H:140:PRO:HD3	1.76	0.48
24:T:14:GLU:OE1	24:T:15:PRO:HD2	2.14	0.48
25:U:20:LEU:HD22	25:U:60:GLN:HE22	1.79	0.48
26:V:122:ARG:CZ	42:V:5817:HOH:O	2.62	0.48
1:0:2630:G:O6	5:A:206:ARG:NH2	2.46	0.47
6:B:177:HIS:O	6:B:181:ILE:HG13	2.14	0.47
7:C:118:THR:CG2	7:C:137:PRO:HB3	2.43	0.47
11:G:16:LYS:O	11:G:20:VAL:HG23	2.14	0.47
17:M:62:HIS:HB3	17:M:65:ASP:OD1	2.13	0.47
17:M:184:ILE:HG22	17:M:185:GLU:N	2.27	0.47
1:0:1701:A:H5''	1:0:1702:U:H3'	1.95	0.47
1:0:2353:A:O2'	17:M:7:LYS:HB3	2.14	0.47
1:0:2401:A:H5'	42:0:8995:HOH:O	2.14	0.47
1:0:2506:A:C1'	42:0:5531:HOH:O	2.62	0.47
1:0:2837:U:H2'	42:0:6313:HOH:O	2.14	0.47
7:C:16:VAL:HG12	7:C:17:ASP:H	1.78	0.47
7:C:76:ARG:HD2	42:C:8439:HOH:O	2.14	0.47
15:K:24:ALA:HB2	15:K:30:ARG:HD2	1.96	0.47
17:M:67:ALA:C	17:M:69:TYR:H	2.22	0.47
21:Q:119:VAL:O	21:Q:119:VAL:HG12	2.14	0.47
26:V:121:PRO:CA	26:V:153:MET:HG2	2.44	0.47
1:0:682:A:H2'	1:0:683:G:O4'	2.14	0.47
5:A:88:ILE:CD1	5:A:100:PRO:HD3	2.42	0.47
6:B:74:ILE:HG13	42:B:8602:HOH:O	2.14	0.47
6:B:307:ARG:HH11	6:B:307:ARG:CB	2.27	0.47
6:B:312:ARG:HD3	6:B:315:VAL:HG13	1.96	0.47
11:G:23:ILE:O	11:G:27:ILE:HG13	2.14	0.47
16:L:61:ILE:HG13	42:L:8627:HOH:O	2.15	0.47
16:L:63:VAL:HG21	16:L:109:PHE:CE1	2.49	0.47
17:M:180:LEU:O	17:M:181:ASP:HB3	2.13	0.47
19:O:91:LYS:O	19:O:95:GLU:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:216:ARG:CD	42:X:8570:HOH:O	2.60	0.47
1:0:380:A:H5'	16:L:48:ARG:NH2	2.28	0.47
1:0:1191:A:N1	1:0:1206:U:O4	2.47	0.47
1:0:1609:C:H2'	1:0:1610:G:H8	1.79	0.47
1:0:2256:G:C2'	1:0:2257:G:H5'	2.44	0.47
7:C:107:ARG:HH11	7:C:107:ARG:CB	2.26	0.47
7:C:129:HIS:HD2	7:C:165:ASP:OD2	1.97	0.47
12:H:31:PHE:CD2	12:H:85:ILE:HG23	2.50	0.47
12:H:113:ALA:N	12:H:114:PRO:HD3	2.30	0.47
13:I:36:VAL:HG12	13:I:37:ALA:N	2.29	0.47
15:K:73:VAL:HG23	15:K:74:THR:H	1.78	0.47
16:L:48:ARG:NH2	42:L:8564:HOH:O	2.47	0.47
16:L:81:ARG:HG3	16:L:85:ARG:HB2	1.96	0.47
26:V:65:VAL:HG12	26:V:116:LEU:HD13	1.96	0.47
1:0:1206:U:H5'	1:0:1206:U:C6	2.42	0.47
1:0:1497:G:H4'	1:0:1627:G:O2'	2.15	0.47
1:0:2252:A:C5	1:0:2253:G:H1'	2.50	0.47
1:0:2730:G:O2'	1:0:2731:G:H5'	2.15	0.47
5:A:96:LEU:HD22	5:A:128:LEU:HD13	1.96	0.47
42:A:8621:HOH:O	29:Y:75:ALA:HB3	2.14	0.47
7:C:246:ARG:CZ	42:C:8430:HOH:O	2.61	0.47
10:F:100:ASP:HB3	42:F:5691:HOH:O	2.15	0.47
13:I:93:ARG:HH11	13:I:93:ARG:CB	2.26	0.47
17:M:143:ARG:HA	17:M:172:PHE:CD2	2.49	0.47
23:S:52:ARG:HB2	23:S:95:ASN:HB3	1.97	0.47
25:U:29:ASN:O	25:U:33:VAL:HG23	2.13	0.47
26:V:154:ARG:HE	26:V:154:ARG:HB3	1.57	0.47
28:X:112:GLU:OE1	28:X:115:ARG:NH1	2.48	0.47
1:0:177:A:H2'	1:0:178:U:O4'	2.15	0.47
1:0:281:U:H3'	42:O:6676:HOH:O	2.15	0.47
1:0:541:C:H2'	1:0:542:A:H5'	1.96	0.47
1:0:858:U:H2'	1:0:859:C:C6	2.50	0.47
1:0:1342:C:C2'	1:0:1343:C:H5'	2.45	0.47
1:0:2781:U:O2'	1:0:2782:G:H5'	2.14	0.47
8:D:158:ASN:HB2	8:D:161:ASP:OD2	2.15	0.47
13:I:46:ILE:HA	42:I:1123:HOH:O	2.14	0.47
15:K:105:TYR:C	15:K:105:TYR:CD1	2.93	0.47
23:S:23:VAL:C	23:S:93:THR:HG21	2.40	0.47
1:0:24:G:N2	1:0:518:G:H1'	2.29	0.47
1:0:92:G:H4'	25:U:44:GLY:HA3	1.96	0.47
1:0:1398:G:O2'	1:0:1399:A:H5'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2100:A:H5'	42:C:8467:HOH:O	2.13	0.47
1:0:2274:A:H4'	16:L:77:PHE:HE1	1.80	0.47
1:0:2312:G:C2'	1:0:2313:C:H5'	2.45	0.47
1:0:2697:A:H2'	1:0:2698:G:O4'	2.14	0.47
1:0:2715:G:N2	6:B:264:GLU:OE1	2.47	0.47
1:0:2831:C:H2'	1:0:2832:C:H5'	1.97	0.47
2:9:3008:G:O6	17:M:11:ARG:NH1	2.48	0.47
40:4:79:BTN:H82	40:4:79:BTN:N2	2.30	0.47
6:B:211:THR:HA	6:B:255:GLY:O	2.15	0.47
7:C:165:ASP:O	7:C:168:ARG:HB3	2.15	0.47
8:D:94:ALA:HB3	8:D:174:VAL:CA	2.45	0.47
8:D:99:ASP:HB2	8:D:103:ASN:H	1.80	0.47
14:J:118:ALA:O	14:J:120:ARG:N	2.48	0.47
17:M:71:TRP:N	42:M:8540:HOH:O	2.47	0.47
18:N:39:THR:HB	42:N:3360:HOH:O	2.13	0.47
22:R:10:VAL:HG11	25:U:36:ALA:HA	1.96	0.47
24:T:52:THR:CG2	24:T:54:THR:HB	2.45	0.47
25:U:39:ALA:O	25:U:41:GLU:N	2.47	0.47
26:V:107:LEU:O	26:V:112:LEU:HB2	2.14	0.47
29:Y:59:HIS:HA	42:Y:8436:HOH:O	2.14	0.47
1:0:1158:G:O2'	1:0:1159:G:H5'	2.14	0.47
1:0:1450:C:C4'	1:0:1451:C:OP2	2.59	0.47
1:0:2320:U:H3'	32:2:2:GLN:HB2	1.97	0.47
1:0:2467:A:H3'	42:0:4934:HOH:O	2.14	0.47
5:A:200:PRO:HD3	42:A:8520:HOH:O	2.14	0.47
5:A:217:ARG:HH11	5:A:217:ARG:CG	2.27	0.47
6:B:108:GLU:HB3	6:B:111:ARG:HD2	1.97	0.47
8:D:103:ASN:ND2	8:D:134:LEU:H	2.12	0.47
10:F:27:GLY:HA3	42:F:5413:HOH:O	2.15	0.47
12:H:117:LYS:O	12:H:119:VAL:HG13	2.15	0.47
19:O:64:GLU:HG2	42:O:169:HOH:O	2.15	0.47
1:0:329:A:OP2	7:C:206:ASN:HB2	2.14	0.47
1:0:820:G:H5'	1:0:821:U:H5'	1.96	0.47
1:0:1450:C:O2'	1:0:1494:A:H5'	2.15	0.47
42:0:3250:HOH:O	23:S:9:LYS:CD	2.62	0.47
42:0:5672:HOH:O	16:L:174:ARG:HD3	2.14	0.47
5:A:194:MET:CE	5:A:199:HIS:HB2	2.39	0.47
7:C:168:ARG:NH2	7:C:190:ALA:O	2.48	0.47
15:K:90:ARG:NH2	15:K:121:ILE:HD11	2.29	0.47
16:L:39:ARG:HA	16:L:63:VAL:HG22	1.97	0.47
17:M:37:ARG:HA	17:M:37:ARG:HD3	1.81	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Q:31:ILE:O	21:Q:32:ALA:C	2.57	0.47
23:S:111:ARG:HB3	23:S:119:ALA:HB2	1.97	0.47
1:0:278:A:H2'	1:0:279:C:O4'	2.15	0.47
1:0:2044:G:OP1	27:W:23:HIS:HE1	1.98	0.47
42:0:9484:HOH:O	15:K:22:ARG:HG2	2.15	0.47
2:9:3006:C:C5'	17:M:37:ARG:HH12	2.23	0.47
5:A:210:GLY:HA3	42:A:8594:HOH:O	2.14	0.47
6:B:66:GLU:OE1	6:B:328:ARG:HD2	2.15	0.47
8:D:93:LEU:HG	42:D:3862:HOH:O	2.13	0.47
10:F:34:ASN:O	10:F:38:LYS:HG3	2.15	0.47
10:F:46:GLU:OE1	10:F:100:ASP:HA	2.14	0.47
12:H:56:ILE:HG22	12:H:61:LEU:CD2	2.43	0.47
16:L:83:SER:HA	16:L:86:MET:HE3	1.97	0.47
19:O:143:ALA:HA	42:O:168:HOH:O	2.15	0.47
26:V:38:THR:HG22	26:V:39:ASP:N	2.30	0.47
26:V:151:GLU:O	26:V:154:ARG:HB3	2.14	0.47
30:Z:28:HIS:CE1	30:Z:31:LYS:HE2	2.50	0.47
1:0:474:C:O3'	7:C:73:LEU:HD21	2.16	0.46
1:0:2862:G:H4'	6:B:336:GLN:O	2.16	0.46
42:0:3883:HOH:O	5:A:11:ARG:CZ	2.63	0.46
42:0:9063:HOH:O	6:B:267:LYS:HD3	2.13	0.46
5:A:95:PRO:HA	5:A:153:ARG:HA	1.98	0.46
6:B:16:ARG:NH1	42:B:8613:HOH:O	2.48	0.46
10:F:34:ASN:HA	16:L:4:ALA:HB2	1.97	0.46
14:J:75:ARG:HG2	14:J:90:PHE:CD2	2.50	0.46
16:L:25:TRP:HE3	16:L:26:HIS:HD2	1.63	0.46
16:L:37:VAL:CG2	16:L:108:LYS:HG3	2.44	0.46
16:L:123:ASP:C	16:L:123:ASP:OD1	2.58	0.46
17:M:73:ALA:HB1	17:M:74:PRO:CD	2.45	0.46
32:2:44:SER:HA	32:2:49:ASP:OD1	2.16	0.46
1:0:1211:G:O2'	1:0:1212:C:H5'	2.15	0.46
1:0:1878:G:O2'	1:0:1879:U:OP2	2.33	0.46
1:0:1883:U:O2'	1:0:1884:G:H5'	2.14	0.46
1:0:1909:A:H2'	1:0:1910:A:C8	2.50	0.46
1:0:2353:A:H4'	1:0:2354:A:O5'	2.15	0.46
2:9:3041:C:C6	8:D:50:VAL:HG21	2.51	0.46
2:9:3055:U:H4'	2:9:3056:A:H8	1.80	0.46
7:C:162:VAL:CG1	7:C:192:ILE:HD11	2.44	0.46
8:D:92:GLU:O	8:D:93:LEU:O	2.33	0.46
10:F:50:VAL:CG2	10:F:63:ILE:HG21	2.45	0.46
12:H:26:LYS:HD2	12:H:28:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:134:ILE:CG2	16:L:141:ILE:HD13	2.46	0.46
17:M:47:LEU:HD13	17:M:97:VAL:HG11	1.96	0.46
21:Q:61:GLN:NE2	42:Q:8541:HOH:O	2.48	0.46
23:S:28:SER:O	23:S:32:ARG:HG3	2.14	0.46
23:S:75:GLU:O	23:S:76:ASP:HB2	2.14	0.46
25:U:27:LEU:HA	25:U:49:LEU:HD13	1.96	0.46
26:V:31:HIS:HB3	42:V:5420:HOH:O	2.14	0.46
30:Z:25:LYS:HD2	31:1:49:GLU:N	2.30	0.46
1:0:622:G:O2'	1:0:623:U:H5'	2.15	0.46
1:0:1304:U:H2'	1:0:1305:C:C6	2.51	0.46
1:0:1666:C:C2'	1:0:1667:A:H5'	2.43	0.46
2:9:3014:G:O2'	17:M:1:ALA:HB2	2.15	0.46
6:B:54:VAL:HB	42:B:8609:HOH:O	2.16	0.46
6:B:125:GLU:OE2	6:B:129:ARG:NH1	2.49	0.46
8:D:140:ARG:HH11	8:D:140:ARG:HG3	1.79	0.46
10:F:99:THR:O	10:F:100:ASP:HB2	2.15	0.46
14:J:9:THR:O	14:J:10:GLN:C	2.59	0.46
14:J:14:LYS:CB	14:J:45:PRO:HG2	2.36	0.46
24:T:39:ASN:HD22	24:T:49:LEU:HD11	1.81	0.46
29:Y:30:GLU:HB2	42:Y:8414:HOH:O	2.15	0.46
32:2:18:GLN:OE1	32:2:73:GLU:HB3	2.16	0.46
1:0:461:C:H2'	42:0:3486:HOH:O	2.15	0.46
1:0:716:G:C2'	1:0:717:C:O5'	2.64	0.46
1:0:2883:A:H2'	1:0:2884:G:O4'	2.16	0.46
42:0:6889:HOH:O	5:A:22:ARG:HD2	2.14	0.46
5:A:35:GLY:O	5:A:36:ASP:CB	2.57	0.46
5:A:36:ASP:O	5:A:37:VAL:C	2.58	0.46
6:B:13:PHE:O	6:B:16:ARG:HD2	2.15	0.46
6:B:101:TRP:HB2	6:B:119:HIS:CD2	2.50	0.46
7:C:118:THR:HG22	7:C:137:PRO:HB3	1.97	0.46
10:F:37:THR:O	10:F:41:GLU:HG3	2.15	0.46
12:H:47:GLU:HG2	12:H:133:ILE:HD12	1.95	0.46
17:M:43:VAL:HG13	17:M:118:ILE:HD11	1.96	0.46
22:R:29:ASP:OD1	22:R:31:ARG:NH1	2.48	0.46
1:0:57:C:H5''	42:0:6233:HOH:O	2.13	0.46
1:0:745:G:H5''	1:0:746:A:OP1	2.16	0.46
1:0:1940:C:H4'	42:0:6815:HOH:O	2.15	0.46
1:0:2090:G:H2'	1:0:2091:G:C8	2.50	0.46
42:0:4307:HOH:O	13:I:47:THR:CB	2.59	0.46
42:0:6926:HOH:O	7:C:188:ARG:CD	2.63	0.46
2:9:3012:C:H5'	2:9:3070:U:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:192:VAL:HG12	5:A:207:GLN:HB3	1.97	0.46
13:I:6:PHE:O	13:I:8:ALA:N	2.48	0.46
15:K:125:PHE:CE1	15:K:140:VAL:HG13	2.51	0.46
17:M:163:PHE:HA	42:M:8519:HOH:O	2.15	0.46
21:Q:39:THR:O	21:Q:40:ALA:C	2.57	0.46
22:R:6:LYS:HB2	22:R:27:ALA:O	2.15	0.46
22:R:81:ILE:HG12	42:R:8336:HOH:O	2.15	0.46
24:T:52:THR:HG22	24:T:54:THR:H	1.81	0.46
25:U:45:ARG:C	25:U:47:LYS:N	2.72	0.46
1:0:308:U:C4	1:0:342:C:H1'	2.50	0.46
1:0:1166:A:H61	1:0:1180:U:H3	1.64	0.46
1:0:2591:C:H2'	1:0:2592:G:O4'	2.16	0.46
6:B:16:ARG:NE	42:B:8551:HOH:O	2.32	0.46
7:C:7:ASP:C	7:C:9:ASP:H	2.24	0.46
12:H:62:GLU:O	12:H:66:VAL:HG23	2.16	0.46
16:L:48:ARG:HH11	16:L:52:LEU:HD21	1.81	0.46
16:L:108:LYS:HE3	42:L:8616:HOH:O	2.15	0.46
22:R:53:ASN:ND2	42:R:8321:HOH:O	2.49	0.46
23:S:20:HIS:ND1	23:S:41:ARG:NE	2.60	0.46
26:V:26:ILE:O	26:V:26:ILE:CG1	2.63	0.46
27:W:66:THR:HG23	27:W:67:PRO:HD2	1.96	0.46
31:1:18:ASN:ND2	31:1:40:ARG:H	2.14	0.46
1:0:432:G:O2'	1:0:433:C:H5'	2.16	0.46
1:0:2247:C:H5''	42:0:6813:HOH:O	2.16	0.46
1:0:2356:A:H2'	1:0:2357:G:O4'	2.16	0.46
1:0:2821:C:H4'	6:B:116:PRO:HB3	1.97	0.46
5:A:69:LEU:C	5:A:69:LEU:HD12	2.40	0.46
6:B:223:ARG:HG3	6:B:232:TRP:O	2.15	0.46
8:D:41:LEU:HA	8:D:44:ILE:CG2	2.45	0.46
8:D:95:THR:OG1	8:D:174:VAL:HG22	2.16	0.46
16:L:84:LYS:HD3	42:L:8532:HOH:O	2.15	0.46
17:M:5:ARG:HG3	20:P:18:PRO:CB	2.45	0.46
17:M:154:LEU:CG	17:M:155:GLU:H	2.27	0.46
1:0:952:G:N3	1:0:2302:A:H2'	2.31	0.46
1:0:962:C:C1'	17:M:5:ARG:NH1	2.72	0.46
1:0:1056:U:H2'	1:0:1057:A:O4'	2.16	0.46
1:0:1097:A:H5''	26:V:125:HIS:NE2	2.31	0.46
1:0:1289:C:H3'	42:0:5886:HOH:O	2.15	0.46
1:0:2010:A:H2'	42:0:5433:HOH:O	2.15	0.46
1:0:2121:G:C2'	1:0:2122:C:H5'	2.46	0.46
1:0:2270:G:H4'	5:A:223:ARG:HH12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:41:PHE:CE1	6:B:79:MET:HG3	2.50	0.46
14:J:55:VAL:CG1	14:J:56:SER:N	2.78	0.46
17:M:82:TYR:C	17:M:82:TYR:CD2	2.94	0.46
23:S:55:PHE:CD2	23:S:77:VAL:HG13	2.50	0.46
26:V:139:GLY:O	26:V:141:HIS:CD2	2.69	0.46
29:Y:39:CYS:O	29:Y:42:CYS:O	2.34	0.46
1:O:21:G:H5''	21:Q:1:GLY:O	2.16	0.46
1:O:447:A:O2'	1:O:448:G:H5'	2.16	0.46
1:O:814:G:H4'	42:O:9626:HOH:O	2.16	0.46
1:O:860:U:H2'	1:O:861:A:C8	2.51	0.46
1:O:1003:U:O2'	12:H:90:PHE:HE1	1.99	0.46
1:O:1120:U:H5''	1:O:1120:U:H6	1.81	0.46
1:O:1391:G:H2'	1:O:1392:A:H5'	1.98	0.46
1:O:2904:U:H4'	27:W:8:ARG:NH1	2.30	0.46
42:O:4422:HOH:O	16:L:82:ARG:HD3	2.16	0.46
3:3:76:A:N6	42:3:7072:HOH:O	2.42	0.46
5:A:105:VAL:HG12	5:A:106:CYS:N	2.31	0.46
5:A:128:LEU:HG	42:A:8583:HOH:O	2.16	0.46
6:B:7:ARG:HG2	6:B:7:ARG:NH1	2.31	0.46
8:D:101:THR:HG22	42:D:7400:HOH:O	2.16	0.46
9:E:20:ILE:HD12	9:E:33:LEU:HD12	1.98	0.46
16:L:69:LYS:HD3	16:L:125:ARG:HA	1.98	0.46
25:U:55:ARG:O	25:U:59:ILE:HG12	2.15	0.46
27:W:25:ARG:HG2	42:W:5356:HOH:O	2.15	0.46
1:O:716:G:H2'	1:O:717:C:O5'	2.16	0.46
1:O:1819:G:H2'	1:O:1820:G:C4'	2.46	0.46
1:O:2459:G:OP2	32:2:64:LYS:HD2	2.16	0.46
5:A:36:ASP:CB	5:A:85:ASP:H	2.28	0.46
5:A:149:ASP:OD1	5:A:151:GLN:HB2	2.15	0.46
5:A:179:MET:HG2	5:A:186:TRP:CB	2.45	0.46
5:A:192:VAL:O	5:A:207:GLN:HG2	2.16	0.46
16:L:87:MET:SD	32:2:46:ILE:HD13	2.55	0.46
23:S:19:ARG:HD3	23:S:67:LEU:O	2.14	0.46
24:T:33:SER:O	24:T:37:GLU:HG3	2.16	0.46
1:O:113:A:OP2	1:O:114:A:H2'	2.16	0.45
1:O:228:C:H2'	1:O:229:G:H5'	1.98	0.45
1:O:512:G:O3'	1:O:513:A:H8	1.99	0.45
1:O:943:A:C5	26:V:23:MET:HE2	2.52	0.45
1:O:2088:C:H1'	1:O:2841:A:N1	2.31	0.45
1:O:2320:U:OP2	32:2:1:MET:HA	2.16	0.45
1:O:2619:U:H5''	1:O:2620:U:OP2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3002:U:OP2	2:9:3002:U:H4'	2.16	0.45
2:9:3007:G:H4'	17:M:55:ASP:OD2	2.15	0.45
7:C:39:GLN:O	7:C:43:LYS:HD3	2.15	0.45
7:C:160:LEU:O	7:C:162:VAL:HG23	2.16	0.45
8:D:173:GLU:O	8:D:174:VAL:C	2.58	0.45
9:E:31:ARG:HH12	9:E:68:HIS:CG	2.33	0.45
19:O:94:TRP:CZ2	19:O:98:ILE:HG13	2.51	0.45
19:O:120:ARG:NH2	19:O:123:TYR:CD2	2.84	0.45
25:U:38:GLY:C	25:U:40:PRO:HD2	2.41	0.45
26:V:76:ASP:O	26:V:77:ALA:C	2.59	0.45
31:1:40:ARG:HA	31:1:45:ASN:ND2	2.30	0.45
1:0:407:A:H2'	1:0:408:A:C8	2.52	0.45
1:0:611:U:H2'	1:0:612:U:C6	2.52	0.45
1:0:1173:A:H2'	42:0:3826:HOH:O	2.16	0.45
1:0:2269:C:H2'	1:0:2270:G:O4'	2.17	0.45
8:D:23:VAL:CG2	8:D:73:VAL:HB	2.44	0.45
8:D:67:ASP:O	8:D:69:ILE:HG13	2.16	0.45
8:D:99:ASP:O	8:D:159:PRO:HG3	2.15	0.45
8:D:99:ASP:HB3	8:D:103:ASN:H	1.81	0.45
12:H:72:VAL:HG11	12:H:81:TYR:CZ	2.51	0.45
14:J:81:ARG:HD3	14:J:87:ARG:NH1	2.30	0.45
22:R:42:GLU:HG2	22:R:49:VAL:HG23	1.98	0.45
24:T:50:GLU:CD	42:T:7349:HOH:O	2.58	0.45
1:0:170:U:H1'	32:2:50:GLY:HA3	1.98	0.45
1:0:282:C:H2'	1:0:283:U:O4'	2.15	0.45
1:0:703:G:O2'	1:0:704:C:H5'	2.17	0.45
1:0:1066:U:H2'	1:0:1067:A:C8	2.51	0.45
1:0:1164:U:O4'	1:0:1165:G:OP1	2.35	0.45
1:0:1205:U:H2'	1:0:1206:U:C5'	2.47	0.45
1:0:1385:G:O3'	27:W:49:ARG:NH1	2.50	0.45
1:0:2432:C:C1'	42:0:3566:HOH:O	2.64	0.45
1:0:2464:C:H5''	1:0:2465:A:OP1	2.16	0.45
5:A:100:PRO:O	5:A:103:VAL:HG23	2.16	0.45
13:I:6:PHE:HB3	13:I:109:TYR:OH	2.16	0.45
17:M:73:ALA:HB2	17:M:163:PHE:CZ	2.51	0.45
21:Q:125:ARG:HG2	42:Q:8543:HOH:O	2.16	0.45
27:W:85:VAL:HG12	27:W:86:GLU:N	2.31	0.45
1:0:316:A:N3	1:0:336:G:O2'	2.43	0.45
1:0:1471:A:H2'	1:0:1472:C:C6	2.51	0.45
1:0:2637:A:H5'	1:0:2638:G:C5'	2.46	0.45
6:B:14:GLY:HA2	6:B:15:PRO:C	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:59:GLY:O	8:D:61:PHE:N	2.41	0.45
9:E:145:ALA:HB1	9:E:168:ILE:CD1	2.47	0.45
14:J:14:LYS:HG3	14:J:32:ILE:O	2.16	0.45
17:M:93:GLN:HG2	42:M:8559:HOH:O	2.15	0.45
32:2:65:THR:HB	32:2:83:TRP:H	1.81	0.45
1:0:100:C:H4'	23:S:16:LEU:HB2	1.99	0.45
1:0:491:C:O2'	1:0:492:C:H5'	2.17	0.45
1:0:2346:C:O3'	8:D:52:THR:HG23	2.16	0.45
42:0:9054:HOH:O	26:V:119:HIS:HE1	1.98	0.45
2:9:3049:G:H2'	2:9:3050:G:O4'	2.17	0.45
27:W:12:ILE:HD12	27:W:36:HIS:ND1	2.32	0.45
1:0:283:U:H5	1:0:284:C:N4	2.15	0.45
1:0:952:G:OP1	20:P:42:LYS:HE2	2.16	0.45
6:B:212:GLN:HB2	6:B:257:THR:CG2	2.38	0.45
9:E:16:ASP:O	9:E:17:HIS:HB2	2.16	0.45
12:H:149:ALA:C	12:H:151:MET:H	2.23	0.45
13:I:79:PHE:HB3	13:I:103:VAL:HG11	1.98	0.45
17:M:77:ASN:OD1	17:M:80:SER:HB2	2.17	0.45
17:M:78:MET:HB2	17:M:79:PRO:HD3	1.98	0.45
1:0:319:A:H4'	1:0:338:C:C4	2.52	0.45
1:0:538:C:H5''	1:0:539:G:C8	2.51	0.45
1:0:926:A:O2'	15:K:41:HIS:HD2	1.99	0.45
1:0:1188:A:C5	1:0:1189:A:C2	3.05	0.45
1:0:1768:C:H2'	1:0:1769:C:O4'	2.17	0.45
1:0:2346:C:O3'	8:D:52:THR:CG2	2.65	0.45
1:0:2768:A:H3'	42:0:3898:HOH:O	2.17	0.45
1:0:2896:A:N3	1:0:2896:A:H2'	2.32	0.45
5:A:186:TRP:CG	5:A:187:PRO:HA	2.52	0.45
15:K:38:HIS:CD2	15:K:39:GLU:HG3	2.52	0.45
20:P:75:ILE:CD1	20:P:84:ILE:HD11	2.47	0.45
23:S:43:ASN:C	23:S:45:GLY:H	2.24	0.45
1:0:1659:A:H2'	1:0:1660:G:O4'	2.17	0.45
5:A:164:ARG:HA	29:Y:69:TYR:CE1	2.52	0.45
8:D:173:GLU:HG3	8:D:174:VAL:N	2.31	0.45
9:E:24:GLY:HA3	9:E:76:VAL:HB	1.98	0.45
9:E:170:ARG:HE	9:E:170:ARG:HB2	1.56	0.45
12:H:95:GLU:HB3	12:H:119:VAL:HG11	1.98	0.45
13:I:52:GLN:HG3	13:I:53:ILE:N	2.32	0.45
16:L:24:MET:HE3	16:L:28:MET:CE	2.40	0.45
21:Q:4:TYR:N	42:Q:8548:HOH:O	2.50	0.45
26:V:88:THR:CG2	26:V:110:GLN:NE2	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2:7:PHE:HE2	32:2:22:VAL:HG21	1.82	0.45
1:0:451:C:O2'	1:0:452:G:H5'	2.17	0.45
1:0:1523:G:H2'	1:0:1524:U:C6	2.52	0.45
1:0:1829:A:C8	1:0:1885:A:C8	3.05	0.45
1:0:1925:G:OP1	32:2:29:ARG:NH2	2.50	0.45
1:0:2735:U:H2'	1:0:2736:U:C6	2.52	0.45
42:0:4203:HOH:O	17:M:21:HIS:HD2	2.00	0.45
7:C:129:HIS:CE1	7:C:231:ARG:HA	2.52	0.45
9:E:23:GLU:HG2	9:E:28:SER:HB2	1.98	0.45
10:F:13:GLU:OE2	10:F:78:GLU:HG2	2.17	0.45
11:G:71:LEU:C	11:G:73:ASP:N	2.75	0.45
17:M:34:LEU:HD13	17:M:47:LEU:HD21	1.98	0.45
21:Q:32:ALA:O	21:Q:33:ARG:C	2.60	0.45
26:V:80:ASP:O	26:V:84:VAL:HG23	2.16	0.45
27:W:74:ALA:HB2	27:W:85:VAL:HG13	1.98	0.45
1:0:317:A:H5''	23:S:52:ARG:HD2	1.98	0.45
1:0:1500:U:OP2	19:O:41:ARG:NH2	2.50	0.45
1:0:1910:A:H2	1:0:2129:U:O4'	2.00	0.45
1:0:1994:A:P	14:J:66:ARG:HH22	2.40	0.45
6:B:42:ALA:HB1	6:B:308:LEU:HD11	1.99	0.45
6:B:279:THR:OG1	6:B:290:VAL:HB	2.17	0.45
6:B:307:ARG:HH11	6:B:307:ARG:CG	2.29	0.45
7:C:236:THR:C	42:C:8452:HOH:O	2.59	0.45
10:F:24:ARG:NH2	42:F:6800:HOH:O	2.51	0.45
20:P:66:LYS:HB2	20:P:70:ALA:O	2.17	0.45
26:V:35:VAL:HA	26:V:36:PRO:HD3	1.78	0.45
27:W:12:ILE:HG23	27:W:36:HIS:CG	2.51	0.45
1:0:1165:G:OP1	1:0:1165:G:C3'	2.61	0.44
1:0:1331:A:OP2	28:X:142:SER:OG	2.34	0.44
1:0:1654:U:H2'	5:A:47:HIS:HD2	1.81	0.44
1:0:2468:A:H61	32:2:48:ASN:HD21	1.64	0.44
1:0:2478:U:H2'	1:0:2479:A:C8	2.52	0.44
1:0:2506:A:H1'	42:0:5531:HOH:O	2.17	0.44
7:C:25:PRO:HD2	42:C:8434:HOH:O	2.15	0.44
8:D:55:LYS:O	8:D:56:ARG:HB2	2.17	0.44
8:D:146:LYS:HE2	17:M:107:ASN:ND2	2.32	0.44
10:F:60:VAL:O	10:F:61:MET:C	2.60	0.44
14:J:118:ALA:C	14:J:120:ARG:N	2.76	0.44
20:P:32:GLU:HA	20:P:71:TYR:OH	2.17	0.44
21:Q:17:MET:HE1	21:Q:19:ARG:CZ	2.45	0.44
21:Q:132:ARG:NH2	42:Q:8585:HOH:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:S:38:ARG:HH11	23:S:38:ARG:HG3	1.81	0.44
1:0:776:A:OP1	30:Z:28:HIS:HE1	1.99	0.44
1:0:1029:U:O2'	1:0:1273:C:OP1	2.31	0.44
1:0:1135:G:H5'	42:0:5403:HOH:O	2.17	0.44
1:0:1159:G:H1	1:0:1208:C:H42	1.65	0.44
1:0:1266:U:H4'	28:X:115:ARG:HH21	1.81	0.44
1:0:1557:G:O2'	1:0:1558:C:H5'	2.17	0.44
1:0:1656:A:H2'	1:0:1657:A:O4'	2.17	0.44
1:0:2505:G:H8	42:0:5114:HOH:O	2.00	0.44
1:0:2825:C:H4'	1:0:2826:G:O5'	2.17	0.44
1:0:2900:G:H2'	1:0:2901:C:O4'	2.17	0.44
11:G:67:LEU:O	11:G:71:LEU:HG	2.17	0.44
26:V:122:ARG:HG2	26:V:122:ARG:NH1	2.26	0.44
27:W:34:ARG:NH1	27:W:48:VAL:O	2.49	0.44
1:0:541:C:O2'	1:0:542:A:H5''	2.18	0.44
1:0:853:C:H2'	1:0:854:G:O4'	2.17	0.44
1:0:1588:G:C6	1:0:1589:G:N1	2.86	0.44
1:0:1634:G:H2'	1:0:1635:U:C6	2.52	0.44
1:0:2281:C:H2'	1:0:2282:U:H5'	1.99	0.44
1:0:2839:C:H2'	1:0:2840:A:H5''	1.99	0.44
5:A:164:ARG:HB2	29:Y:68:CYS:SG	2.57	0.44
6:B:53:LEU:HD21	6:B:270:ILE:HD12	1.98	0.44
7:C:40:ALA:CB	7:C:100:LEU:HD12	2.47	0.44
14:J:22:ASP:C	14:J:22:ASP:OD1	2.60	0.44
14:J:55:VAL:HG12	14:J:56:SER:H	1.82	0.44
26:V:122:ARG:HG2	26:V:152:ALA:O	2.17	0.44
29:Y:11:THR:HG21	29:Y:23:ARG:HB2	1.98	0.44
30:Z:2:GLY:O	30:Z:6:PRO:HG2	2.17	0.44
1:0:170:U:H5'	32:2:48:ASN:HB3	1.98	0.44
1:0:484:A:N1	1:0:506:G:H4'	2.33	0.44
1:0:1252:A:H2'	1:0:1253:C:O4'	2.18	0.44
1:0:1819:G:H5'	42:0:4186:HOH:O	2.18	0.44
1:0:1942:A:H5'	5:A:233:THR:HB	1.98	0.44
1:0:2314:G:C2'	1:0:2315:C:H5'	2.47	0.44
1:0:2326:U:H4'	1:0:2412:G:H4'	2.00	0.44
1:0:2419:U:H5''	1:0:2420:G:C5'	2.43	0.44
5:A:94:LEU:HG	5:A:99:ILE:CD1	2.46	0.44
5:A:105:VAL:HG11	5:A:154:ALA:CB	2.46	0.44
9:E:34:TRP:O	13:I:127:ILE:HD11	2.17	0.44
12:H:26:LYS:CD	12:H:28:ILE:HB	2.47	0.44
12:H:84:ARG:CZ	12:H:135:TRP:CH2	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:84:ARG:CZ	12:H:135:TRP:HH2	2.30	0.44
15:K:53:ARG:NH2	15:K:57:VAL:HG12	2.33	0.44
16:L:46:LEU:HG	42:L:8625:HOH:O	2.17	0.44
24:T:9:CYS:O	24:T:52:THR:HG23	2.18	0.44
25:U:39:ALA:C	25:U:41:GLU:N	2.75	0.44
27:W:31:ILE:O	27:W:35:GLU:HG3	2.16	0.44
27:W:43:VAL:CG1	27:W:44:ASP:N	2.79	0.44
28:X:107:PRO:HB3	28:X:182:PHE:CE2	2.53	0.44
28:X:109:LEU:HA	42:X:8572:HOH:O	2.18	0.44
32:2:1:MET:HG3	32:2:88:LEU:HD12	1.99	0.44
1:0:394:G:H1	16:L:181:GLU:CD	2.26	0.44
1:0:424:C:H2'	1:0:425:U:C6	2.53	0.44
1:0:1593:C:H5'	19:O:116:SER:O	2.17	0.44
1:0:2526:C:C2'	1:0:2527:U:H5'	2.47	0.44
1:0:2720:C:O2	14:J:87:ARG:NH2	2.50	0.44
6:B:22:GLU:HA	6:B:205:VAL:HG21	2.00	0.44
10:F:57:GLU:O	10:F:61:MET:HG3	2.18	0.44
17:M:164:ASP:C	17:M:164:ASP:OD1	2.60	0.44
1:0:960:G:N3	1:0:960:G:C2'	2.79	0.44
1:0:1015:C:H2'	1:0:1016:U:H6	1.79	0.44
1:0:1268:C:H2'	1:0:1269:G:H8	1.83	0.44
1:0:1615:A:H4'	42:0:5359:HOH:O	2.17	0.44
1:0:2372:A:H2'	1:0:2373:U:C6	2.53	0.44
5:A:211:LYS:CB	5:A:212:PRO:HD2	2.31	0.44
8:D:169:THR:C	8:D:170:TYR:HD1	2.25	0.44
9:E:116:THR:CG2	9:E:151:LEU:HD22	2.47	0.44
11:G:12:ILE:HG13	42:G:6833:HOH:O	2.18	0.44
16:L:52:LEU:HD13	16:L:116:ASN:CG	2.42	0.44
18:N:107:GLU:O	18:N:108:GLY:C	2.61	0.44
25:U:1:THR:CG2	25:U:2:VAL:H	2.25	0.44
25:U:55:ARG:NH2	42:U:4428:HOH:O	2.45	0.44
1:0:344:C:H2'	1:0:345:G:O4'	2.17	0.44
1:0:635:A:H2'	1:0:636:G:H5''	1.98	0.44
1:0:1151:G:OP1	11:G:16:LYS:NZ	2.49	0.44
1:0:1589:G:N2	1:0:1605:G:H1'	2.33	0.44
1:0:1592:G:H2'	1:0:1593:C:C6	2.53	0.44
1:0:1735:C:H2'	1:0:1736:A:C8	2.51	0.44
1:0:2064:U:H5'	1:0:2652:U:O3'	2.18	0.44
1:0:2326:U:H4'	1:0:2412:G:C4'	2.47	0.44
1:0:2420:G:H4'	42:0:3581:HOH:O	2.18	0.44
1:0:2443:C:H3'	42:0:9967:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:178:LYS:NZ	36:A:8509:CL:CL	2.86	0.44
5:A:192:VAL:O	5:A:192:VAL:CG1	2.65	0.44
13:I:90:LYS:HB2	36:I:8502:CL:CL	2.55	0.44
17:M:155:GLU:O	17:M:156:GLU:HG3	2.18	0.44
19:O:16:VAL:CG1	19:O:17:GLY:N	2.81	0.44
22:R:32:ALA:HA	22:R:36:GLU:OE1	2.17	0.44
23:S:49:GLU:OE2	23:S:97:ARG:HD2	2.18	0.44
26:V:4:LEU:HD23	26:V:4:LEU:HA	1.75	0.44
26:V:65:VAL:HA	26:V:68:THR:CG2	2.47	0.44
26:V:122:ARG:CG	26:V:152:ALA:O	2.66	0.44
32:2:60:LYS:HG3	32:2:61:PRO:HD2	2.00	0.44
1:0:450:C:H4'	7:C:46:TYR:CE1	2.53	0.44
1:0:536:A:H3'	42:0:4522:HOH:O	2.17	0.44
1:0:951:A:O2'	1:0:952:G:H5'	2.18	0.44
1:0:1007:A:H2'	12:H:19:TYR:CZ	2.53	0.44
1:0:1329:A:C2	42:0:4159:HOH:O	2.56	0.44
1:0:2256:G:H2'	1:0:2257:G:C5'	2.48	0.44
42:0:5686:HOH:O	6:B:2:GLN:CD	2.61	0.44
2:9:3030:C:OP1	8:D:137:PRO:O	2.35	0.44
2:9:3057:A:O2'	8:D:152:PRO:HD2	2.18	0.44
5:A:211:LYS:HD3	42:A:8618:HOH:O	2.17	0.44
7:C:196:THR:HG23	42:C:8406:HOH:O	2.16	0.44
8:D:99:ASP:CB	8:D:103:ASN:HB2	2.47	0.44
12:H:141:ASN:CA	42:H:8366:HOH:O	2.61	0.44
16:L:173:LEU:HA	16:L:183:VAL:HG11	2.00	0.44
19:O:7:LYS:CD	19:O:21:VAL:CG2	2.96	0.44
21:Q:29:LYS:HD3	42:Q:8533:HOH:O	2.18	0.44
24:T:38:ASN:O	24:T:42:LEU:HG	2.18	0.44
24:T:52:THR:HG22	24:T:54:THR:HB	2.00	0.44
28:X:115:ARG:NE	42:X:8557:HOH:O	2.51	0.44
28:X:235:GLU:CD	28:X:235:GLU:N	2.76	0.44
31:1:22:PRO:HB2	31:1:24:TRP:CD1	2.53	0.44
1:0:166:A:N7	15:K:25:GLY:HA2	2.33	0.44
1:0:596:C:H2'	1:0:597:A:C8	2.53	0.44
1:0:1819:G:H2'	1:0:1820:G:C5'	2.48	0.44
2:9:3028:U:H2'	2:9:3029:C:C6	2.53	0.44
5:A:36:ASP:CA	5:A:83:GLY:HA3	2.46	0.44
5:A:107:ASN:OD1	5:A:120:ARG:HD2	2.18	0.44
6:B:154:VAL:HG12	6:B:156:LYS:HG2	1.98	0.44
7:C:13:ASP:OD1	7:C:13:ASP:O	2.36	0.44
7:C:34:ALA:HB3	7:C:220:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:74:ARG:CD	16:L:91:ILE:HD12	2.48	0.44
18:N:25:VAL:HG23	18:N:26:TRP:N	2.33	0.44
19:O:11:ALA:HB2	19:O:18:LYS:HA	2.00	0.44
21:Q:25:PHE:CE2	21:Q:29:LYS:HE2	2.52	0.44
26:V:52:VAL:HG13	26:V:53:ALA:N	2.32	0.44
27:W:9:VAL:HG22	27:W:88:GLU:OE2	2.18	0.44
27:W:20:GLU:CD	27:W:21:PRO:HD2	2.42	0.44
27:W:43:VAL:HG12	27:W:47:ALA:HB3	1.99	0.44
1:O:111:C:H2'	1:O:112:G:O4'	2.18	0.43
1:O:506:G:N2	1:O:509:A:H5'	2.21	0.43
1:O:711:G:C2	1:O:718:C:C2	3.06	0.43
1:O:737:A:H2'	1:O:738:G:O4'	2.18	0.43
1:O:886:A:OP2	1:O:2113:G:H5'	2.18	0.43
1:O:1596:U:H2'	1:O:1598:A:OP2	2.17	0.43
1:O:1681:G:H5''	1:O:1682:A:H5'	2.00	0.43
42:O:3523:HOH:O	7:C:149:LYS:HE3	2.18	0.43
6:B:215:VAL:O	6:B:219:GLY:HA2	2.17	0.43
6:B:274:GLU:HA	6:B:292:GLY:O	2.18	0.43
8:D:169:THR:O	8:D:170:TYR:HB2	2.18	0.43
10:F:16:ALA:HA	10:F:111:ILE:HD13	1.99	0.43
10:F:28:ALA:HB3	10:F:99:THR:O	2.18	0.43
10:F:28:ALA:CB	10:F:99:THR:HG23	2.48	0.43
10:F:39:SER:HB3	10:F:45:ALA:HB2	1.99	0.43
11:G:20:VAL:O	11:G:24:VAL:HG23	2.18	0.43
12:H:86:ARG:CZ	12:H:130:HIS:CD2	3.01	0.43
14:J:99:ASP:OD1	14:J:99:ASP:C	2.60	0.43
16:L:107:ARG:NH1	42:L:8581:HOH:O	2.51	0.43
17:M:47:LEU:HD12	17:M:92:ALA:HB1	2.00	0.43
17:M:58:LEU:N	17:M:58:LEU:CD1	2.80	0.43
17:M:80:SER:CB	42:M:8537:HOH:O	2.61	0.43
20:P:3:SER:HB3	42:P:5998:HOH:O	2.17	0.43
1:O:2314:G:O2'	1:O:2315:C:H5'	2.18	0.43
1:O:2355:G:H5''	1:O:2356:A:OP2	2.19	0.43
1:O:2597:U:H2'	1:O:2598:U:H5'	1.99	0.43
2:9:3078:G:N2	2:9:3103:A:OP2	2.48	0.43
4:4:75:C:H2'	37:4:76:PPU:O4'	2.18	0.43
5:A:51:ARG:NH2	42:A:8551:HOH:O	2.51	0.43
6:B:139:ASP:CB	6:B:165:ARG:HE	2.31	0.43
12:H:65:ARG:NH1	42:H:8385:HOH:O	2.51	0.43
15:K:34:GLY:HA3	15:K:38:HIS:CE1	2.53	0.43
42:L:8532:HOH:O	32:2:46:ILE:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:S:45:GLY:C	42:S:3851:HOH:O	2.60	0.43
27:W:30:MET:HE3	27:W:55:ASN:OD1	2.18	0.43
28:X:234:VAL:HG12	28:X:235:GLU:N	2.33	0.43
1:0:95:A:H5''	1:0:97:G:O4'	2.18	0.43
1:0:536:A:N1	1:0:2075:G:O2'	2.50	0.43
1:0:644:G:H5'	1:0:644:G:N3	2.33	0.43
1:0:949:U:O2'	20:P:40:HIS:HE1	2.01	0.43
1:0:1189:A:N3	42:0:7150:HOH:O	2.48	0.43
1:0:1494:A:O2'	1:0:1505:U:O2	2.30	0.43
1:0:1771:U:C4'	29:Y:20:LEU:HD21	2.37	0.43
1:0:2300:A:H4'	1:0:2301:A:O5'	2.18	0.43
42:0:6827:HOH:O	5:A:177:HIS:HE1	2.01	0.43
2:9:3031:C:H2'	2:9:3032:G:O4'	2.19	0.43
5:A:55:VAL:HG11	5:A:67:LEU:HD13	2.00	0.43
5:A:192:VAL:CG1	5:A:207:GLN:HB3	2.49	0.43
10:F:111:ILE:O	10:F:115:VAL:HG23	2.19	0.43
12:H:14:TYR:N	12:H:91:HIS:HE1	2.16	0.43
12:H:31:PHE:HE2	12:H:87:LYS:O	2.01	0.43
14:J:65:ARG:CD	42:J:5358:HOH:O	2.66	0.43
18:N:98:LEU:HD12	18:N:98:LEU:HA	1.85	0.43
24:T:6:CYS:SG	24:T:31:PHE:HA	2.58	0.43
1:0:524:A:H5'	21:Q:29:LYS:HE2	2.00	0.43
1:0:629:A:H2'	1:0:630:A:O4'	2.19	0.43
1:0:695:C:H2'	1:0:696:C:C6	2.53	0.43
1:0:702:G:O2'	1:0:703:G:H5'	2.19	0.43
1:0:790:A:H1'	1:0:1710:A:H2'	1.99	0.43
1:0:1470:A:OP1	16:L:93:ARG:HD2	2.18	0.43
42:0:8727:HOH:O	5:A:11:ARG:HD3	2.18	0.43
8:D:19:GLU:O	8:D:133:ASN:HB3	2.19	0.43
8:D:128:LEU:HB2	42:D:6007:HOH:O	2.18	0.43
12:H:127:GLY:O	12:H:128:ALA:CB	2.65	0.43
17:M:175:LEU:HD12	17:M:175:LEU:HA	1.85	0.43
23:S:38:ARG:NH1	23:S:38:ARG:HG3	2.33	0.43
24:T:17:THR:CG2	24:T:18:GLY:N	2.82	0.43
1:0:64:G:H2'	1:0:65:C:O4'	2.19	0.43
1:0:288:A:H2'	1:0:289:G:C8	2.54	0.43
1:0:2010:A:C2'	42:0:5433:HOH:O	2.67	0.43
1:0:2092:G:H2'	1:0:2613:G:OP1	2.19	0.43
1:0:2445:U:H2'	1:0:2446:G:H8	1.84	0.43
1:0:2542:C:H4'	4:4:75:C:O2'	2.19	0.43
1:0:2815:G:OP2	13:I:99:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:30:ARG:HE	5:A:30:ARG:HB3	1.60	0.43
7:C:21:VAL:C	7:C:23:GLU:H	2.26	0.43
8:D:10:PHE:CD1	8:D:11:HIS:N	2.86	0.43
8:D:81:GLU:C	8:D:83:PHE:N	2.75	0.43
9:E:77:THR:OG1	9:E:78:GLU:N	2.50	0.43
9:E:162:PHE:CD1	9:E:162:PHE:N	2.86	0.43
12:H:46:VAL:O	12:H:146:TRP:CH2	2.68	0.43
12:H:57:ARG:C	12:H:59:ASN:N	2.76	0.43
14:J:6:ALA:HB3	14:J:116:GLU:HG2	2.00	0.43
15:K:10:SER:O	15:K:11:ARG:HB3	2.19	0.43
16:L:95:LYS:HG2	16:L:99:ARG:HB3	2.00	0.43
16:L:125:ARG:HD3	42:L:8597:HOH:O	2.18	0.43
16:L:155:HIS:CE1	16:L:158:ARG:HH21	2.36	0.43
17:M:73:ALA:HB1	17:M:74:PRO:HD2	1.99	0.43
19:O:13:VAL:HG13	19:O:14:LEU:N	2.33	0.43
23:S:106:GLU:HG3	42:S:4913:HOH:O	2.17	0.43
25:U:1:THR:C	25:U:3:LEU:N	2.76	0.43
26:V:5:VAL:O	26:V:52:VAL:HG22	2.18	0.43
28:X:117:LEU:HD12	28:X:174:VAL:CG1	2.49	0.43
32:2:55:VAL:HB	32:2:56:PRO:HD2	2.01	0.43
1:0:244:C:H6	1:0:244:C:O5'	2.00	0.43
1:0:283:U:H5''	1:0:284:C:OP2	2.19	0.43
1:0:401:C:C5'	42:0:5268:HOH:O	2.65	0.43
1:0:440:C:H2'	1:0:441:A:C8	2.53	0.43
1:0:1052:G:H2'	1:0:1052:G:N3	2.33	0.43
1:0:1311:G:C2	1:0:1312:G:C8	3.07	0.43
1:0:1677:U:OP2	31:1:8:LYS:NZ	2.48	0.43
1:0:1761:U:H5'	19:O:81:LYS:O	2.18	0.43
1:0:2271:G:N3	1:0:2271:G:H2'	2.33	0.43
1:0:2432:C:H2'	1:0:2433:A:H8	1.84	0.43
1:0:2569:A:H2'	1:0:2570:G:O5'	2.18	0.43
7:C:142:ASP:OD2	7:C:238:SER:OG	2.33	0.43
9:E:108:LEU:HD11	9:E:164:ASP:HB2	2.01	0.43
15:K:26:HIS:HB2	42:K:8512:HOH:O	2.18	0.43
16:L:125:ARG:NH1	42:L:8597:HOH:O	2.51	0.43
16:L:167:GLY:O	16:L:171:ARG:HG3	2.19	0.43
17:M:5:ARG:HG3	20:P:18:PRO:HB3	1.99	0.43
21:Q:83:LYS:HB3	42:Q:8517:HOH:O	2.18	0.43
25:U:27:LEU:CA	25:U:49:LEU:HD13	2.49	0.43
28:X:189:ASN:C	28:X:189:ASN:ND2	2.76	0.43
29:Y:38:LYS:HE2	29:Y:45:LYS:CE	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2:39:GLN:HA	32:2:42:ARG:NH2	2.33	0.43
1:0:327:A:OP1	7:C:149:LYS:NZ	2.42	0.43
1:0:338:C:H4'	7:C:174:ILE:HD11	2.00	0.43
1:0:466:A:H2'	1:0:467:G:O4'	2.17	0.43
1:0:870:G:C3'	1:0:871:G:H5''	2.49	0.43
1:0:1095:U:O2	26:V:120:PRO:HG2	2.18	0.43
1:0:1559:A:C1'	42:0:5338:HOH:O	2.63	0.43
5:A:199:HIS:CD2	5:A:201:PHE:HB2	2.54	0.43
6:B:53:LEU:HD11	6:B:327:VAL:HG22	2.01	0.43
7:C:246:ARG:HB3	7:C:246:ARG:HH11	1.81	0.43
8:D:84:LEU:HA	8:D:87:ALA:HB3	2.01	0.43
8:D:167:GLU:C	8:D:169:THR:H	2.27	0.43
9:E:81:GLU:HG2	9:E:134:SER:CB	2.48	0.43
10:F:38:LYS:NZ	16:L:3:SER:HA	2.33	0.43
10:F:117:GLU:C	10:F:119:ARG:N	2.77	0.43
12:H:36:ASN:ND2	42:H:8382:HOH:O	2.50	0.43
16:L:87:MET:HB2	16:L:91:ILE:HD11	2.00	0.43
16:L:114:VAL:HG21	16:L:159:THR:HG21	2.00	0.43
17:M:127:LEU:HD12	17:M:127:LEU:HA	1.84	0.43
22:R:29:ASP:OD1	22:R:31:ARG:HG3	2.18	0.43
25:U:12:THR:O	25:U:13:PRO:C	2.62	0.43
28:X:126:PRO:HG2	28:X:128:PHE:CZ	2.54	0.43
28:X:189:ASN:HA	28:X:217:ILE:HD11	2.00	0.43
32:2:11:CYS:HA	32:2:12:PRO:HD2	1.83	0.43
1:0:1200:A:H4'	42:0:6810:HOH:O	2.19	0.43
1:0:1419:U:H2'	1:0:1685:A:C2	2.54	0.43
1:0:2078:U:O2'	1:0:2079:G:H5'	2.18	0.43
7:C:79:ARG:O	7:C:87:ARG:HG2	2.19	0.43
15:K:104:ASP:HB2	42:K:8581:HOH:O	2.19	0.43
16:L:87:MET:H	16:L:87:MET:HG3	1.34	0.43
18:N:63:LYS:HG3	18:N:80:ASP:O	2.19	0.43
25:U:57:LYS:HA	25:U:60:GLN:HE21	1.83	0.43
26:V:60:GLU:O	26:V:63:GLU:HB2	2.19	0.43
28:X:144:ARG:NH2	42:X:8612:HOH:O	2.52	0.43
1:0:291:C:H2'	1:0:292:G:O4'	2.19	0.43
1:0:513:A:N3	42:0:3152:HOH:O	2.37	0.43
1:0:583:G:H2'	1:0:584:U:H6	1.83	0.43
1:0:639:A:H2'	1:0:640:G:C8	2.53	0.43
1:0:677:C:H4'	7:C:246:ARG:NH2	2.34	0.43
1:0:1345:A:H2'	1:0:1346:U:C6	2.54	0.43
1:0:1940:C:H5''	5:A:234:GLY:HA3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2749:U:O2'	1:0:2751:C:OP2	2.32	0.43
1:0:2795:C:O2'	1:0:2796:U:H5'	2.18	0.43
1:0:2869:G:H5'	42:0:4971:HOH:O	2.17	0.43
2:9:3091:C:H2'	2:9:3092:G:O4'	2.18	0.43
5:A:153:ARG:HB2	5:A:153:ARG:NH1	2.28	0.43
6:B:60:SER:C	6:B:62:ARG:H	2.27	0.43
7:C:109:LEU:HD12	7:C:109:LEU:O	2.18	0.43
8:D:49:PRO:HA	8:D:73:VAL:HG22	2.00	0.43
8:D:59:GLY:C	8:D:61:PHE:N	2.77	0.43
10:F:47:LEU:HD22	10:F:108:LEU:CD1	2.49	0.43
16:L:82:ARG:NH2	42:L:8624:HOH:O	2.51	0.43
17:M:37:ARG:HD3	36:M:8507:CL:CL	2.56	0.43
17:M:143:ARG:HH12	17:M:173:ASP:CG	2.24	0.43
23:S:24:ARG:HH21	23:S:39:ASN:ND2	2.17	0.43
29:Y:56:MET:HA	29:Y:62:TYR:O	2.19	0.43
1:0:303:C:H2'	1:0:304:G:O4'	2.19	0.43
1:0:1250:C:O2'	1:0:1251:C:H5'	2.19	0.43
1:0:1380:U:H5'	42:0:8728:HOH:O	2.18	0.43
1:0:1743:G:H1'	42:0:4362:HOH:O	2.18	0.43
1:0:2457:U:H1'	32:2:79:LEU:HD13	2.01	0.43
1:0:2547:C:H2'	1:0:2548:C:H6	1.83	0.43
1:0:2769:C:H2'	1:0:2770:G:C5'	2.49	0.43
2:9:3056:A:C3'	2:9:3057:A:H5''	2.49	0.43
6:B:248:ARG:O	6:B:251:VAL:HG13	2.19	0.43
7:C:22:PHE:HA	7:C:116:ALA:HA	2.00	0.43
7:C:234:VAL:O	7:C:234:VAL:HG22	2.18	0.43
9:E:20:ILE:HD12	9:E:33:LEU:CD1	2.49	0.43
12:H:163:PRO:O	12:H:164:ALA:HB2	2.19	0.43
16:L:154:ARG:HD3	42:L:8648:HOH:O	2.17	0.43
23:S:75:GLU:HB3	42:S:4772:HOH:O	2.18	0.43
23:S:96:VAL:HG13	23:S:97:ARG:N	2.34	0.43
28:X:144:ARG:NH1	42:X:8577:HOH:O	2.49	0.43
1:0:195:C:H2'	1:0:196:G:H5'	2.01	0.42
1:0:415:A:O2'	1:0:416:G:H5'	2.19	0.42
1:0:646:G:H2'	1:0:647:U:C6	2.54	0.42
1:0:666:A:H2'	1:0:667:C:O4'	2.19	0.42
1:0:1682:A:H5''	42:0:8957:HOH:O	2.19	0.42
1:0:1734:C:OP1	6:B:234:ARG:HD3	2.19	0.42
1:0:2089:A:C2'	1:0:2090:G:H5'	2.49	0.42
1:0:2346:C:O5'	1:0:2346:C:C6	2.72	0.42
1:0:2634:G:OP2	5:A:204:GLY:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:O:9457:HOH:O	32:2:84:ARG:HB2	2.19	0.42
6:B:313:PRO:O	6:B:314:ALA:C	2.62	0.42
7:C:127:ARG:HD2	7:C:229:PRO:O	2.19	0.42
16:L:123:ASP:OD1	16:L:124:GLY:N	2.52	0.42
17:M:152:GLU:C	17:M:154:LEU:N	2.77	0.42
18:N:7:LEU:HD22	42:N:5650:HOH:O	2.19	0.42
18:N:80:ASP:OD1	18:N:81:PHE:N	2.52	0.42
26:V:54:PHE:CZ	26:V:140:LYS:HB2	2.53	0.42
1:O:51:G:O2'	1:O:52:A:H5'	2.20	0.42
1:O:420:U:H2'	1:O:421:C:C6	2.54	0.42
1:O:958:G:H2'	1:O:959:C:C6	2.53	0.42
1:O:1388:U:H2'	1:O:1389:G:O4'	2.19	0.42
1:O:1788:U:C2	1:O:1805:G:N2	2.87	0.42
1:O:1878:G:H5''	42:O:9293:HOH:O	2.19	0.42
1:O:2084:C:H2'	1:O:2085:A:C8	2.54	0.42
1:O:2409:C:H4'	32:2:17:HIS:CB	2.48	0.42
1:O:2429:A:H2'	1:O:2430:A:C8	2.54	0.42
42:O:6926:HOH:O	7:C:188:ARG:HD2	2.19	0.42
6:B:4:SER:O	6:B:5:ARG:HB2	2.19	0.42
6:B:71:VAL:CG1	6:B:296:LEU:HB3	2.47	0.42
7:C:233:THR:HG22	7:C:234:VAL:H	1.84	0.42
10:F:28:ALA:HB3	10:F:99:THR:HG23	2.00	0.42
16:L:184:ARG:HG3	16:L:185:PRO:HA	2.01	0.42
23:S:40:VAL:HG23	23:S:119:ALA:C	2.44	0.42
1:O:1224:G:H2'	1:O:1225:C:C6	2.54	0.42
1:O:1462:C:H2'	1:O:1463:A:C8	2.54	0.42
1:O:2712:G:H5'	42:O:4697:HOH:O	2.19	0.42
1:O:2894:C:O2'	1:O:2895:C:H5'	2.19	0.42
42:9:7568:HOH:O	17:M:107:ASN:HB3	2.19	0.42
42:3:6229:HOH:O	38:4:77:PHA:HA	2.20	0.42
6:B:162:MET:HG3	6:B:310:ARG:HD3	2.01	0.42
7:C:140:VAL:HG12	7:C:141:SER:N	2.34	0.42
9:E:15:GLN:HG2	9:E:19:ASP:O	2.19	0.42
10:F:104:ALA:C	10:F:106:THR:N	2.76	0.42
12:H:39:GLY:O	12:H:41:THR:N	2.52	0.42
12:H:47:GLU:CB	12:H:133:ILE:CD1	2.91	0.42
12:H:48:LEU:HD13	12:H:146:TRP:HB3	2.00	0.42
16:L:65:VAL:CG2	16:L:105:ALA:HB2	2.47	0.42
28:X:178:HIS:CG	28:X:179:PRO:HD2	2.54	0.42
1:O:684:G:H2'	1:O:685:C:C6	2.54	0.42
1:O:736:A:H2'	1:O:737:A:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1463:A:H2'	1:0:1464:U:C6	2.55	0.42
1:0:2320:U:OP2	32:2:2:GLN:N	2.53	0.42
1:0:2649:A:H5'	1:0:2649:A:H8	1.84	0.42
42:0:4097:HOH:O	5:A:6:GLY:HA3	2.17	0.42
7:C:76:ARG:HG2	7:C:78:ARG:NH1	2.34	0.42
7:C:115:LEU:HD12	7:C:115:LEU:HA	1.88	0.42
8:D:159:PRO:O	8:D:162:ALA:HB3	2.19	0.42
9:E:137:ASP:OD1	9:E:137:ASP:C	2.62	0.42
13:I:107:ASN:HD22	13:I:108:PRO:N	2.17	0.42
14:J:74:VAL:HG12	14:J:75:ARG:HG3	2.00	0.42
18:N:25:VAL:O	18:N:29:VAL:HG23	2.19	0.42
21:Q:99:ALA:CB	21:Q:109:MET:HE1	2.22	0.42
22:R:29:ASP:CG	22:R:31:ARG:NH1	2.78	0.42
22:R:57:THR:C	22:R:59:ASP:H	2.27	0.42
1:0:947:U:O2'	1:0:948:G:H5'	2.20	0.42
1:0:1316:G:H1'	1:0:1340:G:N2	2.34	0.42
1:0:1562:C:O2	1:0:1562:C:H2'	2.19	0.42
1:0:2503:A:OP1	12:H:147:ARG:NH2	2.41	0.42
5:A:75:GLY:HA2	29:Y:63:LYS:O	2.20	0.42
6:B:41:PHE:HB3	6:B:190:MET:CE	2.49	0.42
7:C:184:ARG:HB3	42:C:8369:HOH:O	2.19	0.42
7:C:219:ASN:N	7:C:222:ASP:OD1	2.53	0.42
9:E:81:GLU:HA	9:E:133:VAL:O	2.19	0.42
10:F:60:VAL:HG13	10:F:63:ILE:HG13	2.02	0.42
16:L:134:ILE:O	16:L:136:PRO:HD3	2.19	0.42
21:Q:84:ALA:O	21:Q:88:PHE:HD1	2.03	0.42
23:S:41:ARG:HG2	23:S:41:ARG:HH11	1.85	0.42
23:S:79:LEU:HG	23:S:89:ARG:HB2	2.02	0.42
25:U:1:THR:HG23	25:U:2:VAL:N	2.29	0.42
1:0:168:C:O5'	1:0:168:C:H6	2.02	0.42
1:0:1352:A:N1	7:C:48:SER:HB3	2.35	0.42
42:0:8898:HOH:O	16:L:94:LYS:HE2	2.20	0.42
2:9:3004:G:O2'	17:M:44:ARG:NH2	2.52	0.42
5:A:57:ALA:HA	5:A:67:LEU:HD23	2.01	0.42
6:B:203:ALA:HA	6:B:262:ARG:O	2.19	0.42
6:B:215:VAL:HA	6:B:220:VAL:HG22	2.01	0.42
9:E:139:GLU:CD	42:E:5919:HOH:O	2.62	0.42
12:H:31:PHE:HA	12:H:85:ILE:CG2	2.50	0.42
12:H:46:VAL:HG12	12:H:146:TRP:CZ3	2.46	0.42
12:H:48:LEU:CG	12:H:157:ILE:HG21	2.48	0.42
30:Z:21:ARG:HD2	30:Z:39:PHE:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2:3:MET:HG3	32:2:4:PRO:HD2	2.01	0.42
1:0:87:C:H2'	31:1:28:LYS:O	2.19	0.42
1:0:514:G:OP1	1:0:514:G:H2'	2.20	0.42
1:0:583:G:H2'	1:0:584:U:C6	2.54	0.42
1:0:1098:A:H2'	1:0:1099:G:O4'	2.20	0.42
1:0:1882:C:O2'	1:0:2012:U:OP2	2.34	0.42
1:0:2084:C:H2'	1:0:2085:A:H8	1.84	0.42
1:0:2133:U:H4'	1:0:2134:G:H5'	2.02	0.42
1:0:2291:A:N9	1:0:2309:C:H5'	2.34	0.42
1:0:2561:C:OP1	9:E:153:ARG:NH2	2.52	0.42
1:0:2804:C:H2'	1:0:2805:A:O4'	2.20	0.42
42:0:4827:HOH:O	23:S:3:GLN:HG2	2.19	0.42
8:D:41:LEU:CA	8:D:44:ILE:HG22	2.48	0.42
9:E:24:GLY:N	9:E:76:VAL:HB	2.34	0.42
10:F:48:VAL:HG23	10:F:74:PHE:HB3	1.96	0.42
14:J:4:LEU:HD22	14:J:116:GLU:HB3	2.01	0.42
42:J:7438:HOH:O	24:T:20:MET:HE1	2.19	0.42
16:L:38:VAL:O	16:L:38:VAL:HG12	2.17	0.42
17:M:43:VAL:HG11	17:M:81:ALA:HA	2.02	0.42
17:M:50:LEU:HD12	17:M:50:LEU:HA	1.85	0.42
17:M:152:GLU:HA	17:M:152:GLU:OE1	2.20	0.42
17:M:167:ASP:O	17:M:168:LEU:HD23	2.20	0.42
18:N:26:TRP:CE3	18:N:26:TRP:HA	2.55	0.42
18:N:47:ARG:NH1	42:N:4564:HOH:O	2.52	0.42
21:Q:111:ILE:HG23	21:Q:145:LEU:CD1	2.49	0.42
31:1:24:TRP:CD1	42:1:6863:HOH:O	2.72	0.42
1:0:482:G:H4'	1:0:508:A:N1	2.35	0.42
1:0:812:A:H2'	1:0:813:C:C6	2.55	0.42
1:0:1014:A:H5''	2:9:3101:G:O2'	2.20	0.42
1:0:1461:U:H2'	1:0:1462:C:C6	2.55	0.42
1:0:2050:G:OP1	21:Q:79:ARG:HB3	2.19	0.42
1:0:2815:G:H4'	1:0:2816:A:OP2	2.19	0.42
1:0:2906:A:H5'	1:0:2907:C:O4'	2.19	0.42
42:0:3250:HOH:O	23:S:9:LYS:HD2	2.19	0.42
5:A:103:VAL:HA	5:A:104:PRO:HD3	1.86	0.42
6:B:280:VAL:CG1	6:B:281:ASP:N	2.82	0.42
7:C:141:SER:HB3	42:C:8424:HOH:O	2.20	0.42
7:C:142:ASP:OD1	7:C:236:THR:HG23	2.20	0.42
14:J:128:ALA:HB3	14:J:131:ILE:HD11	2.02	0.42
16:L:80:GLY:O	16:L:81:ARG:HD3	2.19	0.42
16:L:164:THR:HB	42:L:8520:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:P:93:ARG:HG3	20:P:93:ARG:NH1	2.35	0.42
23:S:113:GLU:O	23:S:114:SER:C	2.62	0.42
28:X:148:GLY:O	28:X:154:ARG:HD3	2.20	0.42
29:Y:13:ARG:NH1	42:Y:8418:HOH:O	2.51	0.42
1:0:694:A:C2'	1:0:695:C:H5'	2.50	0.42
1:0:814:G:N2	1:0:815:U:H1'	2.35	0.42
1:0:920:C:H5'	1:0:921:G:N3	2.35	0.42
1:0:945:U:O2'	26:V:43:GLY:HA3	2.20	0.42
1:0:1496:G:H5'	1:0:1572:A:H1'	2.02	0.42
1:0:1702:U:H5''	42:0:6687:HOH:O	2.20	0.42
1:0:2453:G:H2'	1:0:2454:C:C6	2.55	0.42
1:0:2846:C:OP1	6:B:158:LYS:HD3	2.20	0.42
6:B:221:GLN:HE22	14:J:42:ASN:ND2	2.14	0.42
7:C:173:LYS:HB3	7:C:187:ARG:HG3	2.00	0.42
8:D:35:ALA:C	8:D:37:ALA:H	2.26	0.42
12:H:110:GLY:N	42:H:8397:HOH:O	2.52	0.42
15:K:142:LEU:HG	15:K:146:GLY:HA3	2.02	0.42
1:0:259:G:H21	16:L:58:GLN:NE2	2.17	0.42
1:0:314:G:N2	1:0:316:A:H3'	2.34	0.42
1:0:812:A:H1'	42:0:3447:HOH:O	2.20	0.42
1:0:1003:U:O2	12:H:90:PHE:CZ	2.73	0.42
1:0:1603:A:H5''	1:0:1605:G:H5'	2.01	0.42
1:0:1828:G:H2'	1:0:1829:A:H5'	2.00	0.42
1:0:2440:C:H5''	42:0:3309:HOH:O	2.19	0.42
1:0:2533:C:O2'	1:0:2534:C:H5'	2.20	0.42
42:0:9844:HOH:O	20:P:16:ASN:HB2	2.19	0.42
6:B:16:ARG:NH2	42:B:8551:HOH:O	2.40	0.42
6:B:43:GLY:O	6:B:308:LEU:HD12	2.19	0.42
6:B:162:MET:HG3	6:B:310:ARG:NH1	2.35	0.42
6:B:320:GLN:HG3	6:B:321:PRO:CD	2.49	0.42
9:E:11:VAL:HG11	9:E:22:VAL:HG13	2.01	0.42
12:H:6:TYR:HE2	12:H:94:ARG:O	2.03	0.42
12:H:71:TYR:O	12:H:73:GLN:N	2.53	0.42
12:H:83:PHE:HE1	12:H:146:TRP:CZ2	2.38	0.42
12:H:112:ARG:O	12:H:113:ALA:C	2.63	0.42
14:J:118:ALA:HA	14:J:125:ALA:HB2	2.02	0.42
17:M:38:LYS:HE3	17:M:38:LYS:HB2	1.82	0.42
20:P:93:ARG:HG3	20:P:93:ARG:HH11	1.85	0.42
28:X:189:ASN:HD22	28:X:192:ASP:H	1.68	0.42
29:Y:38:LYS:HA	29:Y:45:LYS:HA	2.02	0.42
32:2:34:LYS:HB2	32:2:37:ASP:OD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:324:G:O2'	1:0:325:U:H5'	2.20	0.41
1:0:772:G:H2'	1:0:773:A:O4'	2.20	0.41
1:0:1333:U:H2'	1:0:1334:C:H6	1.85	0.41
1:0:1730:G:H4'	1:0:1731:C:O5'	2.20	0.41
1:0:2271:G:P	42:0:8936:HOH:O	2.77	0.41
1:0:2761:A:C4	1:0:2763:G:C8	3.08	0.41
1:0:2780:C:H2'	1:0:2781:U:C6	2.55	0.41
1:0:2820:A:H2'	1:0:2821:C:C6	2.55	0.41
2:9:3092:G:H22	12:H:52:LYS:NZ	2.18	0.41
5:A:171:LYS:NZ	42:A:8526:HOH:O	2.53	0.41
6:B:171:VAL:HG23	6:B:172:SER:N	2.34	0.41
7:C:162:VAL:O	7:C:162:VAL:CG1	2.68	0.41
7:C:200:PRO:HB3	7:C:212:VAL:CG2	2.50	0.41
9:E:126:ILE:HB	9:E:131:LEU:HD21	2.02	0.41
10:F:22:VAL:CG2	10:F:104:ALA:HB2	2.50	0.41
12:H:113:ALA:N	12:H:114:PRO:CD	2.83	0.41
15:K:89:PHE:N	42:K:8576:HOH:O	2.53	0.41
16:L:78:ASN:O	16:L:79:LYS:HG2	2.20	0.41
1:0:240:C:C5'	16:L:146:GLN:NE2	2.83	0.41
1:0:354:A:H2'	1:0:355:C:C6	2.55	0.41
1:0:488:U:O2'	23:S:82:THR:HG21	2.20	0.41
1:0:522:U:O2'	1:0:1366:C:H5'	2.19	0.41
1:0:675:U:H2'	1:0:676:C:H5'	2.01	0.41
1:0:926:A:O2'	15:K:41:HIS:CD2	2.73	0.41
1:0:1079:A:N1	1:0:2068:G:O2'	2.48	0.41
1:0:2004:U:H1'	42:0:9687:HOH:O	2.20	0.41
10:F:21:GLU:O	10:F:24:ARG:CG	2.67	0.41
15:K:73:VAL:HG11	15:K:118:LEU:HD21	2.02	0.41
16:L:77:PHE:HD1	16:L:79:LYS:O	2.03	0.41
17:M:154:LEU:C	17:M:156:GLU:H	2.27	0.41
18:N:53:GLN:HG2	18:N:56:GLU:OE1	2.20	0.41
23:S:80:GLU:OE2	23:S:84:GLY:HA2	2.20	0.41
27:W:27:ASP:OD2	27:W:27:ASP:N	2.52	0.41
32:2:84:ARG:HB3	42:2:8557:HOH:O	2.20	0.41
1:0:134:U:C2	1:0:145:A:C2	3.09	0.41
1:0:290:C:O2'	1:0:291:C:H5'	2.19	0.41
1:0:710:G:P	18:N:24:ALA:HB3	2.61	0.41
1:0:1137:G:H1'	42:0:3367:HOH:O	2.19	0.41
1:0:1616:A:H5''	1:0:1617:C:OP1	2.20	0.41
1:0:2004:U:H2'	1:0:2005:G:OP1	2.20	0.41
1:0:2488:A:H2	42:0:6747:HOH:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3064:C:C2'	2:9:3065:A:H5'	2.50	0.41
6:B:76:THR:N	6:B:77:PRO:HD3	2.34	0.41
6:B:248:ARG:O	6:B:251:VAL:HG12	2.20	0.41
7:C:37:ALA:HB2	42:C:8387:HOH:O	2.20	0.41
7:C:187:ARG:NH2	42:C:8370:HOH:O	2.42	0.41
8:D:81:GLU:O	8:D:85:GLN:HG3	2.20	0.41
14:J:98:VAL:HG22	14:J:102:GLU:C	2.45	0.41
20:P:16:ASN:HD22	20:P:16:ASN:HA	1.64	0.41
23:S:55:PHE:HB2	42:S:6384:HOH:O	2.19	0.41
26:V:125:HIS:CD2	26:V:127:GLY:H	2.38	0.41
28:X:122:ARG:NH2	42:X:8536:HOH:O	2.53	0.41
1:0:81:G:N3	1:0:98:A:C2	2.88	0.41
1:0:192:A:C4'	16:L:176:GLN:HE22	2.34	0.41
1:0:229:G:O2'	1:0:230:C:H5'	2.20	0.41
1:0:461:C:N3	1:0:479:G:H5'	2.36	0.41
1:0:945:U:H2'	1:0:946:C:C6	2.56	0.41
1:0:1545:C:H2'	1:0:1546:G:O4'	2.20	0.41
1:0:1609:C:H2'	1:0:1610:G:C8	2.56	0.41
1:0:2237:G:H1'	42:0:4324:HOH:O	2.19	0.41
1:0:2435:U:P	32:2:28:GLY:HA3	2.60	0.41
2:9:3026:C:P	42:9:3472:HOH:O	2.77	0.41
5:A:170:VAL:HG22	29:Y:22:ILE:HG23	2.01	0.41
8:D:53:LYS:HA	8:D:67:ASP:O	2.21	0.41
14:J:10:GLN:NE2	14:J:10:GLN:N	2.43	0.41
15:K:75:LEU:N	15:K:75:LEU:HD23	2.35	0.41
16:L:99:ARG:HD2	16:L:167:GLY:HA2	2.02	0.41
16:L:137:ASP:HA	16:L:142:LYS:HE3	2.03	0.41
17:M:69:TYR:HE2	17:M:183:ASP:OD2	2.03	0.41
1:0:305:A:C5	1:0:329:A:C2	3.09	0.41
1:0:401:C:H5'	42:0:5268:HOH:O	2.20	0.41
1:0:459:A:H4'	42:0:8954:HOH:O	2.19	0.41
1:0:1192:A:O2'	1:0:1193:A:OP1	2.29	0.41
1:0:1287:A:O4'	26:V:117:ARG:HD3	2.20	0.41
1:0:1524:U:O2'	1:0:1525:G:P	2.78	0.41
1:0:1634:G:H2'	1:0:1635:U:H6	1.85	0.41
1:0:2324:G:H4'	1:0:2418:G:O2'	2.20	0.41
1:0:2729:C:O2'	1:0:2730:G:H5'	2.21	0.41
1:0:2911:C:H2'	1:0:2912:C:H6	1.84	0.41
42:0:5719:HOH:O	5:A:22:ARG:HG2	2.19	0.41
2:9:3107:C:H5	42:9:3167:HOH:O	2.03	0.41
5:A:65:ARG:C	5:A:66:ARG:HG3	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:123:GLY:HA2	5:A:159:VAL:O	2.21	0.41
5:A:125:ASN:CB	5:A:158:VAL:HG12	2.50	0.41
6:B:302:PRO:C	42:B:8650:HOH:O	2.63	0.41
8:D:35:ALA:HB2	42:D:5858:HOH:O	2.21	0.41
8:D:76:ARG:O	8:D:77:ASP:HB2	2.21	0.41
8:D:104:PHE:CE2	8:D:132:VAL:HB	2.55	0.41
17:M:42:HIS:CG	17:M:62:HIS:HE1	2.37	0.41
18:N:73:ASP:HA	18:N:92:VAL:O	2.20	0.41
22:R:29:ASP:OD2	22:R:31:ARG:NH1	2.54	0.41
24:T:47:ARG:HG3	42:T:4381:HOH:O	2.19	0.41
26:V:121:PRO:HA	26:V:153:MET:HG2	2.02	0.41
29:Y:33:HIS:HE1	29:Y:49:ARG:NE	2.19	0.41
1:0:151:A:H2'	1:0:152:A:O4'	2.21	0.41
1:0:245:C:H2'	1:0:246:G:H5'	2.02	0.41
1:0:508:A:H2'	1:0:509:A:H5''	2.01	0.41
1:0:765:G:O3'	7:C:69:HIS:HB3	2.20	0.41
1:0:1657:A:H2'	1:0:1658:A:C8	2.55	0.41
1:0:1939:U:HO2'	5:A:233:THR:H	1.68	0.41
1:0:2112:A:H2'	1:0:2113:G:C8	2.56	0.41
1:0:2642:G:H2'	1:0:2643:G:O4'	2.19	0.41
1:0:2721:U:H4'	14:J:87:ARG:HG3	2.03	0.41
1:0:2812:A:N7	42:0:6984:HOH:O	2.37	0.41
42:0:3714:HOH:O	21:Q:17:MET:HE2	2.20	0.41
2:9:3045:A:H2'	2:9:3046:C:H6	1.86	0.41
5:A:232:ARG:NH2	5:A:236:GLY:O	2.48	0.41
6:B:23:THR:HG23	6:B:162:MET:HE3	2.02	0.41
10:F:33:THR:HG21	10:F:59:ILE:O	2.21	0.41
12:H:68:ALA:HB2	12:H:149:ALA:HB2	2.03	0.41
13:I:131:THR:HG22	13:I:134:GLU:N	2.21	0.41
16:L:42:ARG:HA	16:L:43:PRO:HD3	1.86	0.41
18:N:23:GLY:C	42:N:3062:HOH:O	2.64	0.41
19:O:134:VAL:O	19:O:137:LEU:HB3	2.20	0.41
23:S:48:VAL:HG22	23:S:97:ARG:C	2.45	0.41
26:V:21:LEU:HD22	26:V:26:ILE:HD13	2.01	0.41
26:V:122:ARG:CG	26:V:122:ARG:NH1	2.80	0.41
1:0:319:A:H4'	1:0:338:C:C5	2.55	0.41
1:0:483:C:C4	1:0:484:A:C6	3.09	0.41
1:0:571:C:O5'	1:0:571:C:H6	2.03	0.41
1:0:711:G:N2	1:0:718:C:C2	2.88	0.41
1:0:823:U:H2'	1:0:824:G:O4'	2.20	0.41
1:0:1159:G:P	42:0:3774:HOH:O	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1485:A:H4'	42:0:9780:HOH:O	2.20	0.41
1:0:1568:G:O2'	1:0:1569:U:H5'	2.20	0.41
1:0:1603:A:H5'	1:0:1605:G:C4'	2.50	0.41
2:9:3003:A:H2	2:9:3021:G:N3	2.18	0.41
8:D:93:LEU:HB3	8:D:97:GLN:OE1	2.20	0.41
12:H:143:GLU:N	42:H:8381:HOH:O	2.53	0.41
12:H:157:ILE:CG2	12:H:158:ASN:H	2.34	0.41
15:K:72:ASN:HB2	42:K:8586:HOH:O	2.20	0.41
16:L:169:ARG:NH1	42:L:8574:HOH:O	2.54	0.41
17:M:67:ALA:HA	17:M:71:TRP:CB	2.51	0.41
17:M:71:TRP:CE3	17:M:175:LEU:CD2	3.03	0.41
18:N:45:LEU:HD12	18:N:88:LYS:HD2	2.01	0.41
20:P:26:PRO:O	20:P:30:VAL:HG23	2.21	0.41
21:Q:59:PHE:HZ	21:Q:81:PRO:HG3	1.84	0.41
26:V:21:LEU:HB3	26:V:26:ILE:CG1	2.51	0.41
27:W:14:LEU:HD12	27:W:67:PRO:O	2.20	0.41
1:0:1055:G:OP2	12:H:94:ARG:NH1	2.54	0.41
1:0:1119:G:N2	1:0:1246:A:H2	2.14	0.41
1:0:1224:G:H2'	1:0:1225:C:H6	1.84	0.41
1:0:1483:C:O2'	1:0:1484:G:H5'	2.21	0.41
1:0:1498:G:O2'	1:0:1499:U:H5'	2.20	0.41
1:0:1969:A:N7	1:0:1970:G:C6	2.89	0.41
1:0:2011:A:P	42:0:5433:HOH:O	2.78	0.41
1:0:2045:G:H2'	1:0:2046:G:O4'	2.21	0.41
1:0:2729:C:H2'	1:0:2730:G:H8	1.86	0.41
1:0:2842:G:H2'	1:0:2843:A:C5'	2.51	0.41
42:0:3336:HOH:O	12:H:11:LYS:HE2	2.20	0.41
7:C:1:MET:HG2	7:C:2:GLN:NE2	2.36	0.41
8:D:52:THR:HB	8:D:70:GLY:O	2.21	0.41
9:E:21:THR:HG23	9:E:30:THR:OG1	2.21	0.41
15:K:89:PHE:N	15:K:89:PHE:CD1	2.88	0.41
16:L:62:VAL:C	16:L:63:VAL:HG23	2.46	0.41
17:M:79:PRO:O	17:M:83:LEU:HG	2.21	0.41
17:M:154:LEU:HD11	17:M:157:PRO:HA	2.03	0.41
17:M:162:ASP:HB3	17:M:163:PHE:H	1.63	0.41
18:N:26:TRP:HA	18:N:26:TRP:HE3	1.85	0.41
22:R:8:PRO:HD2	25:U:32:ALA:HA	2.03	0.41
22:R:11:THR:H	22:R:14:ALA:HB3	1.84	0.41
22:R:80:ARG:HG2	42:R:8336:HOH:O	2.20	0.41
1:0:240:C:O2	1:0:240:C:H2'	2.21	0.41
1:0:241:A:C2	1:0:378:A:H4'	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:396:U:C3'	42:0:3823:HOH:O	2.68	0.41
1:0:488:U:H2'	42:0:3493:HOH:O	2.21	0.41
1:0:963:C:O5'	1:0:963:C:H6	2.04	0.41
1:0:1025:C:H5'	26:V:23:MET:O	2.21	0.41
1:0:1086:A:N6	26:V:11:VAL:HG11	2.36	0.41
1:0:1312:G:OP1	28:X:213:LYS:NZ	2.48	0.41
1:0:1613:C:H2'	1:0:1614:G:O4'	2.20	0.41
1:0:1730:G:C5'	1:0:1731:C:H6	2.33	0.41
1:0:1829:A:H2'	1:0:1830:C:H5'	2.03	0.41
1:0:1972:U:C2'	1:0:1973:A:H5'	2.49	0.41
1:0:2039:A:OP2	6:B:234:ARG:NH2	2.54	0.41
1:0:2265:U:H2'	1:0:2266:A:C8	2.56	0.41
1:0:2415:A:C2	17:M:25:ARG:HB3	2.56	0.41
1:0:2842:G:C2'	1:0:2843:A:H5'	2.50	0.41
2:9:3052:A:H2'	2:9:3053:G:O4'	2.21	0.41
2:9:3056:A:H1'	8:D:14:ARG:HG2	2.03	0.41
2:9:3088:G:N2	2:9:3089:C:C2	2.89	0.41
6:B:69:VAL:HA	6:B:70:PRO:HD3	1.88	0.41
6:B:305:ASP:O	6:B:306:LYS:CB	2.68	0.41
7:C:126:ASP:C	7:C:128:GLY:N	2.79	0.41
8:D:27:ILE:HD11	8:D:37:ALA:CB	2.51	0.41
9:E:7:ILE:HA	9:E:8:PRO:HD3	1.94	0.41
12:H:136:VAL:HG22	12:H:137:ASN:N	2.36	0.41
12:H:160:ASP:C	12:H:160:ASP:OD1	2.63	0.41
13:I:116:LEU:HB2	13:I:119:THR:HG21	2.02	0.41
15:K:1:THR:N	42:K:8583:HOH:O	2.54	0.41
16:L:55:LYS:O	16:L:60:ILE:HD12	2.21	0.41
23:S:23:VAL:HG23	23:S:41:ARG:HG3	2.02	0.41
26:V:119:HIS:CD2	26:V:120:PRO:O	2.73	0.41
29:Y:41:VAL:HG12	29:Y:42:CYS:N	2.35	0.41
29:Y:46:LYS:HE2	42:Y:8434:HOH:O	2.20	0.41
1:0:295:C:H2'	1:0:296:G:O4'	2.21	0.41
1:0:424:C:H2'	1:0:425:U:H6	1.85	0.41
1:0:794:U:H3	1:0:819:A:H61	1.68	0.41
1:0:2362:A:H2'	1:0:2363:G:C8	2.56	0.41
1:0:2831:C:H2'	1:0:2832:C:C5'	2.51	0.41
5:A:94:LEU:N	5:A:94:LEU:CD2	2.84	0.41
8:D:58:VAL:CG1	8:D:59:GLY:N	2.83	0.41
9:E:22:VAL:O	9:E:28:SER:HA	2.21	0.41
12:H:83:PHE:HD1	12:H:134:ALA:HB2	1.84	0.41
13:I:49:ARG:O	13:I:50:GLU:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:63:VAL:HG21	16:L:109:PHE:CZ	2.56	0.41
17:M:34:LEU:HD22	17:M:129:ILE:CD1	2.51	0.41
17:M:154:LEU:CG	17:M:155:GLU:N	2.83	0.41
22:R:25:GLN:HG2	22:R:65:VAL:HG22	2.03	0.41
23:S:40:VAL:HA	23:S:119:ALA:O	2.21	0.41
27:W:76:ARG:NH1	27:W:76:ARG:CG	2.84	0.41
29:Y:13:ARG:NH1	29:Y:14:PHE:CE2	2.88	0.41
1:O:941:G:C5	1:O:942:U:C4	3.09	0.40
1:O:1815:A:H4'	1:O:2751:C:O4'	2.22	0.40
1:O:2610:U:H4'	42:O:8982:HOH:O	2.20	0.40
1:O:2912:C:H2'	1:O:2913:A:O4'	2.21	0.40
42:O:5726:HOH:O	24:T:56:ARG:HD3	2.20	0.40
2:9:3040:C:N4	8:D:51:ARG:HB2	2.36	0.40
2:9:3105:A:H2'	2:9:3106:C:O4'	2.21	0.40
5:A:81:GLN:CB	5:A:92:ASN:ND2	2.83	0.40
7:C:138:VAL:O	7:C:234:VAL:HA	2.21	0.40
7:C:192:ILE:CG2	7:C:234:VAL:HG12	2.51	0.40
8:D:170:TYR:N	8:D:170:TYR:CD1	2.89	0.40
9:E:98:GLU:N	42:E:4191:HOH:O	2.53	0.40
10:F:32:GLY:N	42:F:3111:HOH:O	2.53	0.40
10:F:100:ASP:O	10:F:101:ALA:O	2.39	0.40
17:M:149:GLU:O	17:M:152:GLU:HB2	2.21	0.40
18:N:96:VAL:CG1	18:N:100:GLN:HB2	2.51	0.40
21:Q:18:LEU:HB2	21:Q:143:VAL:HG13	2.03	0.40
21:Q:47:LEU:HB2	21:Q:89:LEU:HD21	2.02	0.40
25:U:23:LEU:HD22	25:U:49:LEU:HD23	2.03	0.40
26:V:6:GLN:HA	26:V:52:VAL:HG23	2.02	0.40
1:O:67:A:H5''	1:O:69:A:C8	2.57	0.40
1:O:90:A:H2'	1:O:91:G:O4'	2.21	0.40
1:O:566:A:H2'	1:O:567:U:O4'	2.21	0.40
1:O:612:U:H2'	1:O:613:C:C6	2.57	0.40
1:O:626:U:C4	1:O:627:G:C6	3.08	0.40
1:O:1003:U:H4'	12:H:86:ARG:O	2.21	0.40
1:O:1268:C:H2'	1:O:1269:G:C8	2.56	0.40
1:O:1477:C:H5'	1:O:1868:G:H5'	2.03	0.40
1:O:2474:A:N7	1:O:2621:U:H4'	2.37	0.40
7:C:21:VAL:C	7:C:23:GLU:N	2.80	0.40
12:H:129:ASN:N	12:H:129:ASN:HD22	2.18	0.40
16:L:168:ARG:NH1	42:L:8604:HOH:O	2.54	0.40
23:S:14:ALA:HA	23:S:15:PRO:HD3	1.94	0.40
29:Y:22:ILE:HG22	29:Y:23:ARG:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:1:10:ARG:HH11	31:1:49:GLU:CD	2.29	0.40
1:0:544:G:H2'	1:0:545:G:C5'	2.46	0.40
1:0:745:G:O6	18:N:68:GLY:HA3	2.22	0.40
1:0:954:U:O2'	1:0:955:A:H5'	2.21	0.40
1:0:1164:U:N3	1:0:1192:A:H2	2.09	0.40
1:0:1307:A:H2'	1:0:1308:A:C8	2.56	0.40
1:0:1515:A:H2'	1:0:1516:C:C6	2.56	0.40
1:0:1711:A:O2'	1:0:1712:A:H5'	2.20	0.40
1:0:1762:C:O2'	1:0:1763:C:H5'	2.21	0.40
1:0:1815:A:H2'	1:0:1816:C:O4'	2.22	0.40
1:0:1992:U:H2'	1:0:1994:A:OP2	2.22	0.40
1:0:2266:A:H2'	1:0:2267:G:H8	1.85	0.40
5:A:130:THR:HG22	5:A:131:HIS:O	2.21	0.40
6:B:258:GLY:HA2	42:B:8555:HOH:O	2.20	0.40
7:C:84:VAL:O	7:C:85:LYS:HB2	2.21	0.40
12:H:26:LYS:CG	12:H:28:ILE:H	2.23	0.40
15:K:61:ALA:HA	42:K:8570:HOH:O	2.21	0.40
15:K:121:ILE:HG12	15:K:141:GLU:HB2	2.02	0.40
17:M:91:ARG:HG3	17:M:186:LEU:CD2	2.49	0.40
17:M:163:PHE:O	17:M:164:ASP:O	2.38	0.40
28:X:99:ALA:HB2	28:X:233:TYR:CE2	2.56	0.40
1:0:39:G:N2	1:0:444:C:C2	2.90	0.40
1:0:40:C:H6	1:0:40:C:O5'	2.05	0.40
1:0:825:U:H5''	1:0:826:U:OP1	2.21	0.40
1:0:1050:G:C6	1:0:1051:C:C4	3.10	0.40
1:0:1624:A:H5'	1:0:1626:A:O4'	2.22	0.40
1:0:1641:A:C2'	1:0:1642:A:H5'	2.49	0.40
1:0:1730:G:C5'	1:0:1731:C:C6	3.04	0.40
1:0:1881:A:OP1	5:A:199:HIS:HE1	2.05	0.40
1:0:2582:G:O3'	14:J:41:LYS:HA	2.21	0.40
1:0:2589:U:H2'	1:0:2590:U:C6	2.57	0.40
1:0:2851:G:C2'	1:0:2852:A:H5'	2.52	0.40
1:0:2897:C:H2'	1:0:2898:G:H8	1.85	0.40
2:9:3056:A:N1	8:D:13:MET:HE3	2.36	0.40
5:A:29:HIS:CE1	5:A:107:ASN:ND2	2.89	0.40
8:D:68:PRO:HG3	42:D:1982:HOH:O	2.21	0.40
16:L:59:GLY:HA3	16:L:141:ILE:CD1	2.50	0.40
20:P:30:VAL:O	20:P:30:VAL:HG12	2.21	0.40
26:V:67:ALA:HB2	26:V:93:ILE:HD13	2.04	0.40
1:0:105:G:O2'	1:0:106:A:H5'	2.21	0.40
1:0:128:A:C8	1:0:128:A:C3'	3.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:187:A:H3'	1:0:188:C:H6	1.86	0.40
1:0:793:A:H5''	19:O:83:LYS:HG2	2.04	0.40
1:0:832:U:H2'	1:0:833:G:C8	2.57	0.40
1:0:1516:C:H2'	1:0:1517:U:C6	2.57	0.40
1:0:1804:A:H2'	1:0:1805:G:C8	2.55	0.40
1:0:2364:A:H5''	20:P:15:LYS:HD3	2.03	0.40
5:A:39:ALA:HB3	5:A:61:GLU:OE2	2.22	0.40
5:A:66:ARG:HH11	5:A:66:ARG:CB	2.35	0.40
5:A:140:LEU:HB3	5:A:141:PRO:HD2	2.04	0.40
7:C:102:LEU:HD12	42:C:8316:HOH:O	2.21	0.40
7:C:154:VAL:O	7:C:158:GLU:HG3	2.21	0.40
8:D:57:THR:HA	8:D:63:ILE:HA	2.03	0.40
8:D:77:ASP:HB3	8:D:78:GLU:H	1.60	0.40
10:F:78:GLU:HG3	42:F:5966:HOH:O	2.20	0.40
12:H:48:LEU:CD1	12:H:157:ILE:HG21	2.50	0.40
18:N:32:ARG:HB2	42:N:4656:HOH:O	2.20	0.40
22:R:73:ASP:OD1	22:R:75:GLN:HB2	2.22	0.40
26:V:7:LEU:HD23	26:V:7:LEU:HA	1.91	0.40
26:V:14:HIS:HB2	26:V:17:ILE:HG13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	A	235/239 (98%)	199 (85%)	32 (14%)	4 (2%)	7	30
6	B	335/337 (99%)	299 (89%)	29 (9%)	7 (2%)	5	25
7	C	244/246 (99%)	220 (90%)	22 (9%)	2 (1%)	16	47
8	D	134/176 (76%)	94 (70%)	26 (19%)	14 (10%)	0	2
9	E	170/177 (96%)	159 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	F	117/119 (98%)	104 (89%)	11 (9%)	2 (2%)	7	30
11	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
12	H	152/167 (91%)	132 (87%)	15 (10%)	5 (3%)	3	17
13	I	140/145 (97%)	127 (91%)	9 (6%)	4 (3%)	3	19
14	J	130/132 (98%)	121 (93%)	7 (5%)	2 (2%)	8	32
15	K	141/164 (86%)	124 (88%)	16 (11%)	1 (1%)	18	49
16	L	192/194 (99%)	174 (91%)	17 (9%)	1 (0%)	24	57
17	M	184/186 (99%)	166 (90%)	11 (6%)	7 (4%)	2	15
18	N	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
19	O	141/148 (95%)	138 (98%)	2 (1%)	1 (1%)	18	49
20	P	93/95 (98%)	86 (92%)	7 (8%)	0	100	100
21	Q	148/154 (96%)	136 (92%)	11 (7%)	1 (1%)	18	49
22	R	79/84 (94%)	74 (94%)	5 (6%)	0	100	100
23	S	117/119 (98%)	110 (94%)	7 (6%)	0	100	100
24	T	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
25	U	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	3	18
26	V	152/154 (99%)	143 (94%)	7 (5%)	2 (1%)	9	35
27	W	80/91 (88%)	71 (89%)	6 (8%)	3 (4%)	2	15
28	X	140/240 (58%)	140 (100%)	0	0	100	100
29	Y	71/73 (97%)	63 (89%)	7 (10%)	1 (1%)	9	34
30	Z	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
31	1	42/48 (88%)	41 (98%)	1 (2%)	0	100	100
32	2	90/92 (98%)	84 (93%)	3 (3%)	3 (3%)	3	17
All	All	3633/4235 (86%)	3293 (91%)	278 (8%)	62 (2%)	7	30

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	139	ASP
8	D	93	LEU
8	D	95	THR
8	D	173	GLU
10	F	101	ALA
12	H	162	SER

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Mol	Chain	Res	Type
15	K	80	ASP
17	M	154	LEU
17	M	164	ASP
17	M	183	ASP
5	A	34	ASP
5	A	132	ASP
6	B	34	GLY
6	B	107	SER
6	B	169	GLY
7	C	8	LEU
8	D	20	LYS
8	D	36	ASN
8	D	137	PRO
12	H	138	PRO
12	H	164	ALA
13	I	5	GLU
14	J	119	GLN
17	M	162	ASP
32	2	57	GLY
5	A	119	ALA
6	B	184	ASP
8	D	11	HIS
8	D	171	ASP
13	I	7	ASP
16	L	140	ALA
17	M	167	ASP
17	M	181	ASP
19	O	116	SER
25	U	43	PRO
26	V	49	ASN
26	V	77	ALA
27	W	77	PHE
27	W	87	ALA
32	2	56	PRO
6	B	185	GLY
8	D	147	ALA
10	F	64	PRO
13	I	76	ASP
13	I	143	LYS
14	J	126	SER
17	M	155	GLU
29	Y	81	LYS

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Mol	Chain	Res	Type
6	B	2	GLN
8	D	16	PRO
8	D	82	GLU
7	C	79	ARG
8	D	61	PHE
8	D	170	TYR
12	H	40	PRO
12	H	72	VAL
5	A	37	VAL
21	Q	106	GLY
25	U	40	PRO
27	W	52	PRO
32	2	25	VAL
8	D	27	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	A	179/181 (99%)	167 (93%)	12 (7%)	15	43
6	B	282/282 (100%)	263 (93%)	19 (7%)	15	43
7	C	193/193 (100%)	177 (92%)	16 (8%)	10	35
8	D	117/147 (80%)	109 (93%)	8 (7%)	14	42
9	E	152/155 (98%)	148 (97%)	4 (3%)	40	68
10	F	92/92 (100%)	91 (99%)	1 (1%)	65	78
11	G	27/283 (10%)	26 (96%)	1 (4%)	30	61
12	H	122/122 (100%)	108 (88%)	14 (12%)	5	23
13	I	118/121 (98%)	110 (93%)	8 (7%)	14	42
14	J	106/106 (100%)	102 (96%)	4 (4%)	29	60
15	K	112/126 (89%)	109 (97%)	3 (3%)	39	67
16	L	166/166 (100%)	159 (96%)	7 (4%)	26	58
17	M	149/149 (100%)	140 (94%)	9 (6%)	17	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	N	93/93 (100%)	89 (96%)	4 (4%)	26	57
19	O	113/116 (97%)	109 (96%)	4 (4%)	32	62
20	P	79/79 (100%)	75 (95%)	4 (5%)	21	52
21	Q	117/121 (97%)	112 (96%)	5 (4%)	26	57
22	R	71/73 (97%)	70 (99%)	1 (1%)	59	76
23	S	105/105 (100%)	101 (96%)	4 (4%)	29	60
24	T	44/52 (85%)	42 (96%)	2 (4%)	24	56
25	U	51/56 (91%)	50 (98%)	1 (2%)	48	72
26	V	130/130 (100%)	121 (93%)	9 (7%)	14	41
27	W	66/73 (90%)	61 (92%)	5 (8%)	12	39
28	X	120/195 (62%)	113 (94%)	7 (6%)	18	48
29	Y	56/56 (100%)	49 (88%)	7 (12%)	4	19
30	Z	46/46 (100%)	46 (100%)	0	100	100
31	1	42/44 (96%)	41 (98%)	1 (2%)	43	69
32	2	79/79 (100%)	74 (94%)	5 (6%)	16	45
All	All	3027/3441 (88%)	2862 (94%)	165 (6%)	19	50

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	3	ARG
5	A	33	GLU
5	A	36	ASP
5	A	55	VAL
5	A	68	ILE
5	A	69	LEU
5	A	94	LEU
5	A	131	HIS
5	A	153	ARG
5	A	175	LYS
5	A	179	MET
5	A	217	ARG
6	B	7	ARG
6	B	11	LEU
6	B	27	ASN
6	B	33	ASP
6	B	63	GLU

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Mol	Chain	Res	Type
6	B	84	LEU
6	B	97	LEU
6	B	98	THR
6	B	103	ASP
6	B	195	ARG
6	B	245	SER
6	B	251	VAL
6	B	254	GLN
6	B	256	GLN
6	B	257	THR
6	B	264	GLU
6	B	304	PRO
6	B	307	ARG
6	B	312	ARG
7	C	2	GLN
7	C	27	ARG
7	C	67	GLN
7	C	91	PRO
7	C	94	THR
7	C	101	ASP
7	C	115	LEU
7	C	136	VAL
7	C	187	ARG
7	C	214	THR
7	C	222	ASP
7	C	223	LEU
7	C	234	VAL
7	C	236	THR
7	C	240	LEU
7	C	243	VAL
8	D	24	HIS
8	D	50	VAL
8	D	95	THR
8	D	99	ASP
8	D	131	THR
8	D	136	ARG
8	D	137	PRO
8	D	149	ARG
9	E	1	PRO
9	E	7	ILE
9	E	86	VAL
9	E	102	VAL

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Mol	Chain	Res	Type
10	F	1	PRO
11	G	64	ASN
12	H	18	GLU
12	H	30	GLN
12	H	59	ASN
12	H	61	LEU
12	H	72	VAL
12	H	73	GLN
12	H	82	LYS
12	H	85	ILE
12	H	86	ARG
12	H	94	ARG
12	H	118	PRO
12	H	142	VAL
12	H	150	LYS
12	H	166	ASN
13	I	46	ILE
13	I	47	THR
13	I	74	ARG
13	I	93	ARG
13	I	120	SER
13	I	125	SER
13	I	127	ILE
13	I	131	THR
14	J	7	ASP
14	J	10	GLN
14	J	49	LEU
14	J	98	VAL
15	K	35	ARG
15	K	117	GLU
15	K	140	VAL
16	L	38	VAL
16	L	46	LEU
16	L	81	ARG
16	L	87	MET
16	L	93	ARG
16	L	99	ARG
16	L	164	THR
17	M	17	ARG
17	M	26	LEU
17	M	43	VAL
17	M	47	LEU

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Mol	Chain	Res	Type
17	M	50	LEU
17	M	127	LEU
17	M	128	ASP
17	M	152	GLU
17	M	163	PHE
18	N	3	THR
18	N	67	SER
18	N	98	LEU
18	N	111	VAL
19	O	52	LYS
19	O	91	LYS
19	O	94	TRP
19	O	98	ILE
20	P	11	ARG
20	P	16	ASN
20	P	57	ASP
20	P	95	GLU
21	Q	13	THR
21	Q	39	THR
21	Q	82	GLU
21	Q	132	ARG
21	Q	143	VAL
22	R	10	VAL
23	S	26	THR
23	S	39	ASN
23	S	48	VAL
23	S	96	VAL
24	T	9	CYS
24	T	28	THR
25	U	43	PRO
26	V	4	LEU
26	V	26	ILE
26	V	35	VAL
26	V	52	VAL
26	V	73	LEU
26	V	122	ARG
26	V	142	ASP
26	V	146	ILE
26	V	154	ARG
27	W	15	ARG
27	W	27	ASP
27	W	52	PRO

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Mol	Chain	Res	Type
27	W	66	THR
27	W	72	VAL
28	X	154	ARG
28	X	163	THR
28	X	172	THR
28	X	189	ASN
28	X	200	THR
28	X	203	VAL
28	X	235	GLU
29	Y	11	THR
29	Y	22	ILE
29	Y	32	LYS
29	Y	42	CYS
29	Y	60	CYS
29	Y	64	ILE
29	Y	68	CYS
31	1	18	ASN
32	2	14	CYS
32	2	42	ARG
32	2	56	PRO
32	2	65	THR
32	2	74	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	5	GLN
5	A	29	HIS
5	A	47	HIS
5	A	92	ASN
5	A	127	GLN
5	A	199	HIS
6	B	27	ASN
6	B	145	HIS
6	B	238	ASN
6	B	243	ASN
6	B	256	GLN
6	B	260	HIS
7	C	2	GLN
7	C	39	GLN
7	C	67	GLN
7	C	129	HIS

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Mol	Chain	Res	Type
7	C	163	HIS
8	D	103	ASN
9	E	66	GLN
9	E	96	ASN
9	E	106	ASN
9	E	119	HIS
9	E	143	GLN
11	G	17	GLN
11	G	64	ASN
12	H	30	GLN
12	H	35	ASN
12	H	36	ASN
12	H	45	GLN
12	H	55	GLN
12	H	58	HIS
12	H	59	ASN
12	H	69	ASN
12	H	74	ASN
12	H	91	HIS
12	H	129	ASN
12	H	130	HIS
12	H	137	ASN
12	H	166	ASN
13	I	25	GLN
13	I	52	GLN
13	I	107	ASN
13	I	126	ASN
14	J	10	GLN
14	J	42	ASN
15	K	18	HIS
15	K	41	HIS
15	K	42	ASN
15	K	55	GLN
15	K	58	GLN
15	K	116	HIS
16	L	26	HIS
16	L	58	GLN
16	L	78	ASN
16	L	176	GLN
17	M	22	GLN
17	M	107	ASN
17	M	140	GLN

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Mol	Chain	Res	Type
17	M	153	GLN
19	O	28	GLN
19	O	50	GLN
19	O	66	GLN
19	O	73	HIS
19	O	118	GLN
20	P	16	ASN
20	P	40	HIS
21	Q	61	GLN
21	Q	94	ASN
21	Q	98	ASN
21	Q	113	HIS
21	Q	117	HIS
21	Q	140	GLN
22	R	9	HIS
22	R	25	GLN
22	R	51	GLN
22	R	53	ASN
22	R	55	GLN
22	R	56	ASN
23	S	39	ASN
23	S	43	ASN
23	S	73	HIS
24	T	39	ASN
24	T	48	ASN
25	U	6	GLN
25	U	60	GLN
26	V	6	GLN
26	V	14	HIS
26	V	27	HIS
26	V	28	HIS
26	V	87	HIS
26	V	110	GLN
26	V	119	HIS
26	V	125	HIS
26	V	141	HIS
27	W	23	HIS
27	W	36	HIS
28	X	119	GLN
28	X	133	HIS
28	X	134	HIS
28	X	149	GLN

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Mol	Chain	Res	Type
28	X	153	GLN
28	X	189	ASN
29	Y	33	HIS
29	Y	70	GLN
30	Z	8	GLN
30	Z	16	HIS
30	Z	28	HIS
31	1	16	ASN
31	1	17	GLN
31	1	18	ASN
31	1	37	HIS
31	1	41	HIS
31	1	45	ASN
32	2	30	GLN
32	2	48	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2747/2922 (94%)	250 (9%)	34 (1%)
2	9	121/122 (99%)	14 (11%)	4 (3%)
3	3	2/3 (66%)	1 (50%)	0
4	4	1/2 (50%)	0	0
All	All	2871/3049 (94%)	265 (9%)	38 (1%)

All (265) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C

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Mol	Chain	Res	Type
1	0	139	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	169	A
1	0	185	G
1	0	186	A
1	0	187	A
1	0	191	A
1	0	192	A
1	0	200	U
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	317	A
1	0	318	C
1	0	336	G
1	0	337	A
1	0	345	G
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G

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Mol	Chain	Res	Type
1	0	559	U
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	701	U
1	0	717	C
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	884	C
1	0	885	G
1	0	898	G
1	0	905	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A

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Mol	Chain	Res	Type
1	0	1087	G
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1137	G
1	0	1151	G
1	0	1162	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1171	A
1	0	1174	A
1	0	1175	G
1	0	1177	A
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1331	A
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1378	G
1	0	1407	A
1	0	1451	C
1	0	1460	G
1	0	1474	C
1	0	1485	A
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A

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Mol	Chain	Res	Type
1	0	1564	C
1	0	1580	A
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1710	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1904	A
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1974	G
1	0	1978	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U

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Mol	Chain	Res	Type
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2103	A
1	0	2110	G
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2317	C
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2466	G
1	0	2467	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2526	C
1	0	2527	U
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2619	U
1	0	2620	U

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Mol	Chain	Res	Type
1	0	2637	A
1	0	2638	G
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2718	C
1	0	2719	A
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2825	C
1	0	2840	A
1	0	2850	C
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3007	G
2	9	3014	G
2	9	3022	G
2	9	3024	U
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3052	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C
3	3	76	A

All (38) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	10	U
1	0	69	A
1	0	129	A
1	0	284	C
1	0	338	C
1	0	603	A
1	0	716	G
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1164	U
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1474	C
1	0	1563	G
1	0	1692	C
1	0	1856	C
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2466	G
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2637	A
1	0	2649	A
1	0	2718	C
1	0	2761	A
1	0	2791	U
2	9	3002	U
2	9	3023	U
2	9	3065	A
2	9	3103	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 236 ligands modelled in this entry, 232 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
37	PPU	4	76	4,38	37,40,41	2.37	3 (8%)	47,57,60	0.88	2 (4%)
40	BTN	4	79	39	15,16,17	1.84	4 (26%)	20,21,23	1.51	3 (15%)
39	ACA	4	78	40,38	6,7,8	2.07	1 (16%)	5,6,8	1.13	0
38	PHA	4	77	39,37	10,11,11	1.10	0	8,13,13	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	PPU	4	76	4,38	-	1/25/43/44	0/4/4/4
40	BTN	4	79	39	-	3/6/27/28	0/2/2/2
39	ACA	4	78	40,38	-	2/5/5/6	-
38	PHA	4	77	39,37	-	0/5/6/6	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	4	76	PPU	C-N3'	12.57	1.61	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	4	76	PPU	OC-CM	-5.70	1.26	1.42
39	4	78	ACA	C3-C2	-4.77	1.32	1.52
40	4	79	BTN	C8-C7	-4.44	1.33	1.52
40	4	79	BTN	C9-C10	-3.65	1.36	1.52
37	4	76	PPU	C3'-N3'	-2.61	1.41	1.45
40	4	79	BTN	C3-N1	-2.59	1.30	1.35
40	4	79	BTN	O3-C3	2.38	1.28	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	4	79	BTN	C2-C4-N2	3.95	117.52	113.34
37	4	76	PPU	C2-N1-C6	2.86	118.83	111.83
40	4	79	BTN	C6-C5-N1	2.49	116.39	113.18
37	4	76	PPU	C-CA-N	2.42	118.52	109.37
40	4	79	BTN	C2-C4-C5	2.11	111.48	108.89

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	4	79	BTN	C7-C8-C9-C10
39	4	78	ACA	C4-C5-C6-N
39	4	78	ACA	C3-C4-C5-C6
40	4	79	BTN	C4-C2-C7-C8
37	4	76	PPU	N-CA-CB-CG
40	4	79	BTN	S1-C2-C7-C8

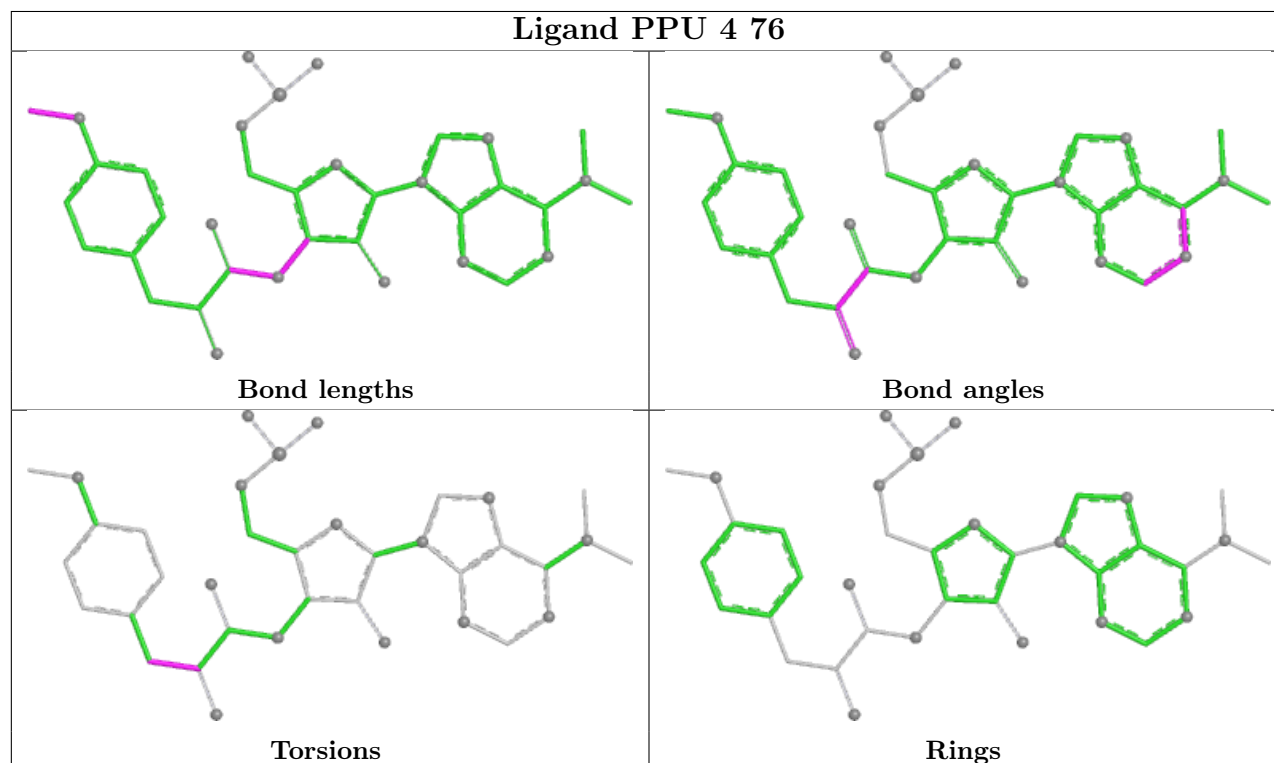
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	4	76	PPU	2	0
40	4	79	BTN	2	0
38	4	77	PHA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2754/2922 (94%)	-0.61	40 (1%) 72 52	11, 39, 86, 141	0
2	9	122/122 (100%)	-0.08	5 (4%) 41 23	28, 60, 91, 145	0
3	3	3/3 (100%)	2.74	3 (100%) 0 0	22, 22, 23, 26	3 (100%)
4	4	2/2 (100%)	-0.08	0 100 100	48, 48, 48, 56	0
5	A	237/239 (99%)	-0.15	4 (1%) 69 48	21, 53, 94, 113	0
6	B	337/337 (100%)	-0.36	1 (0%) 90 80	19, 45, 71, 81	0
7	C	246/246 (100%)	-0.46	1 (0%) 88 76	12, 37, 63, 71	0
8	D	140/176 (79%)	0.74	10 (7%) 22 12	55, 94, 120, 127	0
9	E	172/177 (97%)	-0.10	2 (1%) 76 58	32, 56, 81, 87	0
10	F	119/119 (100%)	0.07	1 (0%) 82 65	41, 66, 94, 104	0
11	G	29/348 (8%)	0.69	2 (6%) 23 12	60, 79, 84, 89	0
12	H	156/167 (93%)	-0.07	4 (2%) 57 36	30, 48, 74, 81	0
13	I	142/145 (97%)	-0.46	0 100 100	26, 38, 60, 77	0
14	J	132/132 (100%)	-0.32	0 100 100	24, 44, 72, 76	0
15	K	145/164 (88%)	0.06	5 (3%) 48 28	16, 68, 97, 109	0
16	L	194/194 (100%)	0.13	22 (11%) 10 5	23, 39, 118, 128	0
17	M	186/186 (100%)	0.21	7 (3%) 44 25	36, 65, 109, 120	0
18	N	115/115 (100%)	-0.21	0 100 100	31, 47, 65, 69	0
19	O	143/148 (96%)	-0.28	1 (0%) 84 68	27, 47, 67, 77	0
20	P	95/95 (100%)	-0.40	1 (1%) 78 59	27, 40, 57, 79	0
21	Q	150/154 (97%)	-0.68	0 100 100	22, 35, 54, 65	0
22	R	81/84 (96%)	-0.30	0 100 100	35, 53, 73, 80	0
23	S	119/119 (100%)	-0.21	1 (0%) 82 65	33, 47, 75, 91	0
24	T	53/66 (80%)	1.47	12 (22%) 2 1	101, 113, 122, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	U	65/70 (92%)	0.17	3 (4%) 37 20	45, 69, 106, 112	0
26	V	154/154 (100%)	-0.42	0 100 100	25, 38, 56, 69	0
27	W	82/91 (90%)	-0.11	4 (4%) 35 18	32, 49, 69, 89	0
28	X	142/240 (59%)	-0.49	1 (0%) 84 68	17, 36, 58, 77	0
29	Y	73/73 (100%)	2.22	36 (49%) 0 0	89, 118, 129, 133	0
30	Z	56/56 (100%)	-0.81	0 100 100	14, 26, 32, 39	0
31	1	46/48 (95%)	-0.11	0 100 100	23, 52, 84, 96	0
32	2	92/92 (100%)	2.65	58 (63%) 0 0	122, 136, 142, 146	0
All	All	6582/7284 (90%)	-0.28	224 (3%) 48 28	11, 45, 105, 146	3 (0%)

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
16	L	89	ASN	7.7
25	U	1	THR	7.3
16	L	80	GLY	7.1
32	2	12	PRO	6.6
16	L	70	GLY	6.2
32	2	60	LYS	6.0
29	Y	22	ILE	5.9
29	Y	16	PRO	5.7
1	0	1173	A	5.6
29	Y	12	GLY	5.5
32	2	79	LEU	5.5
32	2	48	ASN	5.5
16	L	81	ARG	5.3
29	Y	20	LEU	5.2
32	2	83	TRP	4.9
16	L	83	SER	4.7
29	Y	26	VAL	4.7
32	2	35	TRP	4.7
32	2	33	MET	4.7
32	2	39	GLN	4.6
1	0	1925	G	4.6
29	Y	18	TYR	4.5
19	O	116	SER	4.5
29	Y	34	LYS	4.5
32	2	76	LYS	4.5
16	L	82	ARG	4.5

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Mol	Chain	Res	Type	RSRZ
32	2	84	ARG	4.4
29	Y	41	VAL	4.4
32	2	61	PRO	4.4
16	L	71	SER	4.3
1	0	735	C	4.3
16	L	72	SER	4.3
29	Y	40	PRO	4.2
1	0	1168	C	4.2
16	L	88	VAL	4.2
5	A	36	ASP	4.1
29	Y	32	LYS	4.1
32	2	34	LYS	4.1
16	L	78	ASN	4.1
16	L	75	THR	4.0
1	0	1176	C	4.0
1	0	1924	A	3.9
32	2	47	GLY	3.9
32	2	13	HIS	3.8
32	2	17	HIS	3.8
32	2	46	ILE	3.8
8	D	10	PHE	3.8
32	2	7	PHE	3.8
32	2	51	LYS	3.8
8	D	63	ILE	3.7
32	2	36	ILE	3.7
16	L	68	ARG	3.7
27	W	88	GLU	3.7
1	0	1175	G	3.7
32	2	77	ALA	3.7
32	2	88	LEU	3.7
29	Y	13	ARG	3.6
16	L	73	ARG	3.6
29	Y	21	LYS	3.6
32	2	3	MET	3.6
32	2	54	LYS	3.6
29	Y	29	VAL	3.5
32	2	1	MET	3.5
1	0	2433	A	3.5
32	2	4	PRO	3.5
16	L	76	ARG	3.5
32	2	11	CYS	3.5
2	9	3001	U	3.5

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Mol	Chain	Res	Type	RSRZ
32	2	64	LYS	3.4
29	Y	44	PHE	3.4
29	Y	11	THR	3.4
32	2	82	GLY	3.4
32	2	43	ASN	3.4
32	2	63	LYS	3.4
32	2	85	ALA	3.4
32	2	67	LEU	3.3
29	Y	31	ILE	3.3
32	2	52	PHE	3.3
6	B	1	PRO	3.3
1	0	10	U	3.2
16	L	77	PHE	3.2
16	L	86	MET	3.2
29	Y	35	LYS	3.2
29	Y	24	VAL	3.2
29	Y	17	ARG	3.2
1	0	1172	G	3.1
16	L	90	ARG	3.1
3	3	76	A	3.1
1	0	1198	U	3.1
2	9	3002	U	3.1
17	M	168	LEU	3.1
1	0	1193	A	3.1
32	2	31	THR	3.1
32	2	62	THR	3.1
1	0	2436	U	3.0
32	2	78	HIS	3.0
32	2	15	ASN	3.0
24	T	16	GLY	3.0
3	3	74	C	3.0
16	L	74	ARG	2.9
1	0	1162	G	2.9
1	0	1167	G	2.9
24	T	13	ILE	2.9
32	2	8	ASN	2.9
32	2	9	THR	2.9
29	Y	23	ARG	2.9
1	0	1171	A	2.9
29	Y	42	CYS	2.9
1	0	1169	U	2.8
20	P	95	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
32	2	10	TYR	2.8
8	D	62	ASP	2.8
32	2	68	LYS	2.8
32	2	55	VAL	2.8
32	2	53	SER	2.8
32	2	59	ASP	2.7
25	U	40	PRO	2.7
10	F	106	THR	2.7
32	2	22	VAL	2.7
24	T	31	PHE	2.7
1	0	2748	G	2.7
29	Y	64	ILE	2.7
7	C	135	GLU	2.7
29	Y	48	LYS	2.7
24	T	55	ALA	2.7
32	2	56	PRO	2.7
24	T	49	LEU	2.7
1	0	736	A	2.6
1	0	1161	A	2.6
29	Y	14	PHE	2.6
1	0	1160	G	2.6
2	9	3022	G	2.6
15	K	81	VAL	2.6
16	L	79	LYS	2.6
9	E	10	ASP	2.6
32	2	38	ARG	2.6
17	M	167	ASP	2.6
32	2	65	THR	2.6
17	M	169	PRO	2.5
29	Y	15	GLY	2.5
29	Y	19	GLY	2.5
32	2	2	GLN	2.5
11	G	26	MET	2.5
16	L	69	LYS	2.5
24	T	6	CYS	2.5
5	A	37	VAL	2.5
29	Y	27	ALA	2.5
16	L	84	LYS	2.5
17	M	179	LEU	2.5
1	0	1192	A	2.5
1	0	734	U	2.5
25	U	2	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
32	2	42	ARG	2.4
29	Y	33	HIS	2.4
29	Y	54	ILE	2.4
29	Y	30	GLU	2.4
15	K	36	ASP	2.4
1	0	1170	U	2.4
28	X	235	GLU	2.4
29	Y	39	CYS	2.4
32	2	69	TYR	2.4
1	0	1166	A	2.4
32	2	18	GLN	2.3
8	D	107	GLY	2.3
15	K	146	GLY	2.3
29	Y	50	ALA	2.3
1	0	1206	U	2.3
27	W	80	GLU	2.3
1	0	1190	G	2.3
27	W	85	VAL	2.3
1	0	1964	U	2.3
15	K	83	GLU	2.3
29	Y	74	VAL	2.3
17	M	147	ILE	2.3
24	T	51	TRP	2.3
8	D	131	THR	2.3
17	M	186	LEU	2.3
1	0	1165	G	2.3
1	0	737	A	2.3
2	9	3024	U	2.3
16	L	165	SER	2.3
8	D	171	ASP	2.2
9	E	45	ASP	2.2
8	D	59	GLY	2.2
32	2	32	GLY	2.2
1	0	138	U	2.2
1	0	2432	C	2.2
12	H	167	ALA	2.2
12	H	140	PRO	2.2
24	T	54	THR	2.2
29	Y	52	THR	2.2
32	2	44	SER	2.2
24	T	40	ALA	2.2
12	H	40	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
29	Y	53	GLY	2.2
3	3	75	C	2.1
24	T	42	LEU	2.1
12	H	114	PRO	2.1
32	2	57	GLY	2.1
1	0	1279	U	2.1
5	A	38	ILE	2.1
15	K	46	LEU	2.1
1	0	1181	A	2.1
1	0	1923	G	2.1
32	2	14	CYS	2.1
32	2	74	CYS	2.1
1	0	2345	A	2.1
8	D	69	ILE	2.1
17	M	138	ASP	2.1
1	0	1184	C	2.1
1	0	1926	G	2.1
5	A	237	GLY	2.1
32	2	16	GLU	2.1
24	T	22	VAL	2.0
24	T	34	SER	2.0
1	0	1916	C	2.0
2	9	3025	G	2.0
11	G	71	LEU	2.0
8	D	27	ILE	2.0
23	S	1	SER	2.0
1	0	1524	U	2.0
8	D	21	VAL	2.0
27	W	82	GLU	2.0
29	Y	10	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
35	NA	0	8384	1/1	0.41	0.19	87,87,87,87	0
35	NA	0	8329	1/1	0.54	0.33	62,62,62,62	0
35	NA	9	8351	1/1	0.58	0.28	112,112,112,112	0
36	CL	2	8504	1/1	0.60	0.11	104,104,104,104	0
41	CD	2	8404	1/1	0.63	0.36	200,200,200,200	0
41	CD	T	8401	1/1	0.65	0.35	200,200,200,200	0
35	NA	R	8312	1/1	0.65	0.17	84,84,84,84	0
35	NA	0	8382	1/1	0.78	0.28	57,57,57,57	0
35	NA	0	8385	1/1	0.81	0.31	52,52,52,52	0
35	NA	9	8383	1/1	0.83	0.21	57,57,57,57	0
35	NA	0	8344	1/1	0.84	0.02	9,9,9,9	0
35	NA	0	8366	1/1	0.85	0.08	20,20,20,20	0
35	NA	0	8371	1/1	0.86	0.29	47,47,47,47	0
33	MG	9	8095	1/1	0.86	0.16	72,72,72,72	0
35	NA	0	8365	1/1	0.87	0.21	42,42,42,42	0
35	NA	0	8333	1/1	0.87	0.18	25,25,25,25	0
35	NA	Q	8386	1/1	0.88	0.23	62,62,62,62	0
35	NA	0	8331	1/1	0.88	0.38	69,69,69,69	0
35	NA	0	8302	1/1	0.88	0.10	18,18,18,18	0
38	PHA	4	77	11/11	0.88	0.15	64,67,71,71	0
35	NA	0	8340	1/1	0.88	0.16	48,48,48,48	0
34	K	0	8202	1/1	0.88	0.18	69,69,69,69	0
33	MG	0	8049	1/1	0.89	0.11	73,73,73,73	0
36	CL	0	8522	1/1	0.89	0.30	76,76,76,76	0
41	CD	Y	8403	1/1	0.89	0.22	200,200,200,200	0
35	NA	0	8372	1/1	0.89	0.23	73,73,73,73	0
35	NA	0	8332	1/1	0.90	0.14	57,57,57,57	0
33	MG	0	8092	1/1	0.90	0.10	71,71,71,71	0
33	MG	0	8055	1/1	0.90	0.09	82,82,82,82	0
35	NA	0	8360	1/1	0.91	0.15	39,39,39,39	0
33	MG	0	8024	1/1	0.91	0.35	109,109,109,109	0
33	MG	0	8094	1/1	0.91	0.12	54,54,54,54	0
33	MG	0	8101	1/1	0.91	0.10	40,40,40,40	0
36	CL	K	8510	1/1	0.91	0.10	70,70,70,70	0
33	MG	0	8102	1/1	0.91	0.61	135,135,135,135	0
33	MG	0	8070	1/1	0.91	0.21	71,71,71,71	0
40	BTN	4	79	15/16	0.91	0.17	91,104,104,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8334	1/1	0.91	0.17	29,29,29,29	0
33	MG	2	8078	1/1	0.91	0.18	73,73,73,73	0
33	MG	0	8076	1/1	0.91	0.06	70,70,70,70	0
36	CL	I	8502	1/1	0.92	0.06	56,56,56,56	0
35	NA	0	8324	1/1	0.92	0.20	39,39,39,39	0
33	MG	0	8050	1/1	0.92	0.06	78,78,78,78	0
35	NA	0	8355	1/1	0.92	0.24	60,60,60,60	0
35	NA	0	8357	1/1	0.92	0.14	53,53,53,53	0
35	NA	0	8373	1/1	0.92	0.09	51,51,51,51	0
35	NA	0	8381	1/1	0.92	0.12	71,71,71,71	0
35	NA	0	8310	1/1	0.92	0.09	16,16,16,16	0
35	NA	0	8307	1/1	0.93	0.09	40,40,40,40	0
35	NA	0	8374	1/1	0.93	0.16	49,49,49,49	0
33	MG	Y	8105	1/1	0.93	0.08	67,67,67,67	0
35	NA	0	8363	1/1	0.93	0.17	40,40,40,40	0
33	MG	0	8044	1/1	0.93	0.09	35,35,35,35	0
35	NA	0	8352	1/1	0.93	0.07	28,28,28,28	0
35	NA	0	8368	1/1	0.93	0.17	41,41,41,41	0
35	NA	0	8326	1/1	0.93	0.09	38,38,38,38	0
35	NA	H	8322	1/1	0.93	0.11	48,48,48,48	0
35	NA	0	8356	1/1	0.93	0.17	59,59,59,59	0
34	K	0	8201	1/1	0.94	0.26	80,80,80,80	0
35	NA	0	8311	1/1	0.94	0.08	38,38,38,38	0
36	CL	0	8515	1/1	0.94	0.15	72,72,72,72	0
35	NA	0	8377	1/1	0.94	0.14	59,59,59,59	0
35	NA	0	8354	1/1	0.94	0.12	29,29,29,29	0
33	MG	0	8053	1/1	0.94	0.09	38,38,38,38	0
33	MG	0	8066	1/1	0.94	0.09	60,60,60,60	0
37	PPU	4	76	37/38	0.94	0.10	48,55,62,63	0
35	NA	0	8369	1/1	0.94	0.25	67,67,67,67	0
39	ACA	4	78	8/9	0.94	0.16	67,73,85,88	0
35	NA	0	8370	1/1	0.94	0.21	48,48,48,48	0
33	MG	0	8114	1/1	0.94	0.30	161,161,161,161	0
35	NA	0	8358	1/1	0.94	0.20	98,98,98,98	0
35	NA	Q	8337	1/1	0.94	0.06	41,41,41,41	0
36	CL	A	8509	1/1	0.95	0.17	76,76,76,76	0
33	MG	0	8090	1/1	0.95	0.19	65,65,65,65	0
35	NA	0	8321	1/1	0.95	0.16	58,58,58,58	0
36	CL	M	8507	1/1	0.95	0.09	54,54,54,54	0
33	MG	0	8045	1/1	0.95	0.07	44,44,44,44	0
33	MG	0	8093	1/1	0.95	0.07	43,43,43,43	0
35	NA	0	8303	1/1	0.95	0.09	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8378	1/1	0.95	0.11	31,31,31,31	0
35	NA	0	8306	1/1	0.95	0.13	21,21,21,21	0
41	CD	N	8405	1/1	0.95	0.07	111,111,111,111	0
36	CL	0	8514	1/1	0.95	0.05	44,44,44,44	0
33	MG	0	8067	1/1	0.95	0.06	31,31,31,31	0
33	MG	0	8087	1/1	0.95	0.05	36,36,36,36	0
35	NA	0	8349	1/1	0.96	0.09	37,37,37,37	0
35	NA	0	8350	1/1	0.96	0.11	26,26,26,26	0
33	MG	0	8057	1/1	0.96	0.08	30,30,30,30	0
33	MG	0	8072	1/1	0.96	0.05	43,43,43,43	0
35	NA	0	8325	1/1	0.96	0.10	29,29,29,29	0
36	CL	B	8519	1/1	0.96	0.08	51,51,51,51	0
33	MG	0	8103	1/1	0.96	0.10	34,34,34,34	0
33	MG	0	8104	1/1	0.96	0.04	41,41,41,41	0
33	MG	0	8041	1/1	0.96	0.09	50,50,50,50	0
33	MG	0	8046	1/1	0.96	0.04	40,40,40,40	0
35	NA	0	8362	1/1	0.96	0.15	63,63,63,63	0
35	NA	0	8308	1/1	0.96	0.12	44,44,44,44	0
35	NA	0	8364	1/1	0.96	0.14	47,47,47,47	0
33	MG	0	8099	1/1	0.96	0.09	37,37,37,37	0
35	NA	C	8304	1/1	0.96	0.04	25,25,25,25	0
33	MG	0	8100	1/1	0.96	0.14	65,65,65,65	0
35	NA	0	8341	1/1	0.96	0.14	40,40,40,40	0
35	NA	0	8319	1/1	0.96	0.08	50,50,50,50	0
35	NA	0	8314	1/1	0.97	0.06	33,33,33,33	0
33	MG	0	8047	1/1	0.97	0.11	48,48,48,48	0
33	MG	0	8042	1/1	0.97	0.04	40,40,40,40	0
33	MG	0	8011	1/1	0.97	0.16	1,1,1,1	0
35	NA	0	8353	1/1	0.97	0.05	34,34,34,34	0
36	CL	0	8517	1/1	0.97	0.05	57,57,57,57	0
35	NA	0	8301	1/1	0.97	0.07	28,28,28,28	0
33	MG	0	8051	1/1	0.97	0.04	70,70,70,70	0
35	NA	0	8375	1/1	0.97	0.09	40,40,40,40	0
36	CL	I	8501	1/1	0.97	0.05	60,60,60,60	0
33	MG	0	8106	1/1	0.97	0.05	64,64,64,64	0
36	CL	I	8521	1/1	0.97	0.04	39,39,39,39	0
33	MG	0	8111	1/1	0.97	0.04	49,49,49,49	0
36	CL	L	8518	1/1	0.97	0.08	36,36,36,36	0
33	MG	0	8005	1/1	0.97	0.02	26,26,26,26	0
36	CL	N	8508	1/1	0.97	0.07	82,82,82,82	0
36	CL	X	8520	1/1	0.97	0.05	35,35,35,35	0
33	MG	0	8117	1/1	0.97	0.06	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8309	1/1	0.97	0.10	24,24,24,24	0
35	NA	0	8335	1/1	0.97	0.09	47,47,47,47	0
35	NA	0	8339	1/1	0.97	0.05	8,8,8,8	0
33	MG	0	8010	1/1	0.97	0.04	20,20,20,20	0
33	MG	0	8082	1/1	0.97	0.07	43,43,43,43	0
35	NA	0	8367	1/1	0.97	0.06	36,36,36,36	0
35	NA	I	8346	1/1	0.97	0.04	20,20,20,20	0
35	NA	P	8348	1/1	0.97	0.06	45,45,45,45	0
33	MG	0	8108	1/1	0.98	0.08	61,61,61,61	0
35	NA	0	8327	1/1	0.98	0.04	16,16,16,16	0
35	NA	0	8328	1/1	0.98	0.04	41,41,41,41	0
33	MG	0	8085	1/1	0.98	0.09	103,103,103,103	0
35	NA	0	8330	1/1	0.98	0.04	21,21,21,21	0
36	CL	0	8505	1/1	0.98	0.05	57,57,57,57	0
36	CL	0	8511	1/1	0.98	0.07	63,63,63,63	0
36	CL	0	8513	1/1	0.98	0.08	52,52,52,52	0
35	NA	0	8305	1/1	0.98	0.07	19,19,19,19	0
33	MG	0	8098	1/1	0.98	0.13	24,24,24,24	0
36	CL	0	8516	1/1	0.98	0.12	44,44,44,44	0
33	MG	0	8115	1/1	0.98	0.03	58,58,58,58	0
33	MG	0	8116	1/1	0.98	0.05	64,64,64,64	0
33	MG	0	8086	1/1	0.98	0.04	41,41,41,41	0
35	NA	0	8336	1/1	0.98	0.03	30,30,30,30	0
33	MG	0	8043	1/1	0.98	0.03	34,34,34,34	0
33	MG	S	8073	1/1	0.98	0.03	36,36,36,36	0
35	NA	0	8313	1/1	0.98	0.05	59,59,59,59	0
33	MG	0	8088	1/1	0.98	0.07	23,23,23,23	0
35	NA	0	8376	1/1	0.98	0.11	50,50,50,50	0
35	NA	0	8315	1/1	0.98	0.10	32,32,32,32	0
35	NA	0	8316	1/1	0.98	0.06	28,28,28,28	0
36	CL	Q	8506	1/1	0.98	0.04	43,43,43,43	0
35	NA	0	8379	1/1	0.98	0.05	25,25,25,25	0
35	NA	0	8317	1/1	0.98	0.03	23,23,23,23	0
35	NA	0	8318	1/1	0.98	0.04	22,22,22,22	0
33	MG	0	8075	1/1	0.98	0.06	50,50,50,50	0
35	NA	0	8320	1/1	0.98	0.04	15,15,15,15	0
33	MG	0	8091	1/1	0.98	0.04	40,40,40,40	0
33	MG	0	8059	1/1	0.98	0.04	59,59,59,59	0
35	NA	A	8345	1/1	0.98	0.04	40,40,40,40	0
33	MG	0	8064	1/1	0.98	0.09	17,17,17,17	0
35	NA	0	8359	1/1	0.98	0.10	42,42,42,42	0
33	MG	0	8012	1/1	0.99	0.02	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8083	1/1	0.99	0.07	38,38,38,38	0
36	CL	0	8503	1/1	0.99	0.04	49,49,49,49	0
33	MG	0	8084	1/1	0.99	0.09	38,38,38,38	0
33	MG	0	8056	1/1	0.99	0.04	35,35,35,35	0
36	CL	0	8512	1/1	0.99	0.04	34,34,34,34	0
33	MG	0	8014	1/1	0.99	0.05	22,22,22,22	0
33	MG	0	8110	1/1	0.99	0.07	22,22,22,22	0
33	MG	0	8008	1/1	0.99	0.04	42,42,42,42	0
33	MG	0	8112	1/1	0.99	0.06	34,34,34,34	0
33	MG	0	8113	1/1	0.99	0.04	36,36,36,36	0
35	NA	0	8342	1/1	0.99	0.04	19,19,19,19	0
35	NA	0	8343	1/1	0.99	0.03	17,17,17,17	0
33	MG	0	8060	1/1	0.99	0.05	32,32,32,32	0
33	MG	0	8089	1/1	0.99	0.05	50,50,50,50	0
33	MG	0	8063	1/1	0.99	0.04	68,68,68,68	0
33	MG	0	8025	1/1	0.99	0.03	17,17,17,17	0
33	MG	0	8027	1/1	0.99	0.04	37,37,37,37	0
33	MG	A	8065	1/1	0.99	0.05	44,44,44,44	0
33	MG	0	8036	1/1	0.99	0.03	32,32,32,32	0
35	NA	0	8323	1/1	0.99	0.09	34,34,34,34	0
33	MG	0	8040	1/1	0.99	0.07	107,107,107,107	0
33	MG	0	8096	1/1	0.99	0.06	33,33,33,33	0
33	MG	0	8097	1/1	0.99	0.06	30,30,30,30	0
33	MG	0	8003	1/1	0.99	0.03	22,22,22,22	0
35	NA	0	8361	1/1	0.99	0.06	40,40,40,40	0
33	MG	0	8052	1/1	0.99	0.04	36,36,36,36	0
35	NA	K	8380	1/1	0.99	0.07	69,69,69,69	0
35	NA	L	8347	1/1	0.99	0.03	7,7,7,7	0
33	MG	0	8006	1/1	0.99	0.03	28,28,28,28	0
33	MG	0	8081	1/1	0.99	0.03	36,36,36,36	0
35	NA	Q	8338	1/1	0.99	0.03	57,57,57,57	0
33	MG	J	8069	1/1	1.00	0.02	47,47,47,47	0
33	MG	0	8077	1/1	1.00	0.01	21,21,21,21	0
33	MG	X	8109	1/1	1.00	0.04	35,35,35,35	0
33	MG	0	8079	1/1	1.00	0.03	27,27,27,27	0
33	MG	0	8080	1/1	1.00	0.01	42,42,42,42	0
33	MG	0	8039	1/1	1.00	0.04	31,31,31,31	0
33	MG	0	8013	1/1	1.00	0.02	25,25,25,25	0
33	MG	0	8004	1/1	1.00	0.04	30,30,30,30	0
33	MG	0	8015	1/1	1.00	0.02	29,29,29,29	0
33	MG	0	8016	1/1	1.00	0.02	25,25,25,25	0
33	MG	0	8017	1/1	1.00	0.05	15,15,15,15	0

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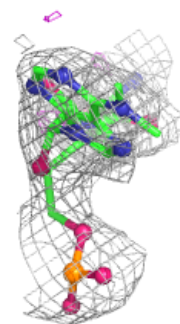
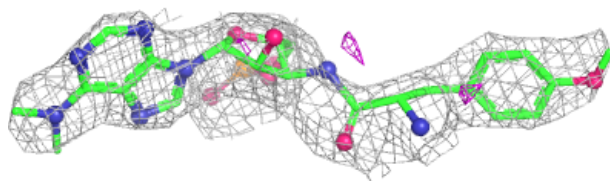
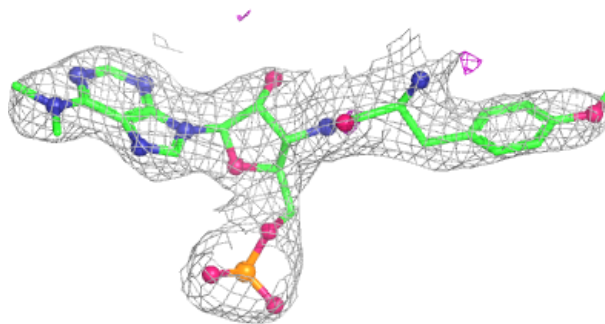
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8018	1/1	1.00	0.02	32,32,32,32	0
33	MG	0	8019	1/1	1.00	0.04	13,13,13,13	0
33	MG	0	8020	1/1	1.00	0.02	16,16,16,16	0
33	MG	0	8048	1/1	1.00	0.02	34,34,34,34	0
33	MG	0	8021	1/1	1.00	0.02	26,26,26,26	0
33	MG	0	8022	1/1	1.00	0.02	30,30,30,30	0
33	MG	0	8023	1/1	1.00	0.03	28,28,28,28	0
33	MG	0	8009	1/1	1.00	0.05	18,18,18,18	0
33	MG	0	8002	1/1	1.00	0.04	33,33,33,33	0
33	MG	0	8054	1/1	1.00	0.02	28,28,28,28	0
33	MG	0	8026	1/1	1.00	0.02	25,25,25,25	0
33	MG	0	8001	1/1	1.00	0.02	21,21,21,21	0
33	MG	0	8028	1/1	1.00	0.04	23,23,23,23	0
33	MG	0	8058	1/1	1.00	0.05	28,28,28,28	0
33	MG	0	8029	1/1	1.00	0.04	23,23,23,23	0
33	MG	0	8030	1/1	1.00	0.02	29,29,29,29	0
33	MG	0	8061	1/1	1.00	0.02	28,28,28,28	0
33	MG	0	8062	1/1	1.00	0.02	37,37,37,37	0
33	MG	0	8107	1/1	1.00	0.01	24,24,24,24	0
33	MG	0	8031	1/1	1.00	0.04	18,18,18,18	0
33	MG	0	8032	1/1	1.00	0.05	29,29,29,29	0
33	MG	0	8033	1/1	1.00	0.01	18,18,18,18	0
33	MG	0	8034	1/1	1.00	0.03	22,22,22,22	0
33	MG	0	8068	1/1	1.00	0.04	58,58,58,58	0
33	MG	0	8035	1/1	1.00	0.04	39,39,39,39	0
33	MG	0	8071	1/1	1.00	0.04	66,66,66,66	0
33	MG	0	8007	1/1	1.00	0.05	18,18,18,18	0
33	MG	0	8074	1/1	1.00	0.03	27,27,27,27	0
33	MG	0	8037	1/1	1.00	0.02	34,34,34,34	0
41	CD	Z	8402	1/1	1.00	0.04	49,49,49,49	0
33	MG	0	8038	1/1	1.00	0.03	23,23,23,23	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PPU 4 76:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.