Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2023 – 07:50 PM EDT

PDB ID	:	1VQ8
Title	:	The structure of CCDA-PHE-CAP-BIO and the antibiotic sparsomycin bound to the large ribosomal subunit of haloarcula marismortui
Authors	:	Schmeing, T.M.; Steitz, T.A.
Deposited on	:	2004-12-16
Resolution	:	2.20 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:

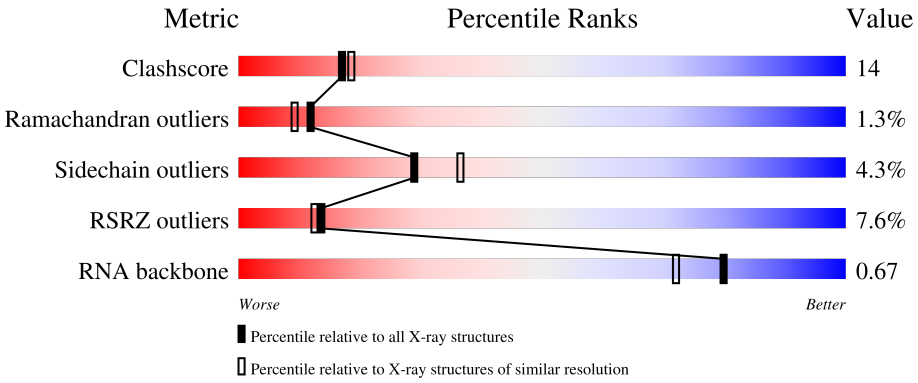
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)
RNA backbone	3102	1032 (2.60-1.80)

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 <=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	3% 65% 24% 5% 6%
2	9	122	5% 53% 37% 8% •
3	4	5	20% 80% 20%
4	A	240	6% 58% 35% 5% •
5	B	338	3% 58% 38% •

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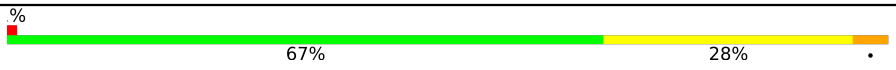
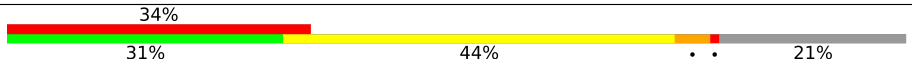
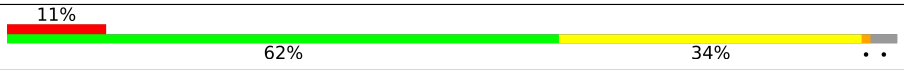
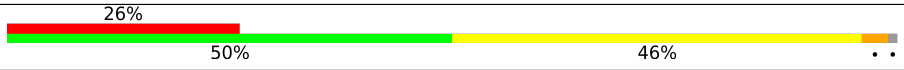
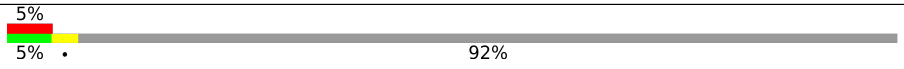
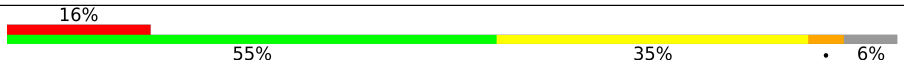
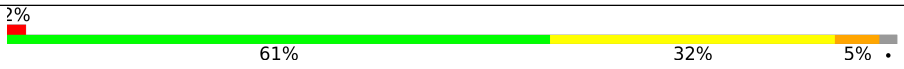
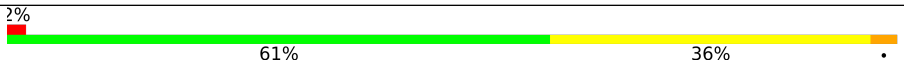
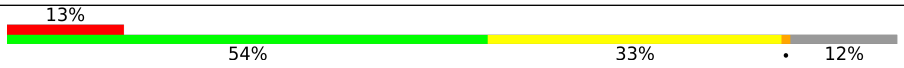
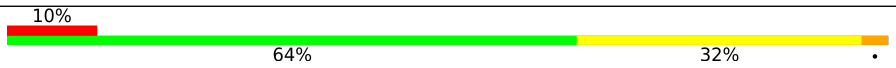
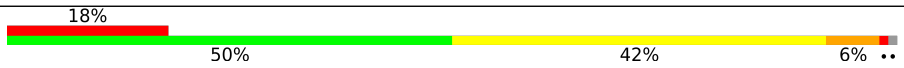
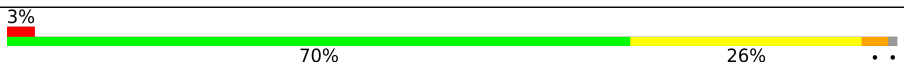
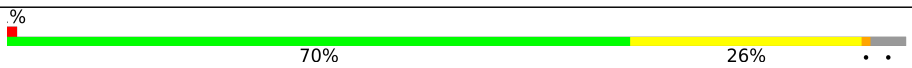
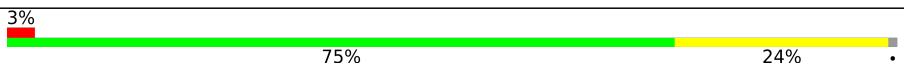
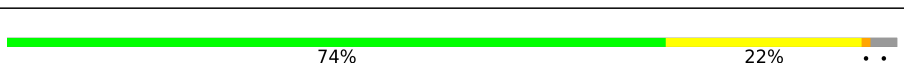
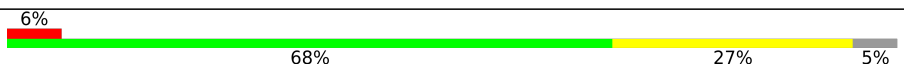
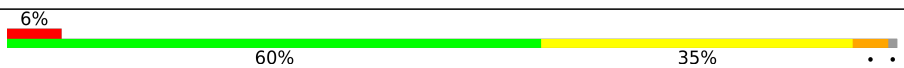
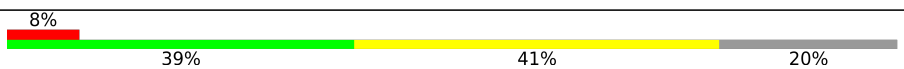
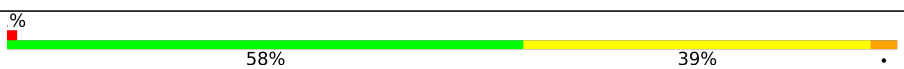
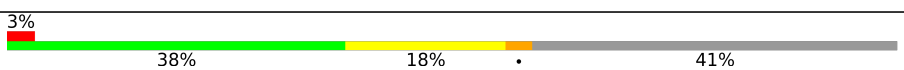
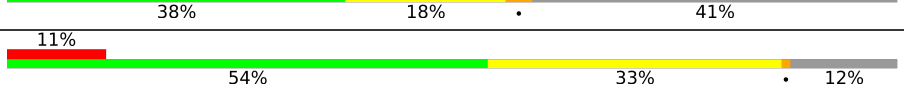
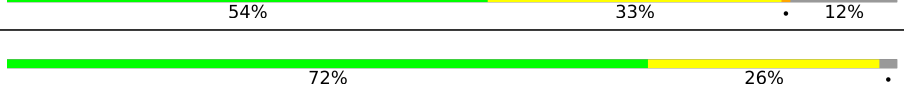
Mol	Chain	Length	Quality of chain
6	C	246	
7	D	177	
8	E	178	
9	F	120	
10	G	348	
11	H	171	
12	J	145	
13	K	132	
14	L	165	
15	M	194	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	
30	2	50	

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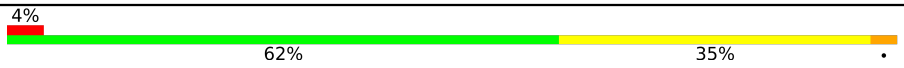
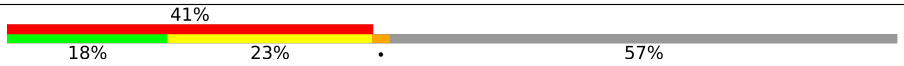
Mol	Chain	Length	Quality of chain
31	3	92	
32	I	162	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	MG	0	8065	-	-	-	X
33	MG	0	8092	-	-	-	X
33	MG	0	8094	-	-	-	X
35	NA	0	9122	-	-	-	X
35	NA	0	9172	-	-	-	X
35	NA	0	9185	-	-	-	X
35	NA	S	9112	-	-	-	X
37	SR	B	9521	-	-	-	X
39	CD	O	9205	-	-	-	X

2 Entry composition (i)

There are 40 unique types of molecules in this entry. The entry contains 99035 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 ribosomal rna.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	0	2754	59021	26350	10878	19048	2745	0	0	0

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

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

- Molecule 3 is a RNA chain called 5'-R(*CP*CP*(DA)*(PHE)*(ACA))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	4	5	73	40	12	19	2	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	A	237	1753	1072	352	324	5	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	B	337	2625	1616	493	511	5	0	0	0

- Molecule 6 is a protein called 50S ribosomal protein L4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	C	246	1859	1131	344	383	1	0	0	0

- Molecule 7 is a protein called 50S ribosomal protein L5P.

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

- Molecule 8 is a protein called 50S ribosomal protein L6P.

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

- Molecule 9 is a protein called 50S ribosomal protein L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 10 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	160	Total	C	N	O	S	0	0	0
			1266	785	237	238	6			

- Molecule 12 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 13 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	conflict	UNP P22450

- Molecule 14 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	L	145	Total	C	N	O	0	0	0
			1118	670	222	226			

- Molecule 15 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1560	943	332	284	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	GB 55231501
M	194	ALA	GLY	conflict	GB 55231501

- Molecule 16 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 17 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	O	115	Total	C	N	O	0	0	0
			865	529	161	175			

- Molecule 18 is a protein called 50S ribosomal protein L19E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	P	143	Total	C	N	O	0	0	0
			1136	683	229	224			

- Molecule 19 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	Q	95	Total	C	N	O	0	0	0
			735	450	141	144			

- Molecule 20 is a protein called 50S ribosomal protein L22P.

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

- Molecule 21 is a protein called 50S ribosomal protein L23P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	T	119	Total	C	N	O	0	0	0
			950	568	180	202			

- Molecule 23 is a protein called 50S ribosomal protein L24E.

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

- Molecule 24 is a protein called 50S ribosomal protein L29P.

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

- Molecule 25 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 26 is a protein called 50S ribosomal protein L31e.

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

- Molecule 27 is a protein called 50S ribosomal protein L32E.

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

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	73	Total	C	N	O	S	0	0	0
			578	346	116	111	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	conflict	GB 55231162

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	88	Total	Mg	0	0
			88	88		
33	9	1	Total	Mg	0	0
			1	1		
33	4	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	65	Total	Na	0	0
			65	65		
35	9	1	Total	Na	0	0
			1	1		
35	B	1	Total	Na	0	0
			1	1		
35	C	1	Total	Na	0	0
			1	1		
35	D	1	Total	Na	0	0
			1	1		
35	J	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	M	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	R	2	Total Na 2 2	0	0
35	S	1	Total Na 1 1	0	0

- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	10	Total Cl 10 10	0	0
36	A	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0
36	J	3	Total Cl 3 3	0	0
36	L	1	Total Cl 1 1	0	0
36	M	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0
36	O	1	Total Cl 1 1	0	0
36	R	1	Total Cl 1 1	0	0
36	Y	1	Total Cl 1 1	0	0
36	3	1	Total Cl 1 1	0	0

- Molecule 37 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	98	Total Sr 98 98	0	0
37	9	3	Total Sr 3 3	0	0

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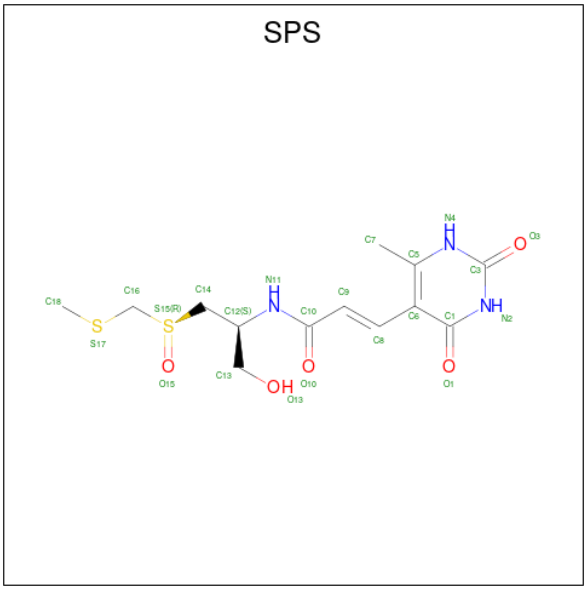
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	A	3	Total Sr 3 3	0	0
37	B	2	Total Sr 2 2	0	0
37	F	1	Total Sr 1 1	0	0
37	H	1	Total Sr 1 1	0	0
37	L	1	Total Sr 1 1	0	0
37	R	1	Total Sr 1 1	0	0
37	S	1	Total Sr 1 1	0	0
37	1	2	Total Sr 2 2	0	0
37	3	1	Total Sr 1 1	0	0

- Molecule 38 is SPARSOMYCIN (three-letter code: SPS) (formula: $C_{13}H_{19}N_3O_5S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	4	1	Total C N O S 23 13 3 5 2	0	0

- Molecule 39 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	O	1	Total Cd 1 1	0	0
39	U	1	Total Cd 1 1	0	0
39	Z	1	Total Cd 1 1	0	0
39	1	1	Total Cd 1 1	0	0
39	3	1	Total Cd 1 1	0	0

- Molecule 40 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	0	5743	Total O 5743 5743	0	0
40	9	136	Total O 136 136	0	0
40	4	2	Total O 2 2	0	0
40	A	120	Total O 120 120	0	0
40	B	135	Total O 135 135	0	0
40	C	172	Total O 172 172	0	0
40	D	48	Total O 48 48	0	0
40	E	42	Total O 42 42	0	0
40	F	27	Total O 27 27	0	0
40	G	16	Total O 16 16	0	0
40	H	71	Total O 71 71	0	0
40	J	51	Total O 51 51	0	0
40	K	58	Total O 58 58	0	0
40	L	87	Total O 87 87	0	0
40	M	127	Total O 127 127	0	0

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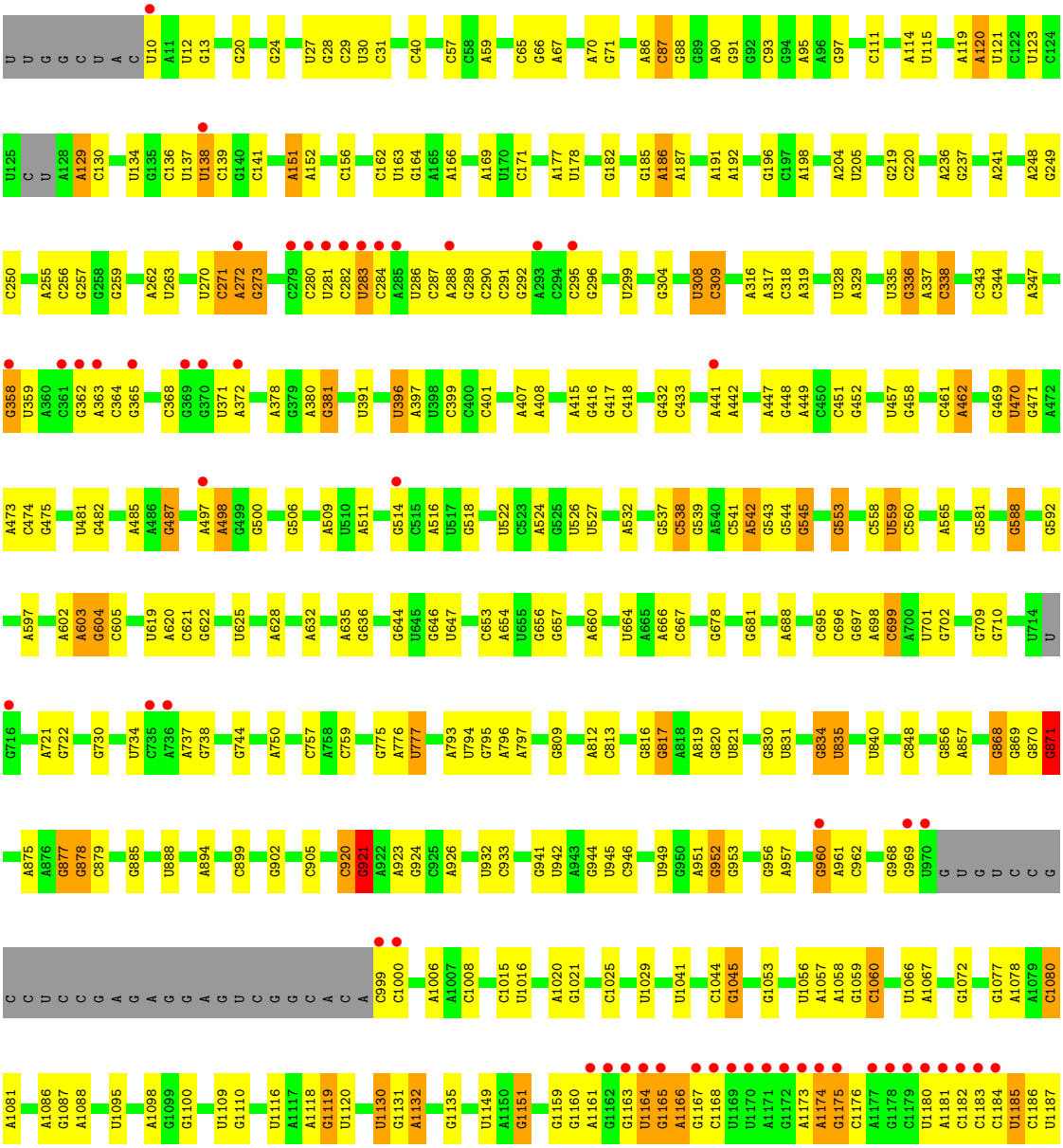
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	N	59	Total O 59 59	0	0
40	O	41	Total O 41 41	0	0
40	P	64	Total O 64 64	0	0
40	Q	58	Total O 58 58	0	0
40	R	85	Total O 85 85	0	0
40	S	30	Total O 30 30	0	0
40	T	36	Total O 36 36	0	0
40	U	28	Total O 28 28	0	0
40	V	15	Total O 15 15	0	0
40	W	68	Total O 68 68	0	0
40	X	23	Total O 23 23	0	0
40	Y	95	Total O 95 95	0	0
40	Z	35	Total O 35 35	0	0
40	1	50	Total O 50 50	0	0
40	2	35	Total O 35 35	0	0
40	3	76	Total O 76 76	0	0
40	I	10	Total O 10 10	0	0

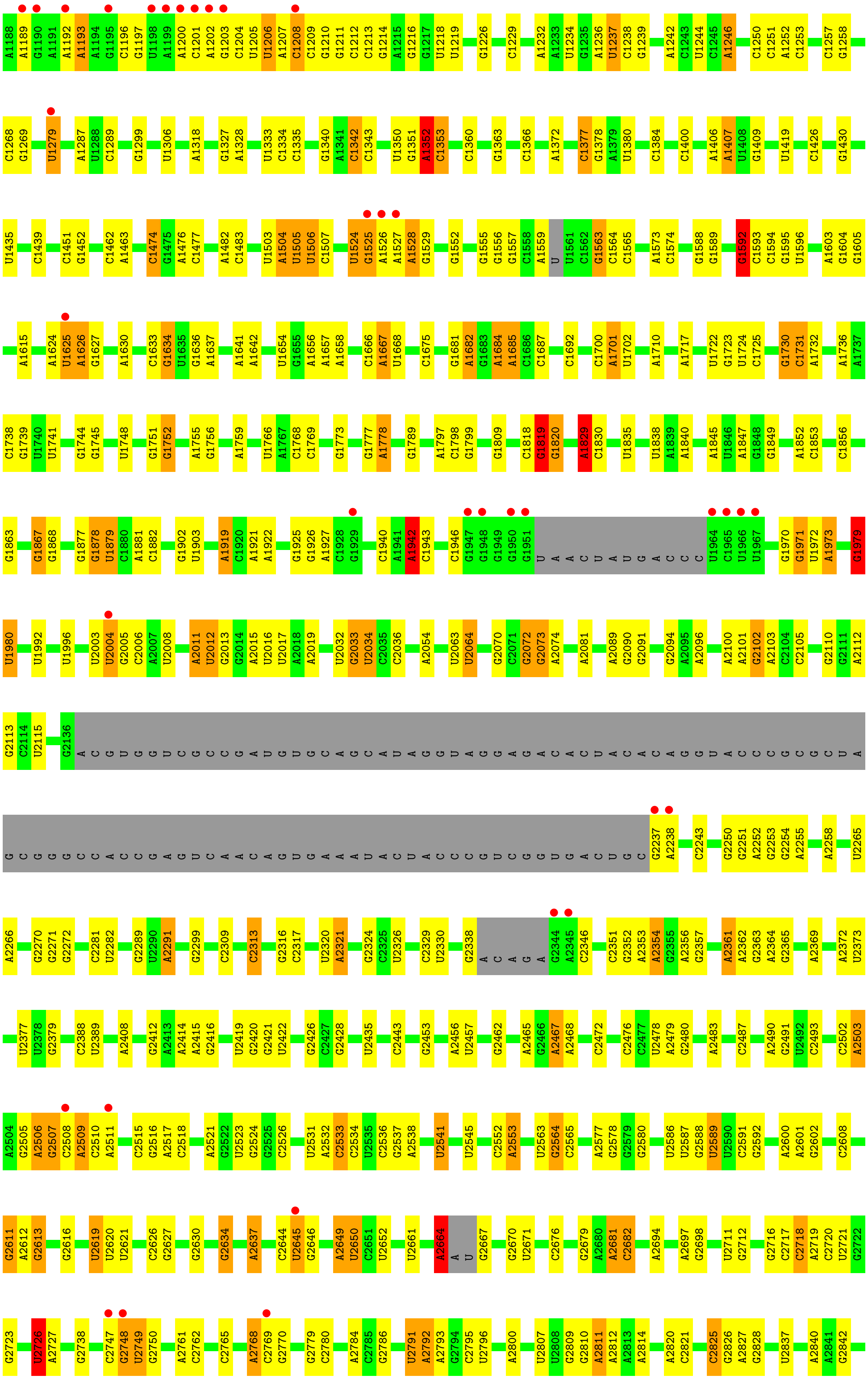
3 Residue-property plots (i)

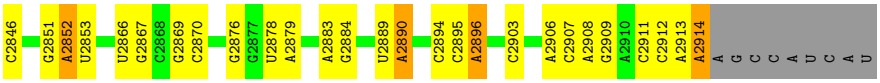
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 ribosomal rna

Chain 0:

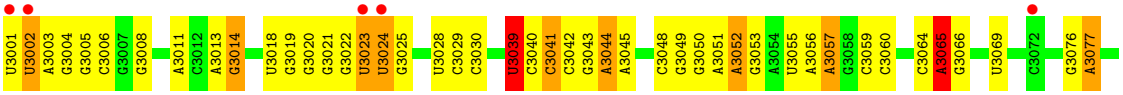


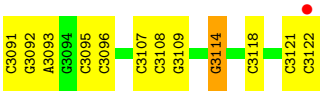

A1188 A1189 G1190 A1191 A1192 A1193 A1194 G1195 C1196 G1197 U1198 A1199 A1200 C1201 A1202 G1203 C1204 U1205 U1206 A1207 C1208 C1209 G1210 G1211 C1212 C1213 G1214 A1215 G1216 G1217 U1218 U1219 G1226 C1229 A1232 A1233 U1234 G1235 A1236 U1237 C1238 G1239 A1242 C1243 U1244 C1245 A1246 C1250 C1251 A1252 C1253 C1257 G1258
C1268 G1269 U1279 A1287 U1288 C1289 G1299 U1306 A1318 G1327 A1328 U1333 C1334 C1335 G1340 A1341 C1342 C1343 U1350 G1351 A1352 C1353 C1360 G1363 C1366 A1372 C1377 G1378 A1379 U1380 C1384 C1400 A1406 A1407 U1408 G1409 U1419 C1426 G1430
U1435 C1439 C1451 G1452 C1462 A1463 C1474 G1475 A1476 C1477 A1482 C1483 U1503 A1504 U1505 U1506 C1507 U1524 G1525 A1526 A1527 A1528 G1529 G1552 G1555 G1556 G1557 C1558 A1559 U U1561 C1562 G1563 C1564 C1565 A1573 C1574 G1588 G1589 G1592 C1593 C1594 G1595 U1596 A1603 G1604 G1605
A1615 A1624 U1625 A1626 G1627 A1630 C1633 G1634 U1635 G1636 A1637 A1641 A1642 U1654 G1655 A1656 A1657 A1658 C1666 A1667 U1668 C1675 G1681 A1682 G1683 A1684 A1685 C1686 C1687 C1692 C1700 A1701 U1702 A1710 A1717 U1722 G1723 U1724 C1725 G1730 C1731 A1732 A1736 A1737
C1738 G1739 U1740 U1741 G1744 G1745 U1748 G1751 G1752 A1755 G1756 A1759 U1766 A1767 C1768 C1769 G1773 G1777 A1778 G1789 A1797 C1798 G1799 G1809 C1818 G1819 G1820 A1829 C1830 U1835 U1838 A1839 A1840 A1845 U1846 A1847 G1848 G1849 A1852 C1853 C1856
G1863 G1867 G1868 G1877 G1878 U1879 C1880 A1881 C1882 G1902 U1903 A1919 C1920 A1921 A1922 G1925 G1926 A1927 C1928 G1929 C1940 A1941 A1942 C1943 C1946 G1947 G1948 G1949 G1950 G1951 U A A C U A U G A C C C U1964 C1965 U1966 U1967 G1970 G1971 U1972 A1973 G1979
U1980 U1992 U1996 U2003 U2004 G2005 C2006 A2007 U2008 A2011 U2012 G2013 G2014 A2015 U2016 U2017 A2018 A2019 U2032 G2033 U2034 C2035 C2036 A2054 U2063 U2064 G2070 C2071 G2072 G2073 A2074 A2081 A2089 G2090 G2091 G2094 A2095 A2096 A2100 A2101 G2102 A2103 C2104 C2105 G2110 G2111 A2112
G2113 C2114 U2115 G2136 A C G U G G U C G C C G A U G U G C A G C A U A G G U A G G A G A C A C U A C A C A G G U A C C C G C G C U A
G C G G G C C A C C G A G U C A A C A G U G A A A U A C U A C C C G U C G G U G A C U G C G2237 A2238 C2243 G2250 G2251 A2252 G2253 G2254 A2255 A2258 U2265
A2266 G2270 G2271 G2272 C2281 U2282 G2289 U2290 A2291 G2299 C2309 C2313 G2316 C2317 U2320 A2321 G2324 C2325 U2326 C2329 U2330 G2338 A C A G A G2344 A2345 C2346 C2351 G2352 A2353 A2354 G2355 A2356 G2357 A2361 A2362 G2363 A2364 G2365 A2369 A2372 U2373
U2377 U2378 G2379 C2388 U2389 A2408 G2412 A2413 A2414 A2415 G2416 U2419 G2420 G2421 U2422 G2426 C2427 G2428 U2435 C2443 G2453 A2456 U2457 G2462 A2465 G2466 A2467 A2468 C2472 C2476 C2477 U2478 A2479 G2480 A2483 C2487 A2490 G2491 U2492 C2493 C2502 A2503
A2504 G2505 A2506 G2507 C2508 A2509 C2510 A2511 C2515 G2516 A2517 C2518 A2521 G2522 U2523 G2524 G2525 C2526 U2531 A2532 C2533 C2534 U2535 C2536 G2537 A2538 U2541 U2545 C2552 A2553 U2563 G2564 C2565 A2577 G2578 G2579 G2580 U2586 U2587 G2588 U2589 U2590 C2591 G2592 A2600 A2601 G2602 C2608
G2611 A2612 G2613 G2616 U2619 U2620 U2621 C2626 C2627 G2630 G2634 A2637 C2644 U2645 G2646 A2649 U2650 C2651 U2652 U2661 A2664 A U G2667 G2670 U2671 C2676 G2679 A2680 A2681 C2682 A2694 A2697 G2698 U2711 G2712 G2716 C2717 C2718 A2719 C2720 U2721 G2722
G2723 U2726 A2727 G2738 C2747 G2748 U2749 G2750 A2761 C2762 C2765 A2768 C2769 G2770 G2779 C2780 A2784 C2785 G2786 U2791 A2792 A2793 G2794 C2795 U2796 A2800 U2807 U2808 G2809 A2810 A2811 A2812 A2813 A2814 A2820 C2821 C2825 G2826 A2827 G2828 U2837 A2840 A2841 G2842



• Molecule 2: 5S ribosomal RNA

Chain 9:



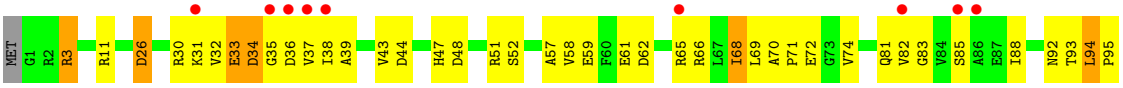


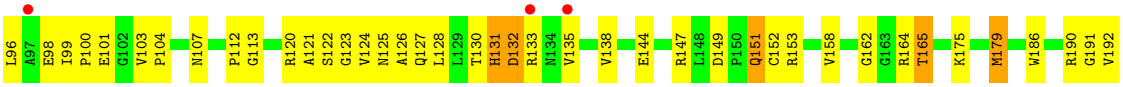
• Molecule 3: 5'-R(*CP*CP*(DA)*(PHE)*(ACA))-3'

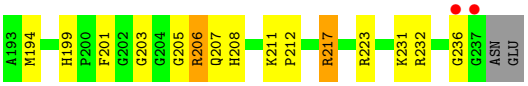
Chain 4:

• Molecule 4: 50S ribosomal protein L2P

Chain A:

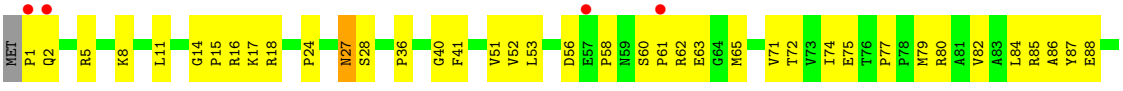


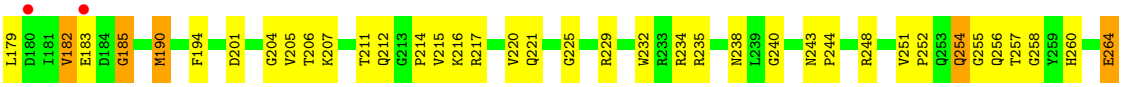


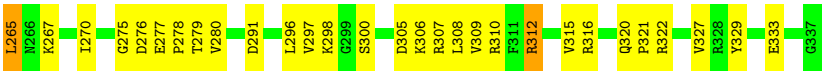


• Molecule 5: 50S ribosomal protein L3P

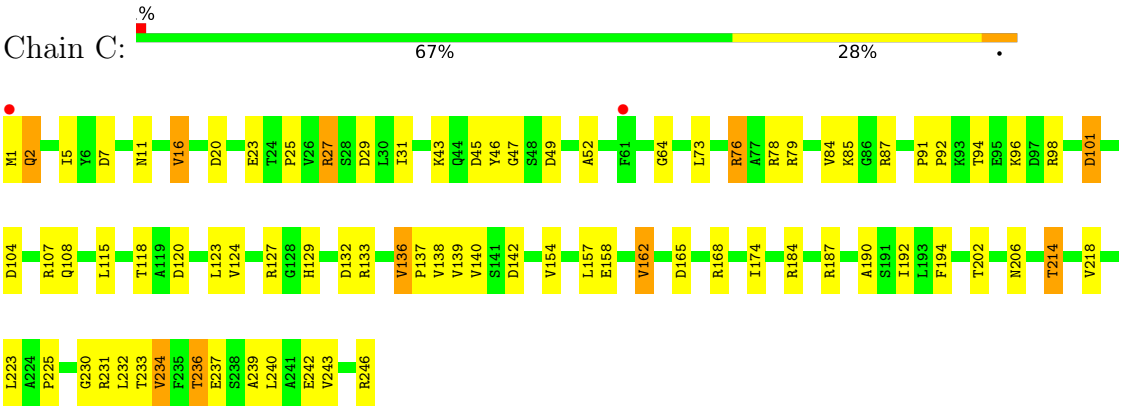
Chain B:



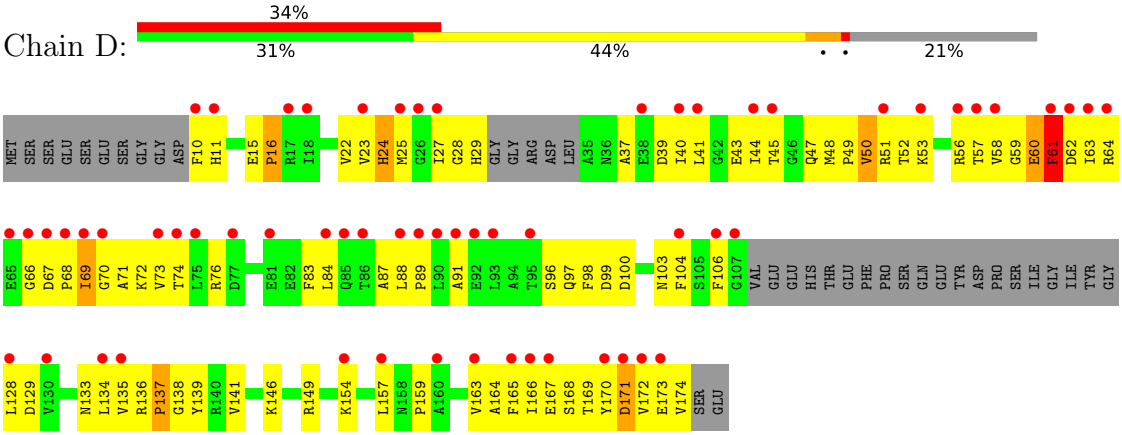




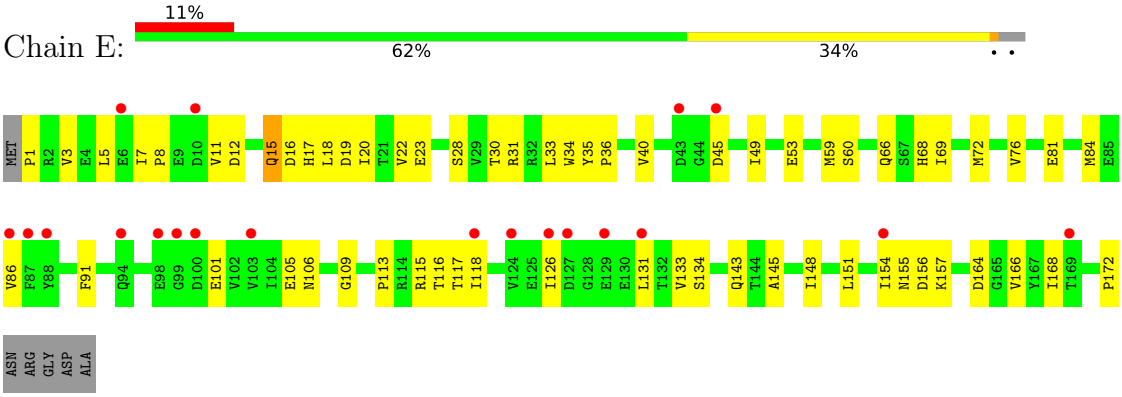
• Molecule 6: 50S ribosomal protein L4E



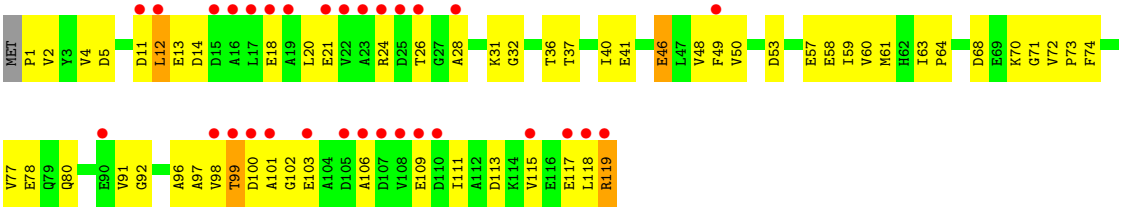
• Molecule 7: 50S ribosomal protein L5P



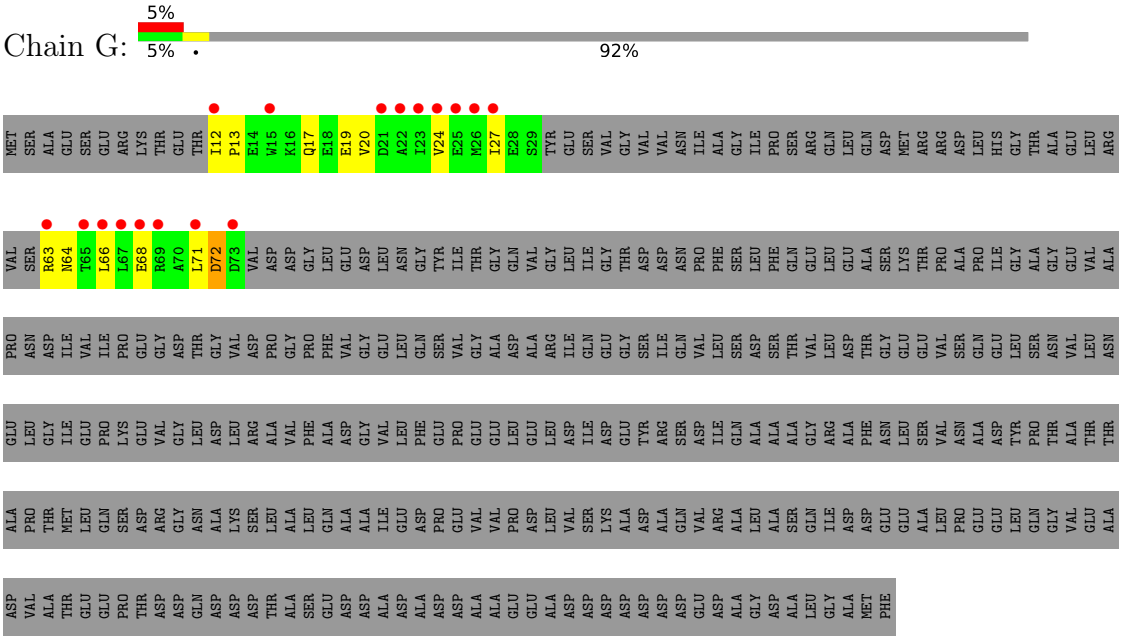
• Molecule 8: 50S ribosomal protein L6P



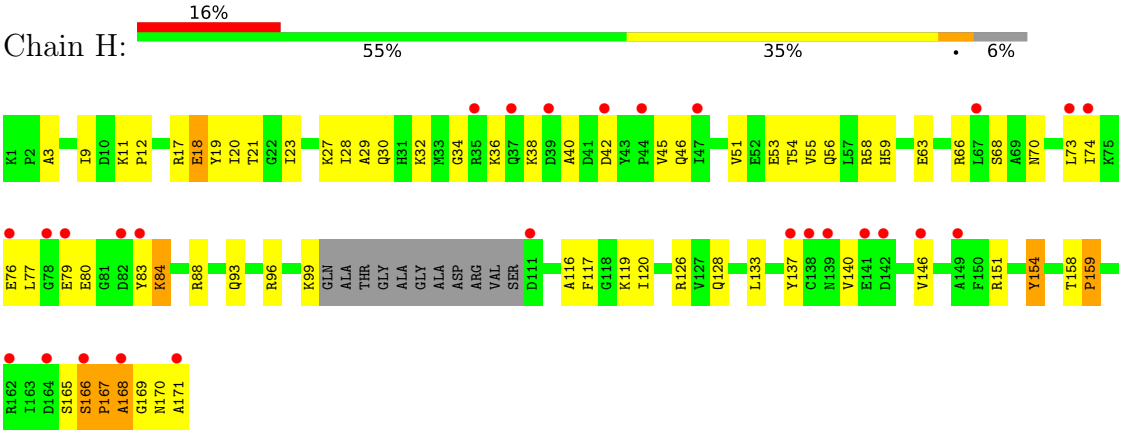
• Molecule 9: 50S ribosomal protein L7AE



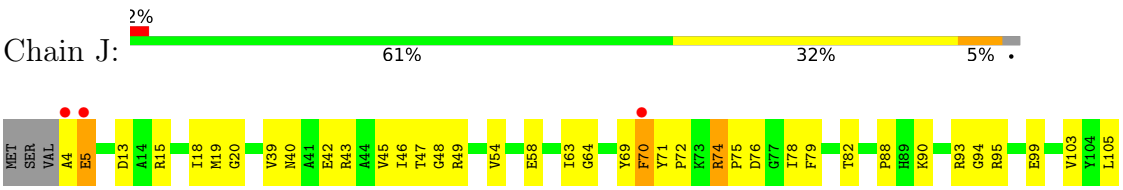
• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



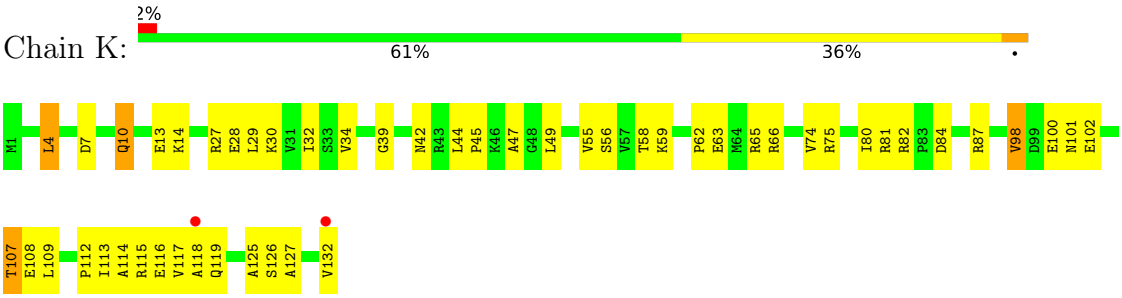
• Molecule 11: 50S RIBOSOMAL PROTEIN L10E



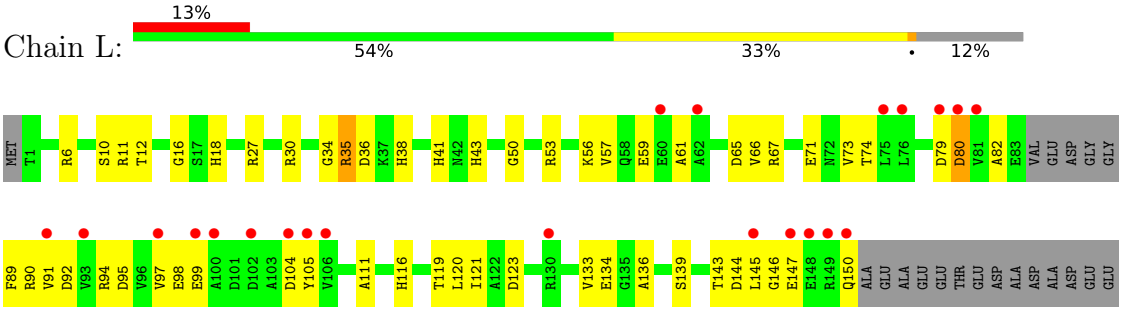
• Molecule 12: 50S ribosomal protein L13P



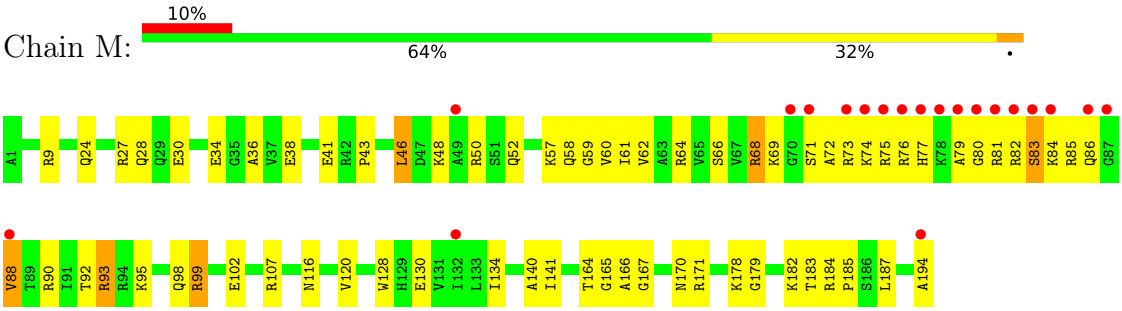
• Molecule 13: 50S ribosomal protein L14P



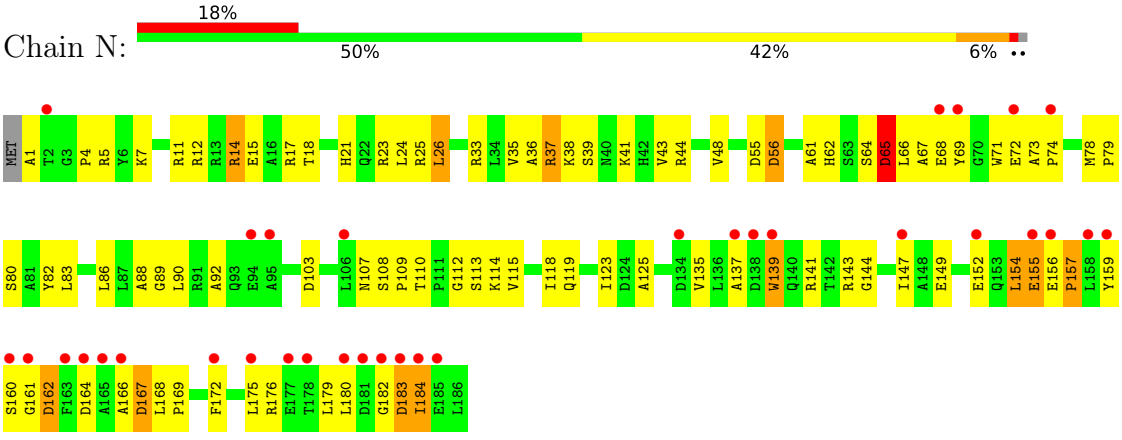
• Molecule 14: 50S ribosomal protein L15P



• Molecule 15: 50S Ribosomal Protein L15E

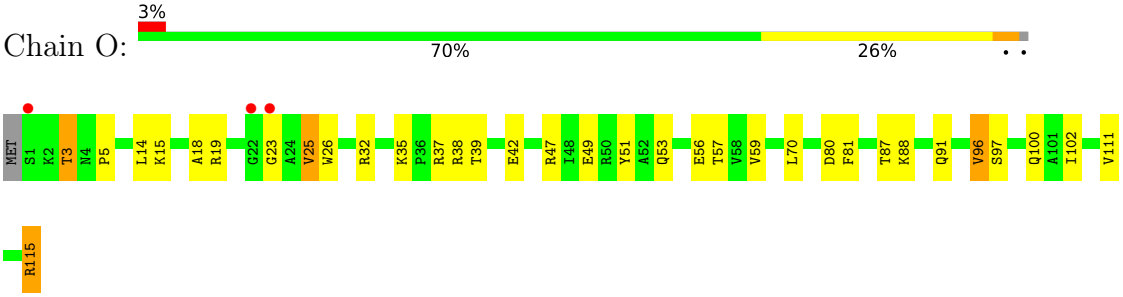


• Molecule 16: 50S ribosomal protein L18P



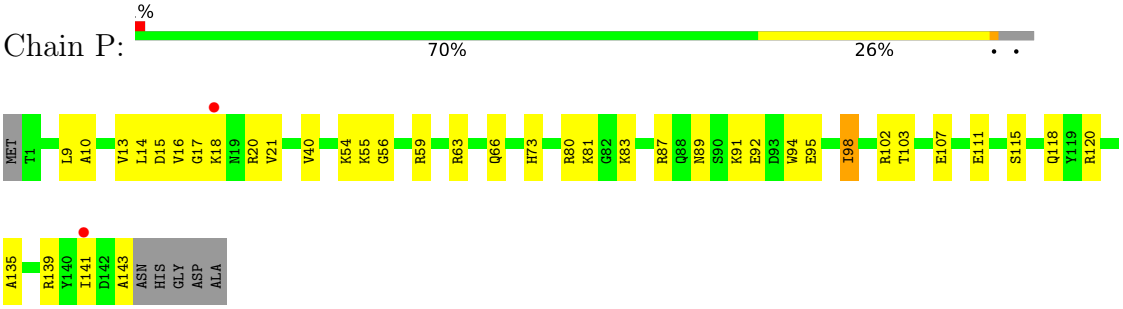
• Molecule 17: 50S ribosomal protein L18e

Chain O:



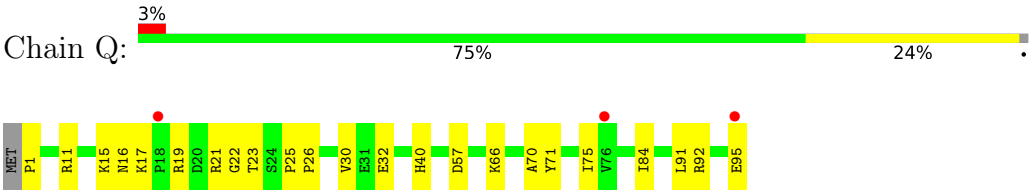
• Molecule 18: 50S ribosomal protein L19E

Chain P:



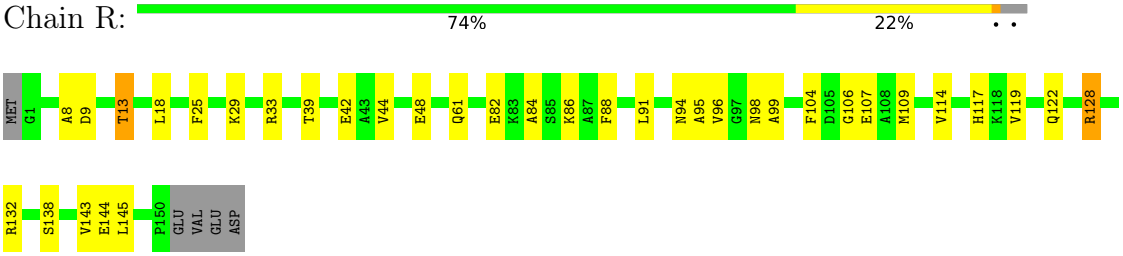
• Molecule 19: 50S ribosomal protein L21e

Chain Q:



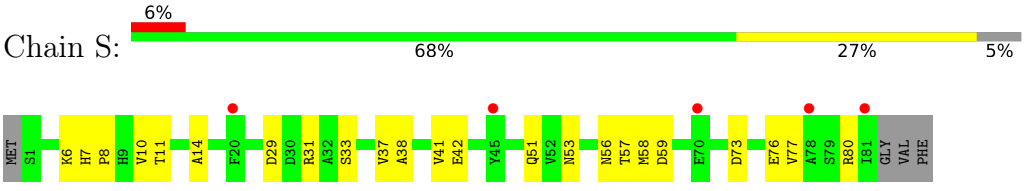
• Molecule 20: 50S ribosomal protein L22P

Chain R:



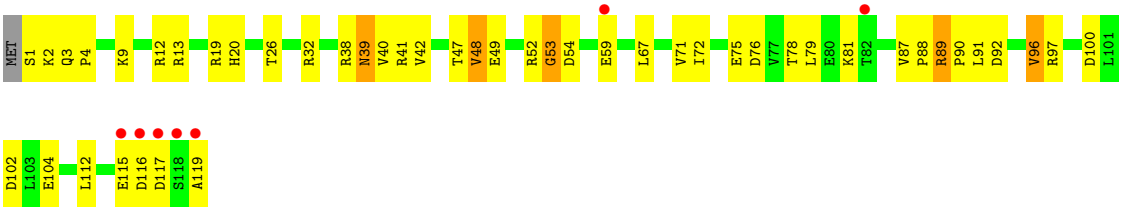
• Molecule 21: 50S ribosomal protein L23P

Chain S:

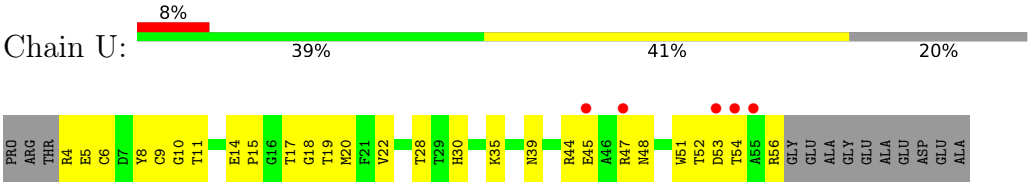


• Molecule 22: 50S ribosomal protein L24P

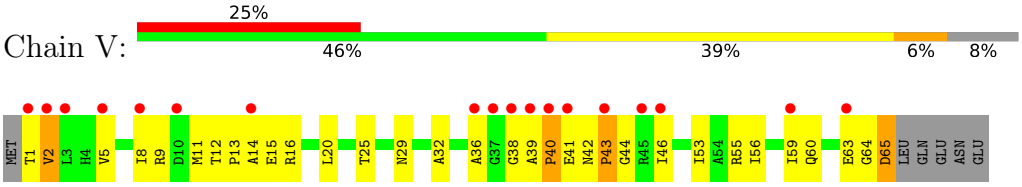
Chain T:



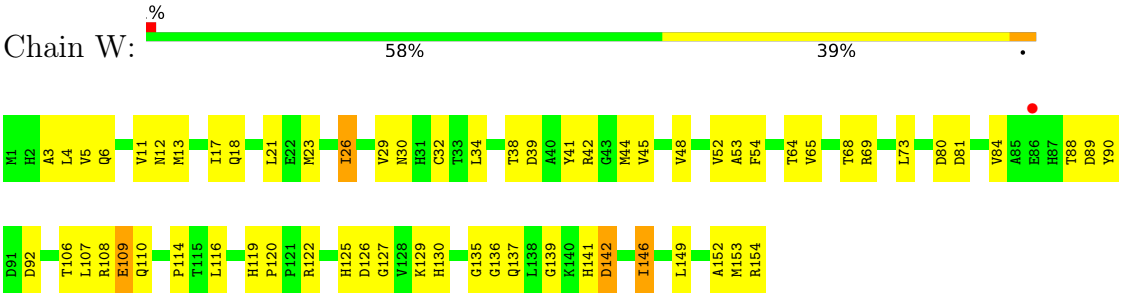
• Molecule 23: 50S ribosomal protein L24E



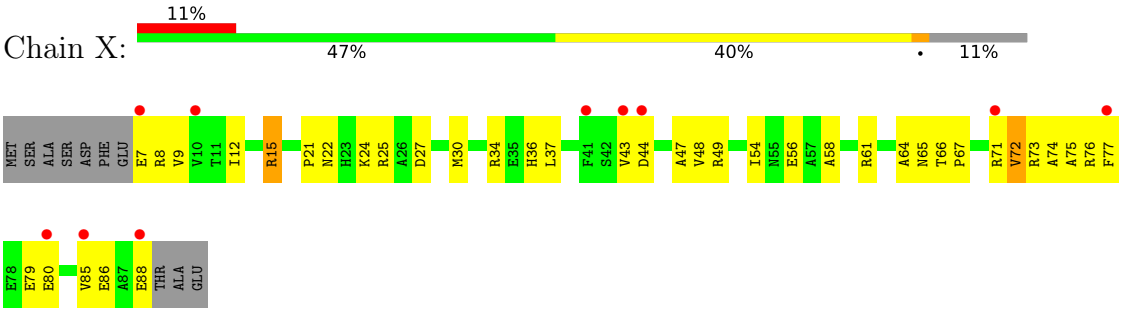
• Molecule 24: 50S ribosomal protein L29P



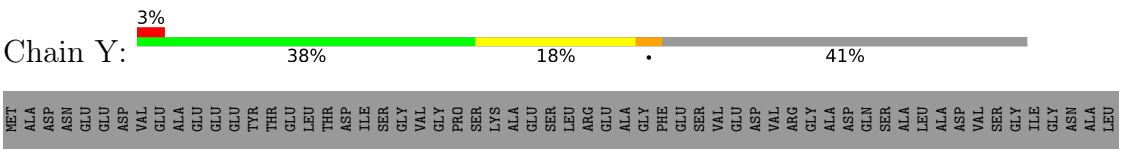
• Molecule 25: 50S ribosomal protein L30P

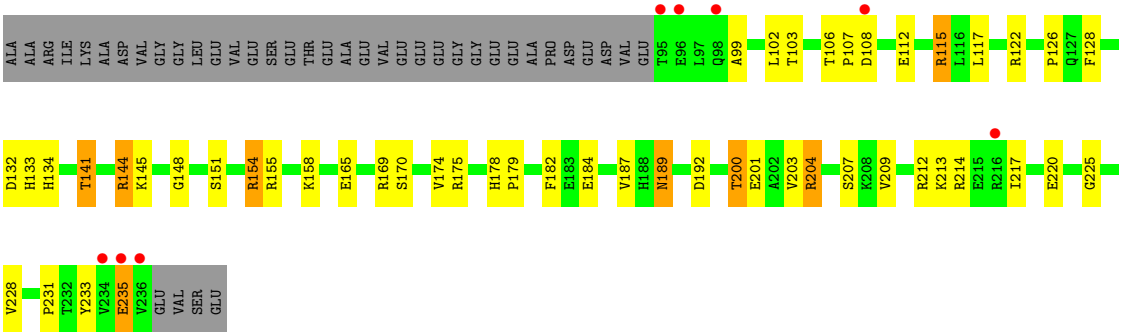


• Molecule 26: 50S ribosomal protein L31e



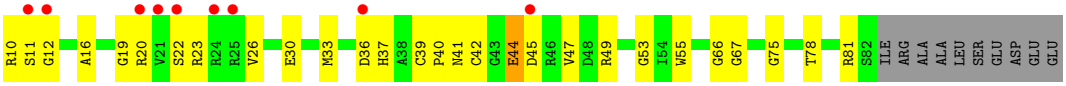
• Molecule 27: 50S ribosomal protein L32E





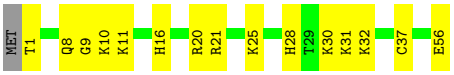
• Molecule 28: 50S ribosomal protein L37Ae

Chain Z:



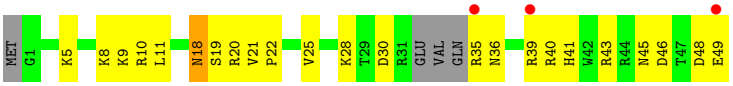
• Molecule 29: 50S ribosomal protein L37e

Chain 1:



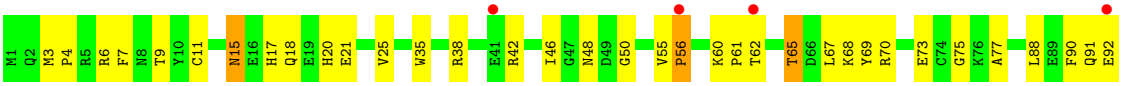
• Molecule 30: 50S ribosomal protein L39e

Chain 2:



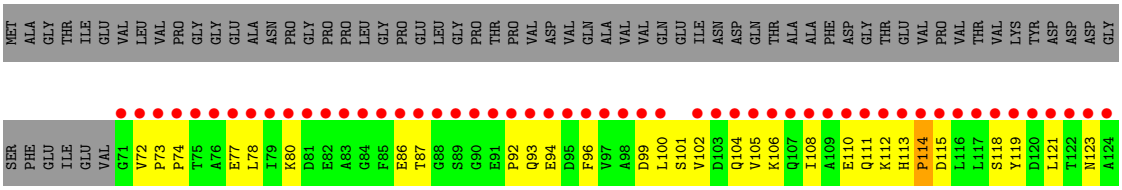
• Molecule 31: 50S ribosomal protein L44E

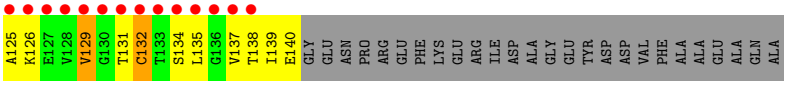
Chain 3:



• Molecule 32: 50S RIBOSOMAL PROTEIN L11P

Chain I:




A125
K126
E127
V128
V129
G130
T131
C132
T133
S134
L135
G136
V137
T138
I139
E140
GLY
GLU
ASN
PRO
ARG
GLU
PHE
LYS
GLU
ARG
ILE
ASP
ALA
GLY
GLU
TYR
ASP
ASP
VAL
PHE
ALA
ALA
GLU
ALA
GLN
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	211.52Å 298.48Å 574.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 49.75 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.1 (50.00-2.20) 90.0 (49.75-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.78 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.247 0.216 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	41.7	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	99035	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 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, SPS, CD, SR, 1MA, CL, MG, ACA, OMG, K, UR3, OMU, PSU

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	0.39	0/65959	0.70	26/102870 (0.0%)
2	9	0.36	0/2905	0.72	1/4528 (0.0%)
3	4	0.54	0/75	0.62	0/110
4	A	0.34	0/1786	0.67	0/2408
5	B	0.34	0/2690	0.66	0/3652
6	C	0.37	0/1884	0.65	0/2551
7	D	0.31	0/1111	0.56	0/1498
8	E	0.34	0/1382	0.58	0/1880
9	F	0.34	0/901	0.56	0/1224
10	G	0.29	0/241	0.46	0/324
11	H	0.34	0/1287	0.64	0/1725
12	J	0.35	0/1136	0.60	0/1530
13	K	0.35	0/1001	0.67	0/1347
14	L	0.34	0/1130	0.67	0/1509
15	M	0.34	0/1584	0.62	0/2119
16	N	0.29	0/1474	0.61	0/1999
17	O	0.33	0/874	0.60	0/1181
18	P	0.34	0/1147	0.57	0/1528
19	Q	0.35	0/749	0.70	1/1005 (0.1%)
20	R	0.36	0/1172	0.67	1/1578 (0.1%)
21	S	0.33	0/648	0.58	0/875
22	T	0.31	0/958	0.61	0/1289
23	U	0.34	0/417	0.56	0/562
24	V	0.28	0/502	0.54	0/675
25	W	0.34	0/1219	0.61	0/1655
26	X	0.33	0/664	0.58	0/895
27	Y	0.35	0/1146	0.65	0/1536
28	Z	0.36	0/589	0.64	0/787
29	1	0.42	0/438	0.66	0/578
30	2	0.35	0/401	0.63	0/529
31	3	0.37	0/771	0.59	0/1024
32	I	0.31	0/526	0.54	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
All	All	0.37	0/98767	0.68	29/147687 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	1	51
2	9	0	2
All	All	1	53

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	1563	G	C2'-C3'-O3'	9.87	131.21	109.50
1	0	871	G	C5'-C4'-O4'	-7.88	99.64	109.10
1	0	1942	A	C5'-C4'-C3'	7.22	127.56	116.00
1	0	1979	G	C2'-C3'-O3'	6.97	124.85	113.70
1	0	1819	G	C5'-C4'-C3'	6.93	127.09	116.00
2	9	3039	U	N1-C1'-C2'	6.83	122.89	114.00
1	0	1592	G	N9-C1'-C2'	6.57	122.54	114.00
1	0	1504	A	C1'-O4'-C4'	-6.28	104.88	109.90
1	0	1819	G	C1'-O4'-C4'	-6.23	104.92	109.90
1	0	777	U	O4'-C1'-N1	6.21	113.17	108.20
1	0	2313	C	C5'-C4'-O4'	5.93	116.21	109.10
1	0	1819	G	C4'-C3'-C2'	-5.71	96.89	102.60
1	0	2467	A	C1'-O4'-C4'	-5.63	105.39	109.90
1	0	2291	A	N9-C1'-C2'	5.63	121.32	114.00
1	0	1352	A	N9-C1'-C2'	5.37	120.98	114.00
1	0	2726	U	N1-C1'-C2'	5.37	120.98	114.00
1	0	1615	A	C5'-C4'-C3'	5.35	124.56	116.00
1	0	129	A	C2'-C3'-O3'	5.31	122.19	113.70
20	R	128	ARG	NE-CZ-NH2	-5.29	117.66	120.30
19	Q	17	LYS	N-CA-C	-5.26	96.81	111.00
1	0	1559	A	C2'-C3'-O3'	5.26	122.11	113.70
1	0	1352	A	OP1-P-O3'	5.24	116.73	105.20
1	0	1504	A	N9-C1'-C2'	5.24	120.81	114.00
1	0	1352	A	C2'-C3'-O3'	5.22	122.06	113.70
1	0	1942	A	C1'-O4'-C4'	-5.22	105.72	109.90
1	0	1452	G	C5'-C4'-C3'	-5.18	107.71	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	921	G	N9-C1'-C2'	5.18	120.73	114.00
1	0	1504	A	O4'-C4'-C3'	-5.02	98.98	104.00
1	0	2664	A	N9-C1'-C2'	5.02	120.53	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (53) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1080	C	Sidechain
1	0	1132	A	Sidechain
1	0	1327	G	Sidechain
1	0	1340	G	Sidechain
1	0	1430	G	Sidechain
1	0	1592	G	Sidechain
1	0	1744	G	Sidechain
1	0	1777	G	Sidechain
1	0	1809	G	Sidechain
1	0	1819	G	Sidechain
1	0	182	G	Sidechain
1	0	1829	A	Sidechain
1	0	1845	A	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1970	G	Sidechain
1	0	2036	C	Sidechain
1	0	2115	U	Sidechain
1	0	2316	G	Sidechain
1	0	24	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2552	C	Sidechain
1	0	2564	G	Sidechain
1	0	2616	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	2630	G	Sidechain
1	0	2664	A	Sidechain
1	0	270	U	Sidechain
1	0	2793	A	Sidechain
1	0	2811	A	Sidechain
1	0	2842	G	Sidechain
1	0	396	U	Sidechain
1	0	458	G	Sidechain
1	0	462	A	Sidechain
1	0	469	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	722	G	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	868	G	Sidechain
1	0	888	U	Sidechain
1	0	952	G	Sidechain
2	9	3039	U	Sidechain
2	9	3065	A	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29811	707	0
2	9	2600	0	1326	58	0
3	4	73	0	42	2	0
4	A	1753	0	1766	110	0
5	B	2625	0	2532	139	0
6	C	1859	0	1816	86	0
7	D	1094	0	1085	83	0
8	E	1357	0	1266	57	0
9	F	890	0	843	55	0
10	G	240	0	231	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	H	1266	0	1268	63	0
12	J	1120	0	1098	62	0
13	K	992	0	1031	57	0
14	L	1118	0	1076	61	0
15	M	1560	0	1567	73	0
16	N	1445	0	1401	96	0
17	O	865	0	873	39	0
18	P	1136	0	1123	38	0
19	Q	735	0	729	19	0
20	R	1149	0	1122	39	0
21	S	641	0	605	20	0
22	T	950	0	923	56	0
23	U	410	0	364	31	0
24	V	499	0	511	43	0
25	W	1196	0	1137	77	0
26	X	654	0	653	39	0
27	Y	1130	0	1133	56	0
28	Z	578	0	539	24	0
29	1	431	0	426	21	0
30	2	396	0	413	26	0
31	3	755	0	728	33	0
32	I	519	0	500	45	0
33	0	88	0	0	0	0
33	4	1	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	65	0	0	0	0
35	9	1	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	2	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	0	0
36	3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	1	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	98	0	0	0	0
37	1	2	0	0	0	0
37	3	1	0	0	0	0
37	9	3	0	0	0	0
37	A	3	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	L	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	4	23	0	19	4	0
39	1	1	0	0	0	0
39	3	1	0	0	0	0
39	O	1	0	0	0	0
39	U	1	0	0	0	0
39	Z	1	0	0	0	0
40	0	5743	0	0	113	0
40	1	50	0	0	1	0
40	2	35	0	0	3	0
40	3	76	0	0	5	0
40	4	2	0	0	1	0
40	9	136	0	0	4	0
40	A	120	0	0	11	0
40	B	135	0	0	23	0
40	C	172	0	0	14	0
40	D	48	0	0	5	0
40	E	42	0	0	1	0
40	F	27	0	0	4	0
40	G	16	0	0	1	0
40	H	71	0	0	6	0
40	I	10	0	0	0	0
40	J	51	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	K	58	0	0	5	0
40	L	87	0	0	10	0
40	M	127	0	0	6	0
40	N	59	0	0	8	0
40	O	41	0	0	6	0
40	P	64	0	0	1	0
40	Q	58	0	0	2	0
40	R	85	0	0	4	0
40	S	30	0	0	1	0
40	T	36	0	0	4	0
40	U	28	0	0	2	0
40	V	15	0	0	1	0
40	W	68	0	0	4	0
40	X	23	0	0	4	0
40	Y	95	0	0	9	0
40	Z	35	0	0	2	0
All	All	99035	0	59957	2109	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 14.

All (2109) 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)
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.28	1.10
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.31	1.10
6:C:236:THR:HG22	6:C:239:ALA:H	1.10	1.09
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.28	1.08
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.36	1.06
25:W:6:GLN:HB2	25:W:26:ILE:HD11	1.37	1.06
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.39	1.04
1:0:156:C:H5"	15:M:171:ARG:HD3	1.44	1.00
5:B:264:GLU:HG2	5:B:267:LYS:HE2	1.41	1.00
2:9:3076:G:H3'	2:9:3077:A:H5"	1.42	0.99
1:0:289:G:H22	1:0:363:A:H2	1.04	0.98
5:B:162:MET:HE2	5:B:310:ARG:HD3	1.44	0.98
1:0:1160:G:H5'	1:0:1161:A:H5'	1.47	0.97
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.47	0.97
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.11	0.95
5:B:86:ALA:HA	40:B:9578:HOH:O	1.66	0.95
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.47	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:238:ASN:HD22	5:B:240:GLY:H	1.10	0.94
5:B:307:ARG:HH11	5:B:307:ARG:HG3	1.31	0.94
7:D:58:VAL:HB	7:D:62:ASP:HB3	1.49	0.93
9:F:91:VAL:HG12	9:F:92:GLY:H	1.34	0.93
18:P:115:SER:H	18:P:118:GLN:HE21	1.11	0.93
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.82	0.93
13:K:10:GLN:NE2	13:K:10:GLN:H	1.64	0.93
15:M:99:ARG:HH21	15:M:170:ASN:HD22	1.10	0.93
1:0:1242:A:H5'	12:J:82:THR:HG23	1.50	0.93
21:S:51:GLN:HE21	21:S:53:ASN:HD21	1.09	0.93
1:0:1701:A:H4'	1:0:1702:U:H5"	1.50	0.92
5:B:140:LEU:HA	40:B:9578:HOH:O	1.71	0.91
1:0:656:G:H5'	17:O:3:THR:HG22	1.53	0.90
1:0:1166:A:H61	1:0:1180:U:H3	1.18	0.90
13:K:10:GLN:HE21	13:K:10:GLN:N	1.69	0.89
16:N:113:SER:HB2	40:N:9354:HOH:O	1.73	0.89
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.02	0.89
25:W:21:LEU:HD22	25:W:26:ILE:HD13	1.52	0.89
4:A:153:ARG:HB2	4:A:153:ARG:HH11	1.38	0.88
1:0:871:G:C8	1:0:871:G:H5'	2.09	0.88
1:0:1372:A:H3'	40:0:7650:HOH:O	1.73	0.88
9:F:46:GLU:OE1	9:F:100:ASP:HA	1.71	0.88
1:0:2840:A:OP1	5:B:211:THR:HG23	1.73	0.88
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.38	0.88
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.55	0.88
1:0:542:A:H5'	1:0:542:A:H8	1.39	0.87
1:0:1474:C:H6	1:0:1474:C:H5'	1.39	0.87
5:B:36:PRO:HA	5:B:168:GLY:HA3	1.56	0.87
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.89	0.87
29:1:25:LYS:HD2	30:2:49:GLU:H	1.40	0.87
13:K:10:GLN:H	13:K:10:GLN:HE21	0.87	0.86
13:K:107:THR:HG22	13:K:108:GLU:HG3	1.54	0.86
13:K:39:GLY:HA2	40:K:4183:HOH:O	1.74	0.86
1:0:2812:A:H2	1:0:2814:A:H62	1.17	0.86
1:0:288:A:H61	1:0:364:C:H42	1.19	0.86
2:9:3056:A:H2'	2:9:3057:A:H5"	1.56	0.86
13:K:4:LEU:HD22	13:K:116:GLU:HB3	1.57	0.86
1:0:1973:A:H5'	1:0:1973:A:H8	1.41	0.86
12:J:93:ARG:HB3	12:J:93:ARG:HH11	1.37	0.85
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.59	0.85
1:0:541:C:H2'	1:0:542:A:H5"	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1206:U:H5'	1:0:1206:U:H6	1.40	0.85
1:0:2586:U:H3	1:0:2592:G:H22	1.26	0.84
8:E:20:ILE:HD11	8:E:40:VAL:HG11	1.59	0.84
6:C:236:THR:HG22	6:C:239:ALA:N	1.92	0.84
1:0:2506:A:O2'	1:0:2507:G:H8	1.61	0.83
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.11	0.83
1:0:2748:G:H5'	40:0:7982:HOH:O	1.77	0.83
1:0:1835:U:H5	1:0:1840:A:N7	1.77	0.83
1:0:2506:A:HO2'	1:0:2507:G:H8	0.85	0.83
8:E:36:PRO:HD3	12:J:127:ILE:HD12	1.60	0.83
1:0:1603:A:H5'	1:0:1605:G:O4'	1.77	0.83
4:A:211:LYS:HG2	4:A:212:PRO:HD2	1.59	0.83
4:A:192:VAL:HB	40:A:9579:HOH:O	1.78	0.82
1:0:2534:C:H1'	40:0:4078:HOH:O	1.80	0.82
6:C:236:THR:CG2	6:C:239:ALA:H	1.91	0.82
13:K:81:ARG:HB2	13:K:87:ARG:NH1	1.94	0.82
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.80	0.81
16:N:144:GLY:O	16:N:147:ILE:HG22	1.80	0.81
1:0:1041:U:H5'	40:L:9495:HOH:O	1.80	0.81
1:0:2054:A:N3	20:R:128:ARG:NH2	2.29	0.81
7:D:136:ARG:HH12	7:D:157:LEU:HA	1.43	0.81
25:W:88:THR:HB	40:W:6679:HOH:O	1.79	0.81
1:0:1116:U:O2'	1:0:1118:A:H2	1.64	0.81
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.63	0.81
15:M:107:ARG:HH11	15:M:107:ARG:HG3	1.44	0.81
40:0:5382:HOH:O	12:J:47:THR:HB	1.81	0.80
6:C:1:MET:HG2	6:C:2:GLN:H	1.45	0.80
1:0:2717:C:C2'	1:0:2718:C:H5"	2.12	0.80
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.63	0.80
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.62	0.80
1:0:541:C:C2'	1:0:542:A:H5"	2.12	0.80
1:0:545:G:H5'	1:0:545:G:H8	1.45	0.80
15:M:80:GLY:O	15:M:81:ARG:HD2	1.81	0.79
27:Y:235:GLU:CD	27:Y:235:GLU:H	1.85	0.79
1:0:2780:C:H1'	8:E:143:GLN:HE21	1.48	0.79
5:B:162:MET:HE1	5:B:308:LEU:HD21	1.61	0.79
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.82	0.79
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.11	0.79
18:P:115:SER:H	18:P:118:GLN:NE2	1.80	0.79
1:0:111:C:O2'	29:1:20:ARG:HG2	1.82	0.79
2:9:3029:C:H2'	2:9:3030:C:H5'	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:139:VAL:HG13	40:C:9249:HOH:O	1.82	0.79
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.46	0.79
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.00	0.79
4:A:192:VAL:HG22	40:A:9617:HOH:O	1.80	0.79
1:0:2003:U:H4'	1:0:2004:U:H5	1.49	0.78
7:D:25:MET:HE2	7:D:41:LEU:HG	1.64	0.78
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.62	0.78
1:0:1878:G:H1'	40:0:6629:HOH:O	1.82	0.78
5:B:162:MET:CE	5:B:310:ARG:HD3	2.12	0.78
1:0:870:G:H2'	1:0:871:G:H5"	1.65	0.78
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.13	0.78
1:0:93:C:H5"	24:V:1:THR:HB	1.65	0.78
11:H:27:LYS:H	11:H:59:HIS:HD2	1.32	0.77
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.66	0.77
7:D:172:VAL:HG12	7:D:173:GLU:H	1.49	0.77
12:J:19:MET:HE3	12:J:132:LEU:HD21	1.66	0.77
25:W:125:HIS:HD2	25:W:127:GLY:H	1.32	0.77
1:0:2541:U:H4'	40:0:5938:HOH:O	1.83	0.77
1:0:797:A:H5'	28:Z:10:ARG:N	1.99	0.77
1:0:871:G:C8	1:0:871:G:C5'	2.68	0.77
4:A:192:VAL:CG1	4:A:207:GLN:HB3	2.15	0.77
6:C:27:ARG:HG3	6:C:29:ASP:OD1	1.85	0.77
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.67	0.76
1:0:871:G:C5'	1:0:871:G:H8	1.96	0.76
4:A:192:VAL:HG12	4:A:207:GLN:HB3	1.67	0.76
27:Y:154:ARG:HH12	27:Y:155:ARG:HG2	1.49	0.76
11:H:21:THR:O	11:H:120:ILE:HD12	1.85	0.76
1:0:796:A:HO2'	28:Z:10:ARG:N	1.83	0.76
4:A:35:GLY:O	4:A:36:ASP:HB3	1.84	0.76
32:I:99:ASP:OD1	32:I:138:THR:HB	1.84	0.76
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.68	0.76
27:Y:151:SER:O	27:Y:155:ARG:HG3	1.86	0.76
1:0:1377:C:H5'	1:0:1377:C:H6	1.50	0.76
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.67	0.76
1:0:289:G:N2	1:0:363:A:H2	1.83	0.76
18:P:115:SER:OG	18:P:118:GLN:HG3	1.85	0.76
1:0:2851:G:C2'	1:0:2852:A:H5'	2.15	0.76
6:C:5:ILE:HD11	6:C:16:VAL:HG22	1.68	0.76
1:0:481:U:H5"	40:0:6177:HOH:O	1.85	0.75
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.68	0.75
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.67	0.75
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.01	0.75
18:P:91:LYS:O	18:P:95:GLU:HG3	1.86	0.75
15:M:99:ARG:NH2	15:M:170:ASN:HD22	1.83	0.75
1:0:2890:A:H1'	23:U:56:ARG:NH2	2.02	0.74
40:9:4707:HOH:O	16:N:147:ILE:HD12	1.87	0.74
5:B:190:MET:HE2	5:B:194:PHE:HD1	1.52	0.74
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.17	0.74
16:N:11:ARG:HG3	16:N:14:ARG:HH12	1.51	0.74
4:A:191:GLY:HA2	4:A:194:MET:HE2	1.69	0.74
24:V:12:THR:HG22	24:V:15:GLU:CG	2.13	0.74
1:0:1667:A:H8	1:0:1667:A:H5'	1.52	0.74
4:A:153:ARG:HB2	4:A:153:ARG:NH1	2.01	0.74
4:A:191:GLY:HA2	4:A:194:MET:CE	2.18	0.74
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.15	0.74
1:0:506:G:H22	1:0:509:A:C5'	2.01	0.74
1:0:1751:G:H2'	1:0:1752:G:H5"	1.69	0.74
1:0:2717:C:H2'	1:0:2718:C:H5"	1.69	0.74
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.03	0.74
31:3:6:ARG:NH1	31:3:21:GLU:HG3	2.02	0.74
6:C:2:GLN:HB3	40:C:9189:HOH:O	1.86	0.74
7:D:154:LYS:H	7:D:154:LYS:HD2	1.52	0.74
25:W:21:LEU:CD2	25:W:48:VAL:HG11	2.13	0.74
1:0:1160:G:C5'	1:0:1161:A:H5'	2.18	0.74
9:F:91:VAL:HG12	9:F:92:GLY:N	2.01	0.74
9:F:96:ALA:HA	40:F:3111:HOH:O	1.88	0.74
1:0:1119:G:N2	1:0:1246:A:C2	2.55	0.73
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.03	0.73
26:X:54:ILE:HD11	26:X:85:VAL:HG12	1.69	0.73
32:I:102:VAL:HG12	32:I:106:LYS:HE3	1.68	0.73
1:0:280:C:H2'	1:0:281:U:O4'	1.89	0.73
1:0:544:G:H2'	1:0:545:G:H5"	1.70	0.73
1:0:1118:A:H62	1:0:1244:U:H3	1.36	0.73
40:0:9966:HOH:O	29:1:1:THR:HA	1.88	0.73
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.69	0.73
1:0:871:G:H5'	1:0:871:G:H8	1.52	0.73
1:0:1205:U:H2'	1:0:1206:U:H5"	1.71	0.73
13:K:32:ILE:HD11	13:K:56:SER:HB3	1.70	0.73
4:A:51:ARG:HB2	40:A:9592:HOH:O	1.89	0.72
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.71	0.72
1:0:1206:U:H2'	1:0:1207:A:O4'	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:199:HIS:HD2	4:A:201:PHE:H	1.38	0.72
6:C:78:ARG:HH11	6:C:78:ARG:HG3	1.54	0.72
14:L:73:VAL:HG23	14:L:74:THR:H	1.55	0.72
1:0:1116:U:HO2'	1:0:1118:A:H2	0.80	0.72
4:A:69:LEU:HD23	4:A:107:ASN:HB2	1.70	0.72
4:A:48:ASP:HB3	40:A:9592:HOH:O	1.90	0.72
10:G:12:ILE:N	10:G:13:PRO:HD3	2.04	0.72
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.04	0.72
32:I:74:PRO:HG2	32:I:77:GLU:OE1	1.89	0.72
24:V:20:LEU:HD22	24:V:60:GLN:HE22	1.55	0.72
1:0:1175:G:H1'	1:0:1193:A:H2'	1.70	0.71
1:0:2644:C:H2'	40:0:7574:HOH:O	1.90	0.71
31:3:38:ARG:HB3	31:3:42:ARG:HH12	1.55	0.71
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.72	0.71
30:2:41:HIS:H	30:2:45:ASN:HD22	1.37	0.71
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.72	0.71
1:0:902:G:N7	14:L:18:HIS:HD2	1.88	0.71
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.72	0.71
17:O:32:ARG:HH21	17:O:35:LYS:HZ2	1.38	0.71
1:0:2346:C:O2'	7:D:52:THR:HG21	1.89	0.71
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.26	0.71
1:0:2716:G:H5"	5:B:206:THR:HG21	1.73	0.71
40:0:7900:HOH:O	5:B:211:THR:HG21	1.91	0.71
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.55	0.71
1:0:474:C:O3'	6:C:73:LEU:HD21	1.91	0.71
1:0:1244:U:OP1	12:J:18:ILE:HD13	1.91	0.71
5:B:16:ARG:NH1	40:B:9610:HOH:O	2.23	0.71
7:D:58:VAL:HG12	7:D:60:GLU:HG2	1.71	0.71
11:H:154:TYR:HB2	40:H:9557:HOH:O	1.91	0.71
16:N:80:SER:HB2	40:N:9332:HOH:O	1.91	0.71
25:W:13:MET:CE	25:W:17:ILE:HG22	2.20	0.70
1:0:1700:C:H5"	1:0:1701:A:OP2	1.91	0.70
21:S:51:GLN:NE2	21:S:53:ASN:HD21	1.87	0.70
1:0:541:C:H2'	1:0:542:A:C5'	2.22	0.70
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.74	0.70
29:1:8:GLN:HE22	29:1:11:LYS:NZ	1.89	0.70
1:0:559:U:H6	1:0:559:U:H5'	1.55	0.70
1:0:1189:A:H3'	40:0:8198:HOH:O	1.91	0.70
2:9:3014:G:H5'	2:9:3014:G:H8	1.56	0.70
1:0:1118:A:H8	1:0:1118:A:H3'	1.56	0.70
1:0:1166:A:H1'	1:0:1192:A:C2	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:82:VAL:HG13	4:A:93:THR:HB	1.74	0.70
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.74	0.70
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.22	0.70
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.71	0.70
25:W:125:HIS:CD2	25:W:127:GLY:H	2.10	0.70
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.15	0.70
1:0:1118:A:H3'	1:0:1118:A:C8	2.27	0.69
1:0:1183:C:N4	1:0:1184:C:H41	1.89	0.69
25:W:52:VAL:HG22	25:W:53:ALA:H	1.56	0.69
9:F:58:GLU:CD	15:M:27:ARG:HH22	1.94	0.69
1:0:1666:C:H2'	1:0:1667:A:H5'	1.73	0.69
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.23	0.69
1:0:381:G:H5"	40:M:9371:HOH:O	1.91	0.69
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.74	0.69
1:0:2468:A:H61	31:3:48:ASN:HD21	1.40	0.69
1:0:1116:U:H3	1:0:1246:A:H62	1.40	0.69
5:B:112:THR:HG23	5:B:158:LYS:NZ	2.07	0.69
9:F:58:GLU:OE1	15:M:27:ARG:NH2	2.25	0.69
11:H:166:SER:HB3	11:H:167:PRO:HD3	1.74	0.69
15:M:164:THR:HG22	15:M:166:ALA:H	1.57	0.69
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.75	0.69
6:C:1:MET:HG2	6:C:2:GLN:N	2.08	0.69
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.74	0.69
22:T:9:LYS:HE3	22:T:13:ARG:HH11	1.53	0.69
22:T:115:GLU:HG3	22:T:116:ASP:N	2.08	0.69
21:S:51:GLN:HE21	21:S:53:ASN:ND2	1.87	0.69
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.23	0.68
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.23	0.68
1:0:1165:G:H1'	1:0:1174:A:H1'	1.74	0.68
40:0:5995:HOH:O	10:G:12:ILE:HA	1.91	0.68
4:A:153:ARG:HH11	4:A:153:ARG:CB	2.06	0.68
5:B:264:GLU:HG2	5:B:267:LYS:CE	2.20	0.68
22:T:26:THR:HA	22:T:39:ASN:HB3	1.76	0.68
24:V:1:THR:HG23	24:V:2:VAL:H	1.57	0.68
1:0:560:C:H42	1:0:597:A:H61	1.41	0.68
5:B:51:VAL:HG23	5:B:329:TYR:O	1.94	0.68
14:L:35:ARG:HB2	14:L:35:ARG:HH11	1.58	0.68
1:0:2807:U:P	5:B:27:ASN:HD21	2.16	0.68
15:M:164:THR:HG22	15:M:166:ALA:N	2.08	0.68
23:U:17:THR:HG22	23:U:18:GLY:N	2.08	0.68
1:0:506:G:H22	1:0:509:A:H5"	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:39:ASP:O	7:D:43:GLU:HG3	1.94	0.68
17:O:32:ARG:NE	17:O:35:LYS:HD2	2.08	0.68
24:V:12:THR:CG2	24:V:15:GLU:HG3	2.16	0.68
24:V:39:ALA:C	24:V:41:GLU:H	1.97	0.68
1:0:316:A:H5'	22:T:54:ASP:OD2	1.94	0.68
1:0:1168:C:H5"	32:I:87:THR:HG23	1.74	0.68
8:E:15:GLN:HG2	8:E:19:ASP:O	1.94	0.68
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.24	0.68
25:W:149:LEU:HG	25:W:153:MET:HE2	1.76	0.68
5:B:125:GLU:O	5:B:129:ARG:HG3	1.94	0.68
32:I:78:LEU:HD12	32:I:112:LYS:NZ	2.09	0.68
16:N:154:LEU:HG	16:N:155:GLU:H	1.59	0.67
24:V:43:PRO:O	24:V:46:ILE:HG22	1.94	0.67
1:0:328:U:O4'	6:C:202:THR:HG22	1.93	0.67
15:M:187:LEU:CD2	15:M:194:ALA:HB3	2.24	0.67
16:N:110:THR:HB	16:N:113:SER:OG	1.93	0.67
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.93	0.67
1:0:87:C:H2'	30:2:28:LYS:O	1.94	0.67
1:0:2005:G:H3'	1:0:2005:G:OP2	1.95	0.67
6:C:132:ASP:HB3	40:C:9166:HOH:O	1.94	0.67
1:0:1730:G:H5'	1:0:1731:C:C5	2.29	0.67
1:0:1973:A:H5'	1:0:1973:A:C8	2.28	0.67
5:B:221:GLN:HE22	13:K:42:ASN:HD22	1.40	0.67
18:P:103:THR:O	18:P:107:GLU:HG3	1.93	0.67
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.77	0.67
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.25	0.67
1:0:2003:U:H4'	1:0:2004:U:C5	2.29	0.67
4:A:57:ALA:HB1	4:A:65:ARG:HE	1.59	0.67
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.74	0.67
1:0:2578:G:H5'	1:0:2578:G:H8	1.58	0.67
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.75	0.67
11:H:27:LYS:N	11:H:59:HIS:HD2	1.91	0.67
14:L:143:THR:HG22	14:L:144:ASP:N	2.10	0.67
23:U:52:THR:HG22	23:U:54:THR:N	2.10	0.67
1:0:962:C:H1'	16:N:5:ARG:NH1	2.10	0.67
16:N:164:ASP:CG	16:N:167:ASP:HA	2.15	0.67
1:0:282:C:O2'	1:0:283:U:H5'	1.95	0.66
7:D:25:MET:HE1	7:D:37:ALA:HB1	1.77	0.66
26:X:71:ARG:HB3	26:X:88:GLU:OE1	1.95	0.66
1:0:1165:G:H4'	1:0:1174:A:O2'	1.95	0.66
15:M:107:ARG:HG3	15:M:107:ARG:NH1	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1159:G:H21	1:0:1189:A:H8	1.42	0.66
22:T:49:GLU:CB	22:T:59:GLU:HG2	2.25	0.66
1:0:1201:C:H2'	1:0:1202:A:H5'	1.76	0.66
1:0:2718:C:H6	1:0:2718:C:H5'	1.60	0.66
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.26	0.66
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.78	0.66
5:B:179:LEU:O	5:B:183:GLU:HG2	1.94	0.66
1:0:447:A:P	22:T:1:SER:HB2	2.35	0.66
1:0:524:A:H5"	20:R:29:LYS:HD3	1.77	0.66
1:0:1701:A:H4'	1:0:1702:U:C5'	2.23	0.66
17:O:14:LEU:HG	17:O:102:ILE:HD11	1.76	0.66
25:W:21:LEU:O	25:W:26:ILE:HG23	1.95	0.66
1:0:681:G:N3	1:0:681:G:H5'	2.11	0.66
1:0:1299:G:O6	14:L:6:ARG:HD3	1.96	0.66
1:0:1838:U:O2'	1:0:2644:C:H5'	1.96	0.66
13:K:49:LEU:HD12	13:K:80:ILE:HG21	1.77	0.66
22:T:71:VAL:HG12	22:T:72:ILE:N	2.11	0.66
1:0:2505:G:O2'	1:0:2506:A:H5'	1.96	0.66
5:B:254:GLN:HG2	5:B:255:GLY:N	2.10	0.66
14:L:133:VAL:HA	40:L:9475:HOH:O	1.96	0.65
15:M:183:THR:HG22	15:M:194:ALA:HB1	1.77	0.65
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.10	0.65
25:W:88:THR:HG22	25:W:89:ASP:N	2.11	0.65
28:Z:22:SER:O	28:Z:26:VAL:HG23	1.96	0.65
9:F:14:ASP:O	9:F:18:GLU:HG3	1.96	0.65
1:0:1187:U:HO2'	1:0:1189:A:H2	1.45	0.65
11:H:46:GLN:HE21	11:H:137:TYR:HE2	1.42	0.65
16:N:33:ARG:NH1	16:N:103:ASP:OD2	2.28	0.65
1:0:291:C:H2'	1:0:292:G:O4'	1.95	0.65
27:Y:144:ARG:CZ	40:Y:9411:HOH:O	2.44	0.65
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.77	0.65
40:0:6989:HOH:O	27:Y:141:THR:HG23	1.97	0.65
4:A:211:LYS:CG	4:A:212:PRO:HD2	2.27	0.65
17:O:32:ARG:O	17:O:32:ARG:HD3	1.97	0.65
25:W:108:ARG:HH21	25:W:114:PRO:HG2	1.61	0.65
27:Y:144:ARG:HH11	27:Y:144:ARG:CG	2.10	0.65
1:0:2480:G:H3'	40:0:4750:HOH:O	1.96	0.65
1:0:2769:C:H2'	1:0:2770:G:O4'	1.97	0.65
1:0:1919:A:H4'	40:0:5395:HOH:O	1.97	0.64
4:A:199:HIS:CD2	4:A:201:PHE:H	2.15	0.64
1:0:470:U:O2'	29:1:16:HIS:HD2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:544:G:C2'	1:0:545:G:H5"	2.26	0.64
1:0:2694:A:H4'	8:E:91:PHE:CE1	2.33	0.64
12:J:75:PRO:HD3	12:J:136:SER:OG	1.96	0.64
25:W:80:ASP:O	25:W:84:VAL:HG23	1.97	0.64
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.28	0.64
1:0:2270:G:H4'	4:A:223:ARG:HH12	1.61	0.64
5:B:238:ASN:ND2	5:B:240:GLY:H	1.90	0.64
5:B:297:VAL:HB	40:B:9599:HOH:O	1.97	0.64
7:D:138:GLY:N	40:D:7597:HOH:O	2.31	0.64
13:K:62:PRO:HG3	13:K:65:ARG:HH21	1.63	0.64
26:X:72:VAL:HG13	26:X:85:VAL:HG13	1.79	0.64
1:0:1183:C:H2'	40:0:6750:HOH:O	1.98	0.64
24:V:39:ALA:N	24:V:40:PRO:HD2	2.12	0.64
1:0:281:U:H2'	1:0:282:C:O4'	1.97	0.64
1:0:949:U:H4'	19:Q:95:GLU:HA	1.80	0.64
2:9:3056:A:C2'	2:9:3057:A:H5"	2.26	0.64
4:A:203:GLY:HA2	40:A:9536:HOH:O	1.97	0.64
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.37	0.64
1:0:1184:C:H1'	40:0:7910:HOH:O	1.98	0.64
1:0:2507:G:H2'	1:0:2510:C:H42	1.61	0.64
25:W:130:HIS:O	25:W:136:GLY:HA3	1.98	0.64
1:0:1666:C:O2'	1:0:1667:A:H5"	1.97	0.64
11:H:166:SER:CB	11:H:167:PRO:CD	2.75	0.64
17:O:57:THR:O	17:O:111:VAL:HG23	1.97	0.64
30:2:20:ARG:HD2	30:2:39:ARG:NH2	2.12	0.64
5:B:307:ARG:HG3	5:B:307:ARG:NH1	2.05	0.64
6:C:118:THR:HG22	6:C:137:PRO:HB3	1.79	0.64
7:D:64:ARG:NE	7:D:67:ASP:HB3	2.13	0.64
30:2:20:ARG:HD2	30:2:39:ARG:HH21	1.62	0.64
1:0:1160:G:H5'	1:0:1161:A:C5'	2.23	0.63
32:I:125:ALA:O	32:I:129:VAL:HG23	1.96	0.63
1:0:123:U:H5'	40:0:7139:HOH:O	1.99	0.63
1:0:2851:G:H2'	1:0:2852:A:H5'	1.79	0.63
5:B:238:ASN:HD22	5:B:240:GLY:N	1.90	0.63
12:J:131:THR:HG22	12:J:134:GLU:H	1.63	0.63
13:K:115:ARG:HG3	13:K:116:GLU:N	2.13	0.63
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.98	0.63
27:Y:165:GLU:HB3	40:Y:9393:HOH:O	1.97	0.63
28:Z:53:GLY:HA2	28:Z:67:GLY:O	1.99	0.63
25:W:48:VAL:O	25:W:48:VAL:HG12	1.98	0.63
4:A:36:ASP:HA	4:A:83:GLY:HA3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1184:C:H4'	32:I:126:LYS:HB3	1.80	0.63
1:0:1377:C:H5'	1:0:1377:C:C6	2.33	0.63
6:C:194:PHE:CD2	6:C:234:VAL:HG11	2.33	0.63
1:0:558:C:H2'	1:0:559:U:H5'	1.80	0.63
2:9:3004:G:H21	16:N:44:ARG:NH1	1.97	0.63
8:E:31:ARG:NH1	8:E:68:HIS:CG	2.67	0.63
9:F:48:VAL:HG12	9:F:97:ALA:HB2	1.79	0.63
15:M:99:ARG:HH21	15:M:170:ASN:ND2	1.89	0.63
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.33	0.63
24:V:55:ARG:O	24:V:59:ILE:HG12	1.99	0.63
4:A:33:GLU:O	4:A:34:ASP:HB2	1.98	0.63
1:0:380:A:OP2	15:M:9:ARG:HD2	1.99	0.63
1:0:1116:U:O2'	1:0:1118:A:C2	2.45	0.63
8:E:20:ILE:CD1	8:E:40:VAL:HG11	2.29	0.63
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.81	0.63
2:9:3013:A:O2'	2:9:3014:G:H5"	1.99	0.63
32:I:110:GLU:HA	32:I:113:HIS:CE1	2.34	0.63
10:G:27:ILE:HD13	10:G:71:LEU:HD23	1.81	0.62
15:M:24:GLN:O	15:M:28:GLN:HG3	1.99	0.62
23:U:45:GLU:HB2	23:U:48:ASN:HD22	1.64	0.62
1:0:1053:G:OP1	11:H:12:PRO:HG3	1.98	0.62
1:0:1333:U:H2'	1:0:1334:C:C6	2.35	0.62
1:0:1426:C:H2'	40:0:3201:HOH:O	1.97	0.62
1:0:1552:G:N2	1:0:1634:G:H1'	2.13	0.62
4:A:33:GLU:H	4:A:33:GLU:CD	2.03	0.62
11:H:166:SER:HB3	11:H:167:PRO:CD	2.29	0.62
14:L:104:ASP:HB2	40:L:9465:HOH:O	1.99	0.62
26:X:15:ARG:HB3	26:X:15:ARG:HH11	1.64	0.62
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.79	0.62
1:0:343:C:O2'	1:0:344:C:H5'	1.99	0.62
6:C:162:VAL:HG22	6:C:232:LEU:HD21	1.80	0.62
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.35	0.62
7:D:172:VAL:HG12	7:D:173:GLU:N	2.14	0.62
11:H:58:ARG:HH11	11:H:58:ARG:HG3	1.63	0.62
18:P:9:LEU:O	18:P:13:VAL:HG12	1.98	0.62
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.79	0.62
25:W:88:THR:HG22	25:W:89:ASP:H	1.64	0.62
1:0:282:C:H1'	1:0:368:C:N4	2.14	0.62
1:0:960:G:H4'	40:0:7877:HOH:O	1.99	0.62
1:0:2878:U:H2'	1:0:2879:A:O4'	1.99	0.62
4:A:194:MET:HE1	4:A:199:HIS:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3069:U:OP1	16:N:4:PRO:HG3	2.00	0.62
4:A:131:HIS:O	4:A:132:ASP:HB2	2.00	0.62
1:0:120:A:H5'	29:1:20:ARG:HH21	1.64	0.62
1:0:656:G:H5'	17:O:3:THR:CG2	2.28	0.62
1:0:1118:A:H8	1:0:1119:G:H5"	1.65	0.62
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.30	0.62
15:M:69:LYS:O	15:M:73:ARG:NH2	2.32	0.62
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.80	0.62
1:0:797:A:C4'	28:Z:10:ARG:N	2.63	0.62
1:0:2073:G:OP2	1:0:2490:A:H5'	1.98	0.62
1:0:2649:A:H5'	1:0:2649:A:H8	1.64	0.62
5:B:88:GLU:HB3	5:B:97:LEU:HD12	1.82	0.62
8:E:31:ARG:HH12	8:E:68:HIS:CD2	2.18	0.62
20:R:99:ALA:HB1	20:R:109:MET:CE	2.30	0.62
22:T:32:ARG:NH1	22:T:38:ARG:HH12	1.98	0.62
22:T:112:LEU:CD2	22:T:119:ALA:HB3	2.29	0.62
1:0:338:C:H4'	6:C:174:ILE:CD1	2.30	0.62
1:0:877:G:H5'	1:0:878:G:OP1	2.00	0.62
1:0:1474:C:H5'	1:0:1474:C:C6	2.28	0.62
1:0:2768:A:H2'	1:0:2769:C:C6	2.35	0.62
18:P:115:SER:N	18:P:118:GLN:HE21	1.92	0.62
1:0:960:G:H3'	1:0:960:G:N3	2.15	0.61
1:0:2533:C:H5'	1:0:2533:C:H6	1.65	0.61
1:0:2769:C:C2'	1:0:2770:G:H5'	2.30	0.61
5:B:58:PRO:HA	5:B:63:GLU:OE2	1.99	0.61
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.65	0.61
25:W:84:VAL:HG12	40:W:6679:HOH:O	1.99	0.61
1:0:545:G:H5'	1:0:545:G:C8	2.31	0.61
11:H:63:GLU:HA	40:H:9545:HOH:O	2.00	0.61
13:K:75:ARG:HD3	13:K:112:PRO:O	2.00	0.61
14:L:35:ARG:HB2	14:L:35:ARG:NH1	2.15	0.61
22:T:38:ARG:NH1	40:T:6217:HOH:O	2.33	0.61
1:0:1926:G:H2'	1:0:1927:A:C8	2.35	0.61
7:D:23:VAL:HG21	7:D:45:THR:HG21	1.81	0.61
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.30	0.61
25:W:137:GLN:NE2	25:W:141:HIS:HE1	1.91	0.61
1:0:164:G:H4'	14:L:30:ARG:HD3	1.83	0.61
1:0:542:A:H5'	1:0:542:A:C8	2.28	0.61
1:0:625:U:H5"	1:0:1044:C:N4	2.15	0.61
1:0:1119:G:H22	1:0:1246:A:H2	1.43	0.61
1:0:1882:C:OP1	4:A:192:VAL:HG23	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:316:A:N3	1:0:336:G:O2'	2.32	0.61
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.81	0.61
8:E:68:HIS:O	8:E:72:MET:HG3	1.99	0.61
17:O:32:ARG:HB2	40:O:4656:HOH:O	2.01	0.61
5:B:72:THR:HB	40:B:9599:HOH:O	1.99	0.61
7:D:149:ARG:HH12	16:N:15:GLU:HA	1.65	0.61
20:R:44:VAL:O	20:R:48:GLU:HG3	1.99	0.61
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.81	0.61
1:0:1189:A:O2'	1:0:1208:C:H2'	2.00	0.61
1:0:1205:U:C2'	1:0:1206:U:H5"	2.30	0.61
7:D:25:MET:SD	7:D:40:ILE:HD11	2.40	0.61
40:0:6053:HOH:O	5:B:298:LYS:HG2	2.00	0.61
8:E:101:GLU:HB2	8:E:116:THR:O	2.00	0.61
20:R:9:ASP:O	20:R:13:THR:HB	2.00	0.61
21:S:57:THR:HG22	21:S:58:MET:N	2.15	0.61
1:0:1058:A:H2'	1:0:1060:C:H5"	1.82	0.61
5:B:154:VAL:HG12	5:B:156:LYS:HG2	1.83	0.61
7:D:51:ARG:HH11	7:D:68:PRO:HB3	1.65	0.61
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.30	0.61
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.83	0.61
1:0:2649:A:H5'	1:0:2649:A:C8	2.36	0.61
7:D:23:VAL:HG22	7:D:73:VAL:HB	1.81	0.61
9:F:37:THR:O	9:F:41:GLU:HG3	2.01	0.61
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.82	0.61
5:B:190:MET:HE2	5:B:194:PHE:CD1	2.36	0.60
12:J:19:MET:CE	12:J:132:LEU:HD11	2.31	0.60
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.31	0.60
1:0:656:G:C5'	17:O:3:THR:HG22	2.29	0.60
5:B:71:VAL:HG11	5:B:296:LEU:HD22	1.82	0.60
7:D:22:VAL:HG22	7:D:74:THR:HG22	1.82	0.60
1:0:553:G:P	27:Y:204:ARG:HH22	2.24	0.60
1:0:2426:G:H1'	40:0:6602:HOH:O	1.99	0.60
9:F:1:PRO:H3	9:F:4:VAL:HG23	1.66	0.60
12:J:76:ASP:HA	40:J:5907:HOH:O	2.00	0.60
16:N:164:ASP:OD1	16:N:167:ASP:HA	2.02	0.60
1:0:1946:C:H2'	1:0:1971:G:C8	2.36	0.60
1:0:2270:G:H4'	4:A:223:ARG:NH1	2.17	0.60
4:A:194:MET:CE	4:A:199:HIS:HB2	2.32	0.60
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.83	0.60
26:X:9:VAL:HG22	26:X:88:GLU:OE2	2.01	0.60
2:9:3020:G:O2'	2:9:3021:G:H5'	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:217:ARG:HG3	5:B:257:THR:HG22	1.82	0.60
12:J:74:ARG:O	12:J:78:ILE:HG12	2.02	0.60
14:L:143:THR:HG22	14:L:144:ASP:H	1.67	0.60
16:N:12:ARG:HD3	16:N:18:THR:OG1	2.02	0.60
4:A:33:GLU:CD	4:A:33:GLU:N	2.55	0.60
11:H:30:GLN:H	11:H:66:ARG:NH1	1.99	0.60
21:S:73:ASP:OD1	21:S:76:GLU:HG3	2.01	0.60
25:W:139:GLY:O	25:W:141:HIS:HD2	1.85	0.60
29:1:10:LYS:HG3	40:1:9489:HOH:O	2.00	0.60
1:0:1159:G:H1	1:0:1208:C:H42	1.50	0.60
4:A:88:ILE:O	4:A:88:ILE:HG22	2.02	0.60
5:B:8:LYS:HG3	5:B:220:VAL:HG12	1.84	0.60
5:B:275:GLY:O	5:B:291:ASP:HA	2.01	0.60
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.31	0.60
1:0:635:A:H2'	1:0:636:G:H5"	1.83	0.60
1:0:1451:C:H5'	1:0:1505:U:C5	2.37	0.60
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.83	0.60
23:U:14:GLU:O	23:U:17:THR:HB	2.02	0.60
23:U:17:THR:CG2	23:U:18:GLY:N	2.64	0.60
23:U:45:GLU:HB2	23:U:48:ASN:ND2	2.16	0.60
26:X:72:VAL:HG13	26:X:85:VAL:CG1	2.32	0.60
1:0:1205:U:H2'	1:0:1206:U:C5'	2.32	0.60
2:9:3040:C:N4	7:D:53:LYS:HE3	2.17	0.60
9:F:99:THR:O	9:F:100:ASP:HB2	2.01	0.60
27:Y:144:ARG:HH11	27:Y:144:ARG:HG3	1.67	0.60
1:0:396:U:O2'	1:0:418:C:H4'	2.02	0.59
1:0:2064:U:H5'	1:0:2652:U:H4'	1.83	0.59
1:0:2524:G:H21	1:0:2526:C:H41	1.48	0.59
1:0:2896:A:N3	1:0:2896:A:H2'	2.17	0.59
4:A:179:MET:HG2	4:A:186:TRP:CB	2.32	0.59
1:0:1119:G:OP2	12:J:49:ARG:HD3	2.02	0.59
1:0:1181:A:H5'	32:I:94:GLU:OE2	2.02	0.59
1:0:2820:A:OP1	5:B:98:THR:HG22	2.03	0.59
1:0:2851:G:O2'	1:0:2852:A:H5'	2.01	0.59
9:F:2:VAL:HG22	9:F:57:GLU:OE1	2.03	0.59
27:Y:212:ARG:HD2	40:Y:9401:HOH:O	2.01	0.59
1:0:1182:C:H1'	1:0:1192:A:H8	1.68	0.59
1:0:2443:C:H5'	14:L:57:VAL:HG21	1.83	0.59
40:0:7995:HOH:O	31:3:60:LYS:HG3	2.02	0.59
5:B:85:ARG:NH1	40:B:9626:HOH:O	2.35	0.59
7:D:170:TYR:O	7:D:171:ASP:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:67:ARG:O	14:L:71:GLU:HG3	2.03	0.59
1:0:1766:U:O2	1:0:1778:A:H5'	2.03	0.59
1:0:2726:U:O2'	26:X:22:ASN:ND2	2.35	0.59
2:9:3029:C:C2'	2:9:3030:C:H5'	2.33	0.59
9:F:12:LEU:HD21	9:F:111:ILE:HG23	1.83	0.59
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.85	0.59
11:H:56:GLN:HE22	11:H:93:GLN:HG2	1.67	0.59
17:O:39:THR:O	17:O:115:ARG:NH2	2.33	0.59
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.17	0.59
1:0:391:U:OP2	15:M:84:LYS:NZ	2.35	0.59
5:B:141:ARG:HG2	5:B:165:ARG:HA	1.84	0.59
5:B:145:HIS:HD2	5:B:146:THR:O	1.86	0.59
14:L:36:ASP:HB2	40:L:9437:HOH:O	2.02	0.59
32:I:92:PRO:C	32:I:94:GLU:H	2.06	0.59
1:0:2644:C:O2'	1:0:2645:U:H5'	2.03	0.59
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.64	0.59
1:0:2291:A:C8	1:0:2309:C:H5'	2.38	0.59
1:0:2338:G:H2'	7:D:129:ASP:OD1	2.03	0.59
1:0:2765:C:H4'	40:0:6053:HOH:O	2.02	0.59
1:0:2827:A:H2'	1:0:2828:G:O4'	2.03	0.59
1:0:516:A:H5'	40:0:6177:HOH:O	2.03	0.59
1:0:2072:G:H4'	40:0:4372:HOH:O	2.02	0.58
40:0:9737:HOH:O	15:M:82:ARG:HD2	2.01	0.58
8:E:23:GLU:HG2	8:E:28:SER:HB3	1.85	0.58
29:1:56:GLU:HG2	29:1:56:GLU:OXT	2.03	0.58
1:0:1201:C:H5"	40:0:6739:HOH:O	2.03	0.58
1:0:2419:U:H5"	1:0:2420:G:H5'	1.84	0.58
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.65	0.58
25:W:88:THR:HG22	25:W:90:TYR:HD1	1.68	0.58
32:I:102:VAL:O	32:I:106:LYS:HG3	2.03	0.58
4:A:179:MET:HA	4:A:179:MET:CE	2.33	0.58
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.36	0.58
7:D:41:LEU:HA	7:D:44:ILE:HG22	1.85	0.58
16:N:162:ASP:HA	40:N:9327:HOH:O	2.02	0.58
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.51	0.58
1:0:138:U:H5"	1:0:139:C:OP2	2.03	0.58
1:0:2524:G:H21	1:0:2526:C:H5	1.49	0.58
7:D:49:PRO:HB3	7:D:73:VAL:HG22	1.84	0.58
16:N:143:ARG:HH21	16:N:169:PRO:HB2	1.69	0.58
18:P:135:ALA:HB1	18:P:139:ARG:HH12	1.67	0.58
1:0:2420:G:O2'	1:0:2421:G:H5'	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:305:ASP:O	5:B:306:LYS:HB2	2.04	0.58
12:J:107:ASN:C	12:J:107:ASN:HD22	2.07	0.58
12:J:107:ASN:ND2	12:J:109:TYR:H	2.01	0.58
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.67	0.58
32:I:78:LEU:HD12	32:I:112:LYS:HZ2	1.66	0.58
1:0:263:U:O4'	9:F:59:ILE:HD13	2.03	0.58
2:9:3039:U:H1'	2:9:3044:A:H61	1.68	0.58
16:N:69:TYR:HE2	16:N:184:ILE:HG13	1.68	0.58
32:I:110:GLU:HA	32:I:113:HIS:NE2	2.18	0.58
2:9:3051:A:H5'	16:N:160:SER:CB	2.34	0.58
24:V:39:ALA:N	24:V:40:PRO:CD	2.66	0.58
31:3:65:THR:HG22	31:3:67:LEU:HG	1.85	0.58
1:0:621:C:H5'	27:Y:132:ASP:OD2	2.03	0.58
4:A:121:ALA:O	4:A:124:VAL:HG22	2.03	0.58
6:C:78:ARG:HG3	6:C:78:ARG:NH1	2.19	0.58
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.85	0.58
13:K:4:LEU:CD2	13:K:116:GLU:HB3	2.32	0.58
14:L:57:VAL:HG12	14:L:57:VAL:O	2.04	0.58
31:3:70:ARG:HB3	40:3:9510:HOH:O	2.04	0.58
32:I:113:HIS:N	32:I:114:PRO:HD2	2.18	0.58
1:0:797:A:C5'	28:Z:10:ARG:N	2.67	0.58
1:0:1168:C:H5"	32:I:87:THR:CG2	2.34	0.58
1:0:1384:C:H5'	26:X:30:MET:HG2	1.85	0.58
1:0:1687:C:O2	29:1:9:GLY:HA2	2.04	0.58
9:F:58:GLU:HA	9:F:61:MET:HG3	1.85	0.58
1:0:441:A:H1'	1:0:442:A:N7	2.19	0.58
1:0:657:G:OP1	6:C:27:ARG:NH2	2.29	0.58
7:D:136:ARG:NH1	7:D:157:LEU:HA	2.16	0.58
1:0:1730:G:H5"	1:0:1731:C:H6	1.69	0.57
27:Y:189:ASN:C	27:Y:189:ASN:HD22	2.07	0.57
1:0:121:U:OP2	30:2:10:ARG:NH2	2.33	0.57
1:0:2795:C:O2'	1:0:2796:U:H5'	2.04	0.57
1:0:2908:A:H2'	1:0:2909:G:O4'	2.02	0.57
31:3:3:MET:HG3	31:3:4:PRO:HD2	1.85	0.57
1:0:506:G:H22	1:0:509:A:H5'	1.69	0.57
1:0:1943:C:H4'	4:A:211:LYS:O	2.05	0.57
1:0:2237:G:H1'	1:0:2238:A:C8	2.40	0.57
1:0:2769:C:O2'	1:0:2770:G:H5'	2.04	0.57
2:9:3018:U:H2'	2:9:3019:G:H8	1.70	0.57
5:B:62:ARG:HA	5:B:65:MET:CE	2.34	0.57
5:B:162:MET:HE2	5:B:310:ARG:CD	2.28	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:175:LEU:O	5:B:175:LEU:HD23	2.05	0.57
9:F:48:VAL:HG12	9:F:97:ALA:CB	2.33	0.57
13:K:81:ARG:HD3	13:K:87:ARG:CZ	2.34	0.57
32:I:118:SER:HB2	32:I:123:ASN:HB2	1.87	0.57
2:9:3014:G:H5'	2:9:3014:G:C8	2.39	0.57
6:C:79:ARG:O	6:C:87:ARG:HG2	2.04	0.57
9:F:13:GLU:OE1	9:F:77:VAL:HG13	2.05	0.57
16:N:23:ARG:HG2	16:N:23:ARG:HH11	1.69	0.57
23:U:47:ARG:HG3	40:U:4381:HOH:O	2.03	0.57
5:B:102:THR:HG21	5:B:182:VAL:O	2.04	0.57
11:H:40:ALA:HB1	11:H:137:TYR:CE2	2.40	0.57
25:W:26:ILE:HB	40:W:5420:HOH:O	2.03	0.57
26:X:43:VAL:HG12	26:X:44:ASP:N	2.19	0.57
32:I:139:ILE:HG22	32:I:140:GLU:N	2.20	0.57
1:0:20:G:H21	20:R:117:HIS:HD2	1.52	0.57
1:0:1634:G:H3'	40:0:4466:HOH:O	2.04	0.57
1:0:2694:A:H4'	8:E:91:PHE:HE1	1.69	0.57
4:A:95:PRO:HG2	4:A:98:GLU:HG2	1.86	0.57
6:C:127:ARG:HD3	6:C:129:HIS:HE1	1.68	0.57
6:C:129:HIS:HD2	6:C:165:ASP:OD2	1.88	0.57
1:0:2676:C:H4'	12:J:70:PHE:CD1	2.39	0.57
5:B:96:PRO:HG3	40:B:9626:HOH:O	2.02	0.57
10:G:64:ASN:HD22	10:G:64:ASN:N	2.01	0.57
1:0:1180:U:O2'	32:I:92:PRO:HD2	2.05	0.57
1:0:1189:A:H1'	1:0:1209:C:O4'	2.04	0.57
5:B:17:LYS:O	5:B:260:HIS:HD2	1.86	0.57
6:C:140:VAL:HB	40:C:9252:HOH:O	2.04	0.57
15:M:24:GLN:NE2	15:M:27:ARG:HH11	2.03	0.57
22:T:41:ARG:HG2	22:T:41:ARG:NH1	2.19	0.57
6:C:127:ARG:CZ	6:C:225:PRO:HG2	2.35	0.57
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.40	0.57
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.87	0.57
20:R:39:THR:HG22	20:R:107:GLU:O	2.05	0.57
21:S:77:VAL:O	21:S:80:ARG:HG2	2.05	0.57
27:Y:154:ARG:HB3	27:Y:154:ARG:HH11	1.69	0.57
40:0:4931:HOH:O	15:M:83:SER:HB3	2.04	0.57
11:H:170:ASN:HD22	11:H:170:ASN:N	2.01	0.57
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.05	0.57
1:0:256:C:H2'	1:0:257:G:O4'	2.05	0.56
2:9:3041:C:O4'	7:D:50:VAL:HG13	2.05	0.56
6:C:242:GLU:HB2	40:C:9186:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2779:G:H21	8:E:143:GLN:NE2	2.03	0.56
7:D:59:GLY:O	7:D:61:PHE:N	2.38	0.56
25:W:5:VAL:O	25:W:52:VAL:HG23	2.04	0.56
31:3:3:MET:O	31:3:90:PHE:HA	2.05	0.56
1:0:500:G:H21	20:R:98:ASN:HD21	1.51	0.56
1:0:1730:G:C5'	1:0:1731:C:C6	2.87	0.56
1:0:2524:G:N2	1:0:2526:C:H41	2.03	0.56
1:0:2717:C:O2'	1:0:2718:C:H5"	2.05	0.56
1:0:2912:C:H2'	1:0:2913:A:O4'	2.05	0.56
15:M:107:ARG:NH1	40:M:9378:HOH:O	2.38	0.56
16:N:115:VAL:HG22	40:N:9354:HOH:O	2.05	0.56
24:V:64:GLY:O	24:V:65:ASP:HB2	2.03	0.56
25:W:4:LEU:O	25:W:32:CYS:HA	2.05	0.56
5:B:267:LYS:HE3	5:B:300:SER:O	2.05	0.56
4:A:113:GLY:HA2	4:A:153:ARG:NH2	2.20	0.56
8:E:20:ILE:HD12	8:E:33:LEU:HD12	1.87	0.56
15:M:187:LEU:HD23	15:M:194:ALA:HB3	1.86	0.56
23:U:4:ARG:HG2	23:U:4:ARG:HH11	1.71	0.56
1:0:871:G:H5"	1:0:871:G:H8	1.70	0.56
1:0:1681:G:H5"	1:0:1682:A:H5'	1.87	0.56
1:0:2105:C:H5'	40:4:7933:HOH:O	2.05	0.56
2:9:3051:A:H5'	16:N:160:SER:HB3	1.87	0.56
11:H:76:GLU:C	11:H:77:LEU:HD23	2.26	0.56
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.87	0.56
25:W:4:LEU:HD11	25:W:45:VAL:HG12	1.88	0.56
1:0:737:A:H2'	1:0:738:G:O4'	2.05	0.56
4:A:206:ARG:H	4:A:206:ARG:HD3	1.71	0.56
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.88	0.56
12:J:74:ARG:NH1	12:J:105:LEU:HD11	2.21	0.56
13:K:55:VAL:HG12	13:K:56:SER:N	2.20	0.56
22:T:48:VAL:HG22	22:T:96:VAL:HG22	1.87	0.56
12:J:93:ARG:HB3	12:J:93:ARG:NH1	2.17	0.56
14:L:79:ASP:HB2	40:L:9459:HOH:O	2.06	0.56
1:0:1595:G:O2'	1:0:1596:U:H5'	2.06	0.56
1:0:2563:U:H2'	1:0:2565:C:O5'	2.05	0.56
5:B:40:GLY:HA3	40:B:9637:HOH:O	2.04	0.56
7:D:57:THR:HG23	7:D:63:ILE:HA	1.88	0.56
11:H:20:ILE:HG23	11:H:120:ILE:HD11	1.87	0.56
16:N:11:ARG:O	16:N:15:GLU:HG3	2.06	0.56
25:W:52:VAL:HG22	25:W:53:ALA:N	2.20	0.56
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:154:ARG:NH1	27:Y:155:ARG:HG2	2.19	0.56
30:2:48:ASP:O	30:2:49:GLU:HB2	2.05	0.56
1:0:1592:G:O2'	1:0:1593:C:O4'	2.24	0.56
9:F:58:GLU:HA	9:F:61:MET:HE2	1.88	0.56
29:1:25:LYS:HD2	30:2:49:GLU:N	2.18	0.56
1:0:95:A:H5"	1:0:97:G:O4'	2.06	0.55
1:0:1878:G:O2'	1:0:1879:U:OP2	2.24	0.55
4:A:123:GLY:HA3	4:A:162:GLY:HA2	1.86	0.55
4:A:135:VAL:HG21	4:A:147:ARG:NH1	2.20	0.55
31:3:62:THR:HB	40:3:9487:HOH:O	2.05	0.55
1:0:2320:U:H4'	1:0:2321:A:O4'	2.06	0.55
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.88	0.55
8:E:34:TRP:O	12:J:127:ILE:HD11	2.06	0.55
16:N:149:GLU:O	16:N:152:GLU:HB3	2.05	0.55
1:0:2453:G:H5"	40:L:9442:HOH:O	2.04	0.55
40:0:6753:HOH:O	23:U:56:ARG:HB3	2.05	0.55
16:N:154:LEU:O	16:N:155:GLU:HB2	2.06	0.55
24:V:11:MET:HB3	24:V:15:GLU:HB2	1.88	0.55
1:0:248:A:H5'	1:0:249:G:OP2	2.07	0.55
2:9:3041:C:H4'	7:D:48:MET:HB3	1.88	0.55
2:9:3076:G:C3'	2:9:3077:A:H5"	2.27	0.55
6:C:236:THR:HG21	40:C:9178:HOH:O	2.05	0.55
14:L:80:ASP:CB	14:L:90:ARG:HB3	2.36	0.55
16:N:183:ASP:O	16:N:184:ILE:O	2.25	0.55
28:Z:10:ARG:HA	40:Z:9215:HOH:O	2.06	0.55
32:I:112:LYS:C	32:I:114:PRO:HD2	2.27	0.55
5:B:120:ASP:OD2	5:B:123:ALA:HB2	2.07	0.55
10:G:12:ILE:N	10:G:13:PRO:CD	2.69	0.55
12:J:70:PHE:CG	12:J:70:PHE:O	2.60	0.55
19:Q:25:PRO:HB2	40:Q:4350:HOH:O	2.07	0.55
22:T:40:VAL:HG22	22:T:41:ARG:N	2.22	0.55
24:V:56:ILE:O	24:V:60:GLN:HG3	2.05	0.55
1:0:558:C:O2'	1:0:559:U:H5"	2.06	0.55
1:0:1200:A:H4'	40:0:7793:HOH:O	2.07	0.55
1:0:1209:C:H2'	1:0:1210:G:H8	1.71	0.55
2:9:3014:G:O2'	16:N:1:ALA:HB2	2.05	0.55
5:B:84:LEU:HB2	5:B:182:VAL:HG21	1.89	0.55
5:B:112:THR:HG23	5:B:158:LYS:HZ1	1.71	0.55
7:D:44:ILE:HG12	7:D:83:PHE:HE1	1.72	0.55
18:P:111:GLU:O	18:P:111:GLU:HG2	2.06	0.55
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:64:THR:O	25:W:68:THR:HG22	2.06	0.55
1:0:870:G:C2'	1:0:871:G:H5"	2.35	0.55
1:0:2072:G:C6	1:0:2533:C:H1'	2.42	0.55
11:H:171:ALA:HA	40:H:9535:HOH:O	2.06	0.55
14:L:136:ALA:HB3	40:L:9475:HOH:O	2.06	0.55
16:N:89:GLY:O	16:N:92:ALA:HB3	2.07	0.55
1:0:272:A:H5'	1:0:273:G:OP2	2.07	0.55
1:0:2521:A:OP2	11:H:3:ALA:HB3	2.07	0.55
1:0:2645:U:C6	1:0:2645:U:OP2	2.59	0.55
5:B:185:GLY:HA2	40:B:9625:HOH:O	2.05	0.55
12:J:75:PRO:HB3	12:J:132:LEU:HB3	1.89	0.55
14:L:91:VAL:HG13	14:L:120:LEU:HD23	1.88	0.55
25:W:13:MET:HE1	25:W:18:GLN:HA	1.89	0.55
1:0:1236:A:C8	12:J:63:ILE:HD11	2.41	0.55
2:9:3057:A:H8	7:D:141:VAL:HG21	1.72	0.55
5:B:62:ARG:HA	5:B:65:MET:HE2	1.88	0.55
6:C:214:THR:HG23	40:C:9237:HOH:O	2.06	0.55
22:T:49:GLU:OE2	22:T:97:ARG:HD2	2.07	0.55
24:V:1:THR:HG23	24:V:2:VAL:N	2.22	0.55
30:2:36:ASN:HB3	30:2:39:ARG:HG3	1.89	0.55
1:0:2365:G:H5"	40:Q:6597:HOH:O	2.06	0.55
1:0:2502:C:C2'	1:0:2503:A:H5'	2.36	0.55
40:0:3147:HOH:O	18:P:81:LYS:HG2	2.06	0.55
40:0:9698:HOH:O	5:B:214:PRO:HD2	2.06	0.55
15:M:79:ALA:HB3	15:M:81:ARG:NH1	2.22	0.55
24:V:42:ASN:HB3	40:V:7247:HOH:O	2.06	0.55
1:0:1406:A:H4'	1:0:1407:A:H5"	1.88	0.54
1:0:1528:A:H2'	1:0:1529:G:O4'	2.07	0.54
1:0:2524:G:H21	1:0:2526:C:N4	2.04	0.54
9:F:13:GLU:OE2	9:F:78:GLU:HG2	2.07	0.54
15:M:68:ARG:O	15:M:68:ARG:HD3	2.08	0.54
1:0:485:A:N3	1:0:487:G:H5"	2.22	0.54
1:0:2416:G:O2'	16:N:25:ARG:HG2	2.06	0.54
5:B:5:ARG:HH11	5:B:8:LYS:HE2	1.72	0.54
5:B:97:LEU:O	5:B:98:THR:HG23	2.06	0.54
8:E:22:VAL:HG12	8:E:76:VAL:HG11	1.89	0.54
17:O:59:VAL:CG2	17:O:111:VAL:HG21	2.37	0.54
1:0:949:U:C4'	19:Q:95:GLU:HA	2.37	0.54
4:A:107:ASN:OD1	4:A:120:ARG:HD2	2.07	0.54
5:B:321:PRO:HA	40:B:9646:HOH:O	2.07	0.54
8:E:31:ARG:HH12	8:E:68:HIS:CG	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:31:LYS:HE3	40:F:2623:HOH:O	2.06	0.54
18:P:16:VAL:HG12	18:P:17:GLY:N	2.23	0.54
21:S:57:THR:CG2	21:S:58:MET:N	2.69	0.54
25:W:41:TYR:HA	25:W:44:MET:HE3	1.88	0.54
32:I:134:SER:O	32:I:135:LEU:HD23	2.07	0.54
1:0:1067:A:H5'	40:0:4901:HOH:O	2.06	0.54
4:A:34:ASP:OD1	4:A:35:GLY:N	2.41	0.54
17:O:59:VAL:HG23	17:O:111:VAL:CG2	2.37	0.54
1:0:2670:G:O2'	1:0:2671:U:H5'	2.07	0.54
1:0:2717:C:OP1	5:B:207:LYS:HG3	2.08	0.54
4:A:101:GLU:OE2	4:A:131:HIS:HB2	2.08	0.54
11:H:79:GLU:C	11:H:80:GLU:HG3	2.28	0.54
24:V:56:ILE:HG22	24:V:60:GLN:HE21	1.72	0.54
25:W:65:VAL:HG12	25:W:116:LEU:HD13	1.89	0.54
32:I:72:VAL:HG11	32:I:111:GLN:O	2.07	0.54
1:0:2720:C:O2	13:K:87:ARG:NH2	2.41	0.54
1:0:2748:G:OP1	1:0:2749:U:H5"	2.07	0.54
7:D:104:PHE:CE2	7:D:166:ILE:HD13	2.42	0.54
18:P:98:ILE:O	18:P:98:ILE:HD13	2.08	0.54
1:0:2866:U:H4'	1:0:2867:G:H5'	1.89	0.54
2:9:3029:C:O3'	7:D:138:GLY:HA2	2.07	0.54
1:0:656:G:OP2	17:O:37:ARG:HD2	2.08	0.54
1:0:1667:A:H2'	1:0:1668:U:C6	2.43	0.54
40:0:3309:HOH:O	5:B:254:GLN:HG3	2.08	0.54
5:B:321:PRO:HG3	40:B:9595:HOH:O	2.08	0.54
11:H:169:GLY:C	11:H:170:ASN:HD22	2.11	0.54
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.13	0.54
15:M:66:SER:HB3	15:M:128:TRP:CD1	2.43	0.54
1:0:12:U:H2'	1:0:13:G:H5'	1.90	0.54
1:0:1853:C:OP1	4:A:231:LYS:HG3	2.08	0.54
2:9:3114:G:O6	16:N:11:ARG:HD3	2.07	0.54
1:0:151:A:H2'	1:0:152:A:O4'	2.07	0.54
1:0:834:G:H4'	1:0:835:U:OP2	2.08	0.54
1:0:2894:C:O2'	1:0:2895:C:H5'	2.07	0.54
1:0:286:U:H2'	1:0:287:C:C6	2.43	0.53
1:0:1641:A:H2'	1:0:1642:A:H5'	1.90	0.53
1:0:1902:G:H2'	1:0:1903:U:O4'	2.08	0.53
14:L:80:ASP:HB2	14:L:90:ARG:O	2.06	0.53
15:M:58:GLN:HG3	40:M:9405:HOH:O	2.07	0.53
1:0:757:C:OP1	14:L:27:ARG:HD2	2.07	0.53
1:0:1335:C:OP2	27:Y:207:SER:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:154:ILE:HD11	8:E:157:LYS:HB2	1.89	0.53
1:0:156:C:H5"	15:M:171:ARG:CD	2.27	0.53
1:0:1189:A:H1'	1:0:1209:C:C1'	2.38	0.53
4:A:94:LEU:HD23	4:A:94:LEU:N	2.24	0.53
5:B:139:ASP:HB3	40:B:9552:HOH:O	2.08	0.53
6:C:236:THR:HA	40:C:9252:HOH:O	2.07	0.53
9:F:60:VAL:O	9:F:60:VAL:HG12	2.09	0.53
14:L:150:GLN:HB3	40:L:9471:HOH:O	2.08	0.53
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.38	0.53
1:0:558:C:H2'	1:0:559:U:C5'	2.38	0.53
1:0:709:G:O2'	17:O:25:VAL:CG1	2.56	0.53
1:0:1819:G:H2'	1:0:1820:G:H4'	1.89	0.53
6:C:194:PHE:HA	6:C:234:VAL:HG13	1.91	0.53
8:E:145:ALA:HB1	8:E:168:ILE:CD1	2.38	0.53
22:T:47:THR:HB	22:T:100:ASP:HB3	1.90	0.53
1:0:40:C:H4'	40:0:7476:HOH:O	2.08	0.53
1:0:2711:U:H1'	40:0:4024:HOH:O	2.08	0.53
4:A:165:THR:HG22	40:A:9604:HOH:O	2.09	0.53
5:B:41:PHE:CD1	5:B:79:MET:HE2	2.42	0.53
5:B:310:ARG:HD2	40:B:9587:HOH:O	2.08	0.53
10:G:20:VAL:O	10:G:24:VAL:HG23	2.08	0.53
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.09	0.53
16:N:169:PRO:O	16:N:172:PHE:HB3	2.09	0.53
23:U:5:GLU:HG2	23:U:10:GLY:O	2.07	0.53
6:C:20:ASP:O	6:C:23:GLU:HB2	2.08	0.53
15:M:77:HIS:HD2	15:M:79:ALA:O	1.91	0.53
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.91	0.53
1:0:793:A:H5"	18:P:83:LYS:HG2	1.91	0.53
1:0:1555:G:H4'	1:0:1630:A:H2	1.73	0.53
15:M:60:VAL:C	15:M:61:ILE:HD12	2.28	0.53
20:R:122:GLN:HB3	20:R:138:SER:HB2	1.89	0.53
1:0:1363:G:OP1	6:C:76:ARG:NH2	2.42	0.53
4:A:164:ARG:CZ	40:A:9572:HOH:O	2.56	0.53
13:K:58:THR:HG22	13:K:59:LYS:HG3	1.90	0.53
15:M:167:GLY:O	15:M:171:ARG:HG3	2.09	0.53
31:3:70:ARG:HH11	31:3:70:ARG:HG2	1.74	0.53
1:0:538:C:OP2	27:Y:134:HIS:HE1	1.91	0.53
1:0:1476:A:O2'	1:0:1477:C:H5'	2.08	0.53
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.38	0.53
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.65	0.53
32:I:138:THR:HG22	32:I:139:ILE:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1118:A:C8	1:0:1119:G:H5"	2.44	0.53
1:0:2812:A:C2	1:0:2814:A:N6	2.65	0.53
5:B:264:GLU:CG	5:B:267:LYS:HE2	2.29	0.53
8:E:3:VAL:HG22	8:E:49:ILE:HB	1.91	0.52
8:E:20:ILE:CD1	8:E:33:LEU:HD12	2.39	0.52
15:M:30:GLU:O	15:M:34:GLU:HG3	2.09	0.52
1:0:1268:C:O2'	27:Y:169:ARG:HB2	2.09	0.52
1:0:1626:A:H2'	1:0:1627:G:O4'	2.08	0.52
1:0:1666:C:H2'	1:0:1667:A:C5'	2.37	0.52
1:0:1730:G:H5'	1:0:1731:C:H5	1.74	0.52
1:0:2541:U:H5'	1:0:2541:U:H6	1.74	0.52
2:9:3049:G:O2'	2:9:3050:G:H5'	2.10	0.52
22:T:19:ARG:HD3	22:T:67:LEU:O	2.09	0.52
25:W:38:THR:HG22	25:W:39:ASP:N	2.24	0.52
32:I:99:ASP:O	32:I:100:LEU:HD23	2.09	0.52
1:0:288:A:H2'	1:0:289:G:C8	2.43	0.52
1:0:951:A:C2'	1:0:952:G:H5'	2.39	0.52
1:0:1352:A:O2'	1:0:1353:C:OP1	2.24	0.52
6:C:84:VAL:HG12	6:C:85:LYS:HG2	1.92	0.52
17:O:87:THR:O	17:O:91:GLN:HG3	2.08	0.52
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.24	0.52
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.90	0.52
32:I:105:VAL:HG11	32:I:129:VAL:CG2	2.39	0.52
1:0:1166:A:H1'	1:0:1192:A:N3	2.25	0.52
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.23	0.52
25:W:88:THR:HG22	25:W:90:TYR:CD1	2.45	0.52
27:Y:235:GLU:CD	27:Y:235:GLU:N	2.59	0.52
1:0:949:U:O2'	19:Q:40:HIS:HE1	1.93	0.52
1:0:1878:G:O2'	1:0:1879:U:C6	2.60	0.52
2:9:3008:G:O6	16:N:11:ARG:NH1	2.42	0.52
5:B:232:TRP:HD1	5:B:235:ARG:HD2	1.74	0.52
5:B:232:TRP:CD1	5:B:235:ARG:HD2	2.44	0.52
14:L:134:GLU:HG3	40:L:9458:HOH:O	2.10	0.52
19:Q:75:ILE:HD13	19:Q:84:ILE:HD11	1.91	0.52
1:0:1878:G:O2'	1:0:1879:U:P	2.68	0.52
1:0:2032:U:H2'	1:0:2033:G:C5'	2.40	0.52
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.91	0.52
1:0:894:A:N1	6:C:87:ARG:NH2	2.57	0.52
6:C:233:THR:HG22	6:C:234:VAL:N	2.25	0.52
15:M:57:LYS:HE2	15:M:140:ALA:O	2.10	0.52
22:T:32:ARG:NH1	22:T:38:ARG:NH1	2.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:750:A:O3'	6:C:101:ASP:HB2	2.09	0.52
1:0:2626:C:H2'	1:0:2627:G:C8	2.45	0.52
4:A:217:ARG:HH11	4:A:217:ARG:CG	2.23	0.52
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.90	0.52
14:L:73:VAL:HG23	14:L:74:THR:N	2.25	0.52
14:L:92:ASP:HB3	14:L:95:ASP:OD2	2.10	0.52
27:Y:117:LEU:HA	27:Y:174:VAL:HG11	1.92	0.52
1:0:364:C:H2'	1:0:365:G:O4'	2.10	0.52
1:0:848:C:H5'	40:0:7728:HOH:O	2.09	0.52
1:0:1187:U:O2'	1:0:1189:A:H2	1.91	0.52
1:0:2346:C:H6	1:0:2346:C:O5'	1.93	0.52
14:L:119:THR:HG23	14:L:139:SER:OG	2.10	0.52
16:N:72:GLU:O	16:N:72:GLU:HG2	2.10	0.52
32:I:114:PRO:HG2	32:I:115:ASP:H	1.75	0.52
1:0:1738:C:H1'	40:0:7770:HOH:O	2.10	0.51
1:0:2415:A:N3	16:N:26:LEU:HD13	2.25	0.51
40:0:7093:HOH:O	27:Y:155:ARG:HD2	2.08	0.51
15:M:98:GLN:O	15:M:102:GLU:HG3	2.10	0.51
1:0:962:C:H1'	16:N:5:ARG:HH12	1.75	0.51
1:0:1060:C:H6	1:0:1060:C:H5'	1.76	0.51
1:0:1328:A:OP1	27:Y:169:ARG:HD2	2.10	0.51
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.45	0.51
2:9:3042:C:O2	7:D:76:ARG:NH1	2.43	0.51
4:A:128:LEU:HD21	4:A:131:HIS:HE1	1.75	0.51
8:E:35:TYR:HA	12:J:127:ILE:CD1	2.41	0.51
14:L:92:ASP:HA	14:L:121:ILE:HB	1.92	0.51
25:W:149:LEU:HG	25:W:153:MET:CE	2.40	0.51
9:F:48:VAL:HG23	9:F:74:PHE:CB	2.40	0.51
11:H:116:ALA:O	11:H:117:PHE:C	2.49	0.51
16:N:154:LEU:O	16:N:155:GLU:CB	2.58	0.51
27:Y:144:ARG:CG	27:Y:144:ARG:NH1	2.71	0.51
1:0:920:C:H5"	1:0:921:G:O5'	2.10	0.51
1:0:1181:A:N1	1:0:1192:A:O2'	2.40	0.51
1:0:1242:A:C5'	12:J:82:THR:HG23	2.31	0.51
1:0:2064:U:H5'	1:0:2652:U:O3'	2.10	0.51
2:9:3049:G:C2'	2:9:3050:G:H5'	2.41	0.51
5:B:258:GLY:H	5:B:260:HIS:CE1	2.28	0.51
8:E:11:VAL:HG12	8:E:12:ASP:N	2.24	0.51
8:E:154:ILE:HG13	8:E:156:ASP:OD1	2.10	0.51
27:Y:112:GLU:HA	27:Y:112:GLU:OE1	2.10	0.51
28:Z:42:CYS:SG	28:Z:44:GLU:HB2	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:53:ASP:OD1	9:F:80:GLN:HB2	2.11	0.51
13:K:74:VAL:HG11	13:K:113:ILE:CG1	2.32	0.51
13:K:125:ALA:C	13:K:127:ALA:H	2.13	0.51
15:M:71:SER:O	15:M:73:ARG:NH1	2.43	0.51
20:R:39:THR:HB	20:R:42:GLU:HG3	1.93	0.51
1:0:2769:C:H2'	1:0:2770:G:C5'	2.40	0.51
6:C:154:VAL:O	6:C:158:GLU:HG3	2.11	0.51
8:E:23:GLU:HG2	8:E:28:SER:CB	2.41	0.51
9:F:28:ALA:CB	9:F:99:THR:HG23	2.41	0.51
11:H:170:ASN:N	11:H:170:ASN:ND2	2.59	0.51
24:V:25:THR:HG22	24:V:29:ASN:HD21	1.75	0.51
32:I:113:HIS:N	32:I:114:PRO:CD	2.73	0.51
1:0:1234:U:N3	5:B:244:PRO:HB3	2.26	0.51
1:0:1594:C:OP2	18:P:120:ARG:HD2	2.10	0.51
1:0:2505:G:C2'	1:0:2506:A:H5'	2.41	0.51
6:C:136:VAL:HG22	6:C:137:PRO:HA	1.93	0.51
7:D:128:LEU:HB2	40:D:6007:HOH:O	2.11	0.51
9:F:48:VAL:HG23	9:F:74:PHE:HB3	1.93	0.51
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.91	0.51
28:Z:26:VAL:O	28:Z:30:GLU:HG3	2.10	0.51
1:0:1730:G:C5'	1:0:1731:C:H6	2.23	0.51
1:0:2712:G:H5'	40:K:4183:HOH:O	2.11	0.51
9:F:91:VAL:CG1	9:F:92:GLY:H	2.14	0.51
11:H:56:GLN:NE2	11:H:126:ARG:HE	2.09	0.51
12:J:88:PRO:O	12:J:94:GLY:HA3	2.11	0.51
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.31	0.51
15:M:64:ARG:HD2	40:M:9384:HOH:O	2.09	0.51
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.46	0.51
1:0:299:U:H5'	40:0:7789:HOH:O	2.11	0.51
1:0:475:G:OP1	6:C:73:LEU:CD2	2.58	0.51
1:0:1351:G:OP1	6:C:96:LYS:NZ	2.39	0.51
1:0:1400:C:H4'	26:X:56:GLU:HG2	1.92	0.51
1:0:1701:A:H5"	1:0:1702:U:H3'	1.93	0.51
5:B:215:VAL:HB	5:B:234:ARG:HH12	1.76	0.51
5:B:254:GLN:HG2	5:B:255:GLY:H	1.76	0.51
20:R:82:GLU:O	20:R:86:LYS:HG3	2.11	0.51
25:W:5:VAL:O	25:W:52:VAL:CG2	2.59	0.51
25:W:38:THR:O	25:W:42:ARG:HB2	2.10	0.51
1:0:134:U:H6	1:0:134:U:H5"	1.75	0.51
1:0:328:U:O4'	6:C:202:THR:CG2	2.59	0.51
1:0:2456:A:H2'	1:0:2457:U:C6	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3002:U:OP2	2:9:3003:A:H5'	2.10	0.51
8:E:35:TYR:HA	12:J:127:ILE:HD12	1.93	0.51
9:F:36:THR:HG23	9:F:97:ALA:HB2	1.92	0.51
12:J:4:ALA:O	12:J:5:GLU:HB2	2.11	0.51
14:L:145:LEU:HD23	14:L:145:LEU:O	2.10	0.51
1:0:776:A:OP1	29:1:28:HIS:HE1	1.95	0.50
1:0:1218:U:H2'	1:0:1219:U:C6	2.46	0.50
1:0:2718:C:H5'	1:0:2718:C:C6	2.44	0.50
8:E:49:ILE:HD11	8:E:69:ILE:HD12	1.92	0.50
12:J:107:ASN:HD22	12:J:109:TYR:H	1.58	0.50
15:M:72:ALA:HB2	15:M:93:ARG:HG2	1.93	0.50
23:U:9:CYS:HA	23:U:52:THR:HG23	1.93	0.50
25:W:139:GLY:O	25:W:141:HIS:CD2	2.63	0.50
27:Y:112:GLU:CD	27:Y:115:ARG:NH1	2.64	0.50
1:0:588:G:O6	25:W:154:ARG:NH1	2.45	0.50
1:0:1462:C:H2'	1:0:1463:A:C8	2.47	0.50
1:0:2896:A:H5"	40:X:5399:HOH:O	2.10	0.50
40:9:1361:HOH:O	16:N:41:LYS:HE3	2.10	0.50
5:B:41:PHE:CD2	5:B:190:MET:HE3	2.47	0.50
17:O:42:GLU:HB2	40:O:2176:HOH:O	2.10	0.50
32:I:101:SER:H	32:I:104:GLN:NE2	2.09	0.50
1:0:870:G:OP2	4:A:3:ARG:HD3	2.12	0.50
1:0:945:U:H2'	1:0:946:C:C6	2.46	0.50
1:0:2661:U:H3	1:0:2812:A:H62	1.60	0.50
2:9:3057:A:C8	7:D:141:VAL:HG21	2.46	0.50
4:A:36:ASP:C	4:A:38:ILE:H	2.15	0.50
23:U:9:CYS:O	23:U:52:THR:HG23	2.11	0.50
32:I:105:VAL:HG11	32:I:129:VAL:HG22	1.92	0.50
1:0:241:A:C2	1:0:378:A:H4'	2.47	0.50
1:0:407:A:H2'	1:0:408:A:C8	2.47	0.50
1:0:2414:A:H2'	1:0:2415:A:C8	2.47	0.50
1:0:2487:C:H1'	40:0:5938:HOH:O	2.10	0.50
4:A:192:VAL:HG11	4:A:207:GLN:HB3	1.93	0.50
14:L:104:ASP:O	14:L:105:TYR:HB3	2.11	0.50
14:L:143:THR:O	14:L:147:GLU:HG3	2.10	0.50
17:O:53:GLN:HE21	17:O:56:GLU:CD	2.15	0.50
1:0:447:A:OP2	22:T:1:SER:HB2	2.11	0.50
1:0:2726:U:O2	1:0:2749:U:O5'	2.30	0.50
5:B:307:ARG:HB3	40:B:9642:HOH:O	2.11	0.50
6:C:236:THR:HG22	6:C:239:ALA:CB	2.41	0.50
7:D:25:MET:HE1	7:D:37:ALA:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:38:LYS:HE2	11:H:42:ASP:HB2	1.93	0.50
15:M:164:THR:CG2	15:M:165:GLY:N	2.74	0.50
20:R:119:VAL:HG12	20:R:119:VAL:O	2.11	0.50
22:T:71:VAL:CG1	22:T:72:ILE:N	2.74	0.50
32:I:138:THR:HG22	32:I:139:ILE:N	2.26	0.50
1:0:1350:U:H2'	1:0:1351:G:O4'	2.11	0.50
4:A:39:ALA:HB3	4:A:61:GLU:OE2	2.11	0.50
5:B:16:ARG:NH2	40:B:9557:HOH:O	2.39	0.50
5:B:162:MET:CE	5:B:308:LEU:HD21	2.36	0.50
15:M:41:GLU:HG3	40:M:9344:HOH:O	2.12	0.50
15:M:48:LYS:O	15:M:52:GLN:HG3	2.12	0.50
1:0:119:A:H2'	1:0:120:A:H5"	1.93	0.50
1:0:2265:U:H2'	1:0:2266:A:C8	2.47	0.50
1:0:2507:G:H2'	1:0:2510:C:N4	2.27	0.50
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.41	0.50
12:J:47:THR:HG22	12:J:48:GLY:N	2.26	0.50
13:K:28:GLU:HB3	13:K:59:LYS:HB2	1.93	0.50
13:K:132:VAL:HG11	23:U:22:VAL:HG22	1.93	0.50
21:S:33:SER:O	21:S:37:VAL:HG23	2.10	0.50
31:3:35:TRP:HB2	40:3:9493:HOH:O	2.12	0.50
1:0:292:G:H2'	1:0:358:G:N2	2.27	0.50
1:0:1477:C:H5'	1:0:1868:G:C5'	2.41	0.50
1:0:2524:G:N2	1:0:2526:C:H5	2.10	0.50
40:0:3164:HOH:O	25:W:119:HIS:HE1	1.95	0.50
4:A:191:GLY:HA2	4:A:194:MET:HE3	1.91	0.50
7:D:136:ARG:HB3	7:D:137:PRO:HD2	1.93	0.50
11:H:158:THR:HB	11:H:159:PRO:HD3	1.94	0.50
12:J:13:ASP:OD1	12:J:15:ARG:HB3	2.12	0.50
16:N:36:ALA:O	16:N:37:ARG:HD2	2.12	0.50
1:0:65:C:O2'	1:0:66:G:H5'	2.12	0.50
6:C:104:ASP:O	6:C:108:GLN:HG3	2.12	0.50
7:D:25:MET:CE	7:D:41:LEU:HG	2.38	0.50
8:E:20:ILE:HD11	8:E:40:VAL:CG1	2.39	0.50
10:G:12:ILE:HD12	40:G:692:HOH:O	2.11	0.50
40:0:5157:HOH:O	4:A:206:ARG:HD3	2.11	0.49
2:9:3023:U:O2'	2:9:3024:U:H4'	2.12	0.49
8:E:7:ILE:HG22	8:E:45:ASP:O	2.11	0.49
8:E:166:VAL:HG12	40:E:3134:HOH:O	2.12	0.49
17:O:97:SER:OG	17:O:100:GLN:HG3	2.12	0.49
18:P:141:ILE:C	18:P:143:ALA:H	2.14	0.49
20:R:84:ALA:O	20:R:88:PHE:HD1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:29:ASP:OD1	21:S:31:ARG:NH1	2.45	0.49
27:Y:115:ARG:NE	40:Y:9356:HOH:O	2.45	0.49
1:0:1279:U:O2	1:0:1279:U:H2'	2.12	0.49
1:0:2072:G:H3'	1:0:2073:G:C5'	2.42	0.49
5:B:212:GLN:HB2	5:B:257:THR:CG2	2.38	0.49
7:D:25:MET:CE	7:D:40:ILE:HD11	2.42	0.49
16:N:114:LYS:O	16:N:118:ILE:HG13	2.12	0.49
24:V:39:ALA:O	24:V:41:GLU:N	2.44	0.49
32:I:74:PRO:C	32:I:112:LYS:HZ1	2.14	0.49
1:0:944:G:H21	25:W:44:MET:CE	2.26	0.49
1:0:2541:U:C2	1:0:2619:UR3:H3U2	2.47	0.49
1:0:2911:C:O2'	1:0:2912:C:H5'	2.12	0.49
11:H:27:LYS:H	11:H:59:HIS:CD2	2.20	0.49
20:R:104:PHE:HB3	20:R:109:MET:HE1	1.94	0.49
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.77	0.49
27:Y:203:VAL:CG1	27:Y:228:VAL:HG22	2.42	0.49
28:Z:30:GLU:HG2	28:Z:33:MET:HE3	1.95	0.49
1:0:2889:U:H4'	1:0:2890:A:H5'	1.95	0.49
4:A:232:ARG:NH2	4:A:236:GLY:O	2.37	0.49
6:C:236:THR:H	6:C:239:ALA:HB3	1.77	0.49
11:H:58:ARG:HG3	11:H:58:ARG:NH1	2.27	0.49
20:R:29:LYS:NZ	40:R:9451:HOH:O	2.45	0.49
1:0:926:A:O2'	14:L:41:HIS:HD2	1.96	0.49
1:0:1200:A:H3'	40:0:6281:HOH:O	2.11	0.49
1:0:2502:C:H2'	1:0:2503:A:H5'	1.95	0.49
6:C:118:THR:O	6:C:136:VAL:HG13	2.11	0.49
11:H:45:VAL:HA	11:H:167:PRO:O	2.12	0.49
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.94	0.49
29:1:25:LYS:O	29:1:25:LYS:HG2	2.12	0.49
1:0:309:C:OP1	22:T:97:ARG:NH2	2.39	0.49
1:0:678:G:OP2	6:C:107:ARG:NH2	2.45	0.49
1:0:1592:G:H2'	1:0:1593:C:C6	2.48	0.49
1:0:2100:A:H4'	6:C:64:GLY:O	2.12	0.49
1:0:2346:C:H4'	7:D:52:THR:CG2	2.42	0.49
4:A:217:ARG:HH11	4:A:217:ARG:HG3	1.76	0.49
5:B:320:GLN:HE21	5:B:321:PRO:HD2	1.77	0.49
7:D:24:HIS:HB2	7:D:72:LYS:CB	2.43	0.49
12:J:142:ASN:O	12:J:144:THR:N	2.46	0.49
14:L:144:ASP:HA	14:L:147:GLU:OE1	2.11	0.49
21:S:8:PRO:HD2	24:V:32:ALA:HA	1.95	0.49
1:0:820:G:O2'	1:0:856:G:H4'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1118:A:C8	1:0:1118:A:C3'	2.90	0.49
2:9:3052:A:O2'	2:9:3053:G:H5'	2.13	0.49
6:C:27:ARG:O	6:C:31:ILE:HG13	2.13	0.49
8:E:81:GLU:HG2	8:E:134:SER:CB	2.42	0.49
11:H:46:GLN:NE2	11:H:137:TYR:HE2	2.08	0.49
12:J:45:VAL:HG22	12:J:46:ILE:N	2.27	0.49
13:K:62:PRO:HG3	13:K:65:ARG:NH2	2.26	0.49
27:Y:145:LYS:HE2	40:Y:9405:HOH:O	2.11	0.49
1:0:1666:C:C2'	1:0:1667:A:C5'	2.91	0.49
7:D:24:HIS:HB2	7:D:72:LYS:HB3	1.94	0.49
16:N:110:THR:HB	16:N:113:SER:HG	1.75	0.49
1:0:542:A:H2'	1:0:543:G:O4'	2.12	0.49
7:D:50:VAL:O	7:D:71:ALA:HA	2.13	0.49
9:F:111:ILE:O	9:F:115:VAL:HG23	2.13	0.49
16:N:82:TYR:OH	16:N:176:ARG:NH1	2.46	0.49
20:R:132:ARG:NH2	40:R:9494:HOH:O	2.46	0.49
22:T:112:LEU:HD23	22:T:119:ALA:HB3	1.93	0.49
1:0:775:G:OP1	29:1:16:HIS:HE1	1.96	0.49
1:0:797:A:H4'	28:Z:10:ARG:N	2.28	0.49
1:0:1506:U:H6	1:0:1506:U:H5'	1.78	0.49
1:0:2090:G:H2'	1:0:2091:G:C8	2.47	0.49
1:0:2846:C:H4'	40:0:5619:HOH:O	2.11	0.49
5:B:265:LEU:HD21	5:B:316:ARG:HD3	1.95	0.49
30:2:35:ARG:HB2	40:2:2691:HOH:O	2.11	0.49
40:0:4331:HOH:O	22:T:9:LYS:HD3	2.13	0.48
6:C:246:ARG:NH1	40:C:9174:HOH:O	2.45	0.48
8:E:69:ILE:HA	8:E:72:MET:CE	2.43	0.48
16:N:36:ALA:C	16:N:37:ARG:HD2	2.34	0.48
16:N:167:ASP:C	16:N:168:LEU:HG	2.34	0.48
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.94	0.48
22:T:71:VAL:HG13	22:T:91:LEU:O	2.13	0.48
22:T:89:ARG:O	22:T:89:ARG:HG3	2.13	0.48
24:V:64:GLY:O	24:V:65:ASP:CB	2.60	0.48
1:0:920:C:H4'	1:0:921:G:C2	2.49	0.48
1:0:999:C:H2'	1:0:1000:C:O4'	2.12	0.48
1:0:1119:G:N2	1:0:1246:A:N1	2.61	0.48
17:O:14:LEU:CG	17:O:102:ILE:HD11	2.43	0.48
1:0:475:G:OP1	6:C:73:LEU:HD22	2.12	0.48
1:0:2408:A:H4'	31:3:15:ASN:O	2.13	0.48
4:A:52:SER:HB2	4:A:164:ARG:HH11	1.78	0.48
5:B:190:MET:CE	5:B:194:PHE:CD1	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:104:ASP:HA	6:C:107:ARG:NH1	2.27	0.48
7:D:25:MET:CE	7:D:37:ALA:HB1	2.42	0.48
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.49	0.48
28:Z:36:ASP:HB3	28:Z:45:ASP:O	2.13	0.48
1:0:319:A:H4'	1:0:338:C:C5	2.48	0.48
1:0:1183:C:H5	1:0:1192:A:OP1	1.96	0.48
1:0:1527:A:H1'	1:0:1528:A:C8	2.48	0.48
1:0:2102:G:H5"	1:0:2538:A:C2	2.48	0.48
1:0:2508:C:H2'	40:0:7232:HOH:O	2.12	0.48
26:X:34:ARG:NH1	26:X:48:VAL:O	2.46	0.48
6:C:157:LEU:HD22	6:C:162:VAL:CG1	2.43	0.48
16:N:36:ALA:HB1	16:N:118:ILE:HD12	1.96	0.48
22:T:38:ARG:NH1	22:T:38:ARG:HG3	2.29	0.48
24:V:39:ALA:C	24:V:41:GLU:N	2.65	0.48
1:0:1921:A:O2'	1:0:1922:A:H5'	2.14	0.48
1:0:2472:C:O2'	1:0:2634:G:H4'	2.13	0.48
1:0:2509:A:H2'	1:0:2510:C:O4'	2.13	0.48
11:H:34:GLY:HA3	11:H:84:LYS:HA	1.95	0.48
16:N:69:TYR:CE2	16:N:184:ILE:HG13	2.49	0.48
16:N:73:ALA:N	40:N:9360:HOH:O	2.45	0.48
17:O:80:ASP:OD1	17:O:81:PHE:N	2.45	0.48
1:0:666:A:H2'	1:0:667:C:O4'	2.14	0.48
1:0:2032:U:H2'	1:0:2033:G:H5'	1.94	0.48
4:A:72:GLU:HG3	28:Z:66:GLY:HA2	1.95	0.48
5:B:56:ASP:HB3	5:B:322:ARG:HE	1.79	0.48
12:J:131:THR:HB	12:J:134:GLU:OE1	2.14	0.48
13:K:27:ARG:HD2	40:K:4747:HOH:O	2.14	0.48
14:L:10:SER:O	14:L:11:ARG:HB3	2.14	0.48
15:M:24:GLN:NE2	15:M:24:GLN:HA	2.28	0.48
15:M:59:GLY:HA3	15:M:141:ILE:HD12	1.95	0.48
26:X:7:GLU:HA	26:X:74:ALA:O	2.14	0.48
1:0:969:G:H1	1:0:999:C:H42	1.62	0.48
1:0:1724:U:H5"	40:0:4309:HOH:O	2.12	0.48
1:0:2883:A:H2'	1:0:2884:G:O4'	2.14	0.48
9:F:60:VAL:O	9:F:60:VAL:CG1	2.61	0.48
12:J:107:ASN:HD21	12:J:109:TYR:HB2	1.78	0.48
14:L:97:VAL:HG12	14:L:98:GLU:O	2.13	0.48
14:L:123:ASP:O	14:L:146:GLY:HA2	2.13	0.48
15:M:184:ARG:HG3	15:M:185:PRO:HA	1.96	0.48
18:P:98:ILE:HD12	18:P:102:ARG:CZ	2.43	0.48
25:W:65:VAL:CG1	25:W:116:LEU:HD13	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:653:C:H2'	1:0:654:A:C8	2.48	0.48
1:0:2587:OMU:O5'	1:0:2587:OMU:H6	2.13	0.48
6:C:84:VAL:O	6:C:85:LYS:HB2	2.14	0.48
9:F:46:GLU:O	9:F:73:PRO:HD2	2.14	0.48
15:M:182:LYS:O	15:M:194:ALA:HB2	2.14	0.48
21:S:56:ASN:O	30:2:8:LYS:NZ	2.42	0.48
1:0:558:C:C2'	1:0:559:U:H5"	2.44	0.48
1:0:1739:G:H1'	1:0:2726:U:O4	2.13	0.48
1:0:1789:G:O6	18:P:73:HIS:HE1	1.97	0.48
1:0:2769:C:H2'	1:0:2770:G:H5'	1.95	0.48
40:0:5826:HOH:O	25:W:122:ARG:NH2	2.41	0.48
8:E:5:LEU:HD21	8:E:66:GLN:HG3	1.95	0.48
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.28	0.48
14:L:91:VAL:CG1	14:L:120:LEU:HD23	2.43	0.48
16:N:64:SER:C	16:N:66:LEU:H	2.17	0.48
17:O:96:VAL:HG13	17:O:100:GLN:HB2	1.96	0.48
24:V:1:THR:CG2	24:V:2:VAL:H	2.20	0.48
24:V:8:ILE:HG21	24:V:59:ILE:HG13	1.96	0.48
25:W:142:ASP:HB2	40:W:2729:HOH:O	2.14	0.48
1:0:1044:C:H5"	40:0:9649:HOH:O	2.13	0.47
1:0:1603:A:H5"	1:0:1605:G:H5'	1.96	0.47
1:0:1736:A:H1'	40:0:8086:HOH:O	2.14	0.47
1:0:2852:A:H5"	40:0:5770:HOH:O	2.14	0.47
5:B:41:PHE:CG	5:B:190:MET:HE3	2.49	0.47
14:L:61:ALA:HB2	14:L:105:TYR:CZ	2.49	0.47
15:M:43:PRO:HG3	15:M:62:VAL:HG21	1.95	0.47
15:M:79:ALA:HB3	15:M:81:ARG:HH12	1.79	0.47
1:0:2112:A:H2'	1:0:2113:G:C8	2.49	0.47
1:0:2895:C:H4'	40:X:4132:HOH:O	2.13	0.47
2:9:3048:C:H4'	16:N:141:ARG:HH21	1.79	0.47
5:B:267:LYS:HD2	40:B:9530:HOH:O	2.13	0.47
13:K:14:LYS:HG3	13:K:32:ILE:O	2.13	0.47
14:L:35:ARG:C	14:L:35:ARG:HD3	2.35	0.47
20:R:106:GLY:HA2	20:R:109:MET:CE	2.44	0.47
1:0:1730:G:H5"	1:0:1731:C:C6	2.49	0.47
1:0:2749:U:H5'	40:0:8433:HOH:O	2.13	0.47
1:0:2812:A:N7	40:0:7959:HOH:O	2.35	0.47
4:A:149:ASP:OD1	4:A:151:GLN:HB2	2.14	0.47
5:B:58:PRO:HA	5:B:63:GLU:CD	2.34	0.47
13:K:55:VAL:CG1	13:K:56:SER:N	2.77	0.47
22:T:81:LYS:HD2	22:T:87:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:154:ARG:HH12	27:Y:155:ARG:CG	2.21	0.47
1:0:1972:U:H2'	1:0:1973:A:C5'	2.44	0.47
1:0:2611:G:H5'	1:0:2613:G:C8	2.49	0.47
5:B:51:VAL:HG22	5:B:52:VAL:N	2.29	0.47
26:X:74:ALA:CB	26:X:85:VAL:HG22	2.44	0.47
31:3:11:CYS:HB2	31:3:20:HIS:CE1	2.50	0.47
1:0:317:A:OP1	22:T:52:ARG:O	2.33	0.47
1:0:558:C:C2'	1:0:559:U:C5'	2.93	0.47
40:0:7351:HOH:O	15:M:178:LYS:HB2	2.14	0.47
5:B:53:LEU:HD21	5:B:270:ILE:HD12	1.97	0.47
6:C:133:ARG:HH11	6:C:133:ARG:HG3	1.79	0.47
12:J:130:VAL:HG12	12:J:131:THR:N	2.30	0.47
16:N:152:GLU:C	16:N:154:LEU:H	2.16	0.47
17:O:59:VAL:HG21	17:O:111:VAL:HG21	1.94	0.47
23:U:11:THR:HG22	23:U:53:ASP:OD2	2.15	0.47
32:I:106:LYS:O	32:I:110:GLU:HG3	2.14	0.47
1:0:1979:G:O2'	1:0:1980:U:OP1	2.27	0.47
1:0:2545:U:OP2	5:B:2:GLN:NE2	2.47	0.47
1:0:2681:A:H4'	1:0:2682:C:H5'	1.97	0.47
1:0:2717:C:H2'	1:0:2718:C:C5'	2.40	0.47
1:0:2906:A:H5'	1:0:2907:C:O4'	2.15	0.47
2:9:3018:U:H2'	2:9:3019:G:C8	2.50	0.47
5:B:5:ARG:NH1	5:B:8:LYS:HE2	2.30	0.47
6:C:25:PRO:HG2	40:C:9125:HOH:O	2.14	0.47
11:H:29:ALA:HB3	11:H:66:ARG:HH12	1.80	0.47
16:N:166:ALA:O	16:N:167:ASP:O	2.33	0.47
1:0:29:C:C2'	1:0:30:U:H5'	2.44	0.47
1:0:185:G:H4'	1:0:186:A:H4'	1.96	0.47
1:0:1185:U:H2'	1:0:1186:C:C6	2.48	0.47
1:0:1406:A:H4'	1:0:1407:A:C5'	2.45	0.47
1:0:1881:A:OP1	4:A:199:HIS:HE1	1.97	0.47
1:0:2421:G:H4'	40:0:5324:HOH:O	2.13	0.47
1:0:2443:C:H1'	14:L:56:LYS:HE3	1.97	0.47
40:0:3822:HOH:O	32:I:92:PRO:HD3	2.13	0.47
2:9:3059:C:H2'	2:9:3060:C:C6	2.50	0.47
6:C:218:VAL:N	40:C:9225:HOH:O	2.48	0.47
7:D:84:LEU:HA	7:D:87:ALA:HB3	1.97	0.47
7:D:146:LYS:NZ	16:N:107:ASN:HD21	2.13	0.47
8:E:106:ASN:ND2	8:E:109:GLY:HA2	2.30	0.47
11:H:56:GLN:HE21	11:H:126:ARG:HE	1.61	0.47
13:K:98:VAL:HG22	13:K:102:GLU:C	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:80:ASP:HB2	14:L:90:ARG:HB3	1.96	0.47
14:L:98:GLU:O	14:L:99:GLU:HB2	2.15	0.47
23:U:52:THR:HG22	23:U:54:THR:H	1.77	0.47
24:V:5:VAL:CG1	24:V:9:ARG:NH1	2.78	0.47
26:X:25:ARG:HD2	40:X:5356:HOH:O	2.15	0.47
27:Y:184:GLU:OE1	27:Y:204:ARG:NH1	2.48	0.47
1:0:710:G:H5'	17:O:25:VAL:HG13	1.97	0.47
1:0:932:U:H2'	1:0:933:C:C6	2.50	0.47
1:0:1992:U:OP2	13:K:66:ARG:HD2	2.14	0.47
1:0:2503:A:P	11:H:151:ARG:HH22	2.38	0.47
5:B:41:PHE:HB3	5:B:190:MET:HE1	1.97	0.47
6:C:133:ARG:NE	6:C:138:VAL:HG22	2.29	0.47
9:F:118:LEU:O	9:F:119:ARG:HB3	2.15	0.47
14:L:53:ARG:HH22	14:L:57:VAL:HG12	1.80	0.47
32:I:131:THR:O	32:I:135:LEU:HG	2.15	0.47
1:0:1066:U:H2'	1:0:1067:A:C8	2.49	0.47
6:C:133:ARG:HE	6:C:138:VAL:HG22	1.79	0.47
13:K:101:ASN:O	13:K:102:GLU:HB2	2.15	0.47
26:X:61:ARG:HB2	26:X:65:ASN:HB2	1.97	0.47
26:X:66:THR:HG23	26:X:67:PRO:HD2	1.96	0.47
27:Y:99:ALA:HB2	27:Y:233:TYR:CE2	2.50	0.47
27:Y:187:VAL:HG23	27:Y:192:ASP:HB3	1.96	0.47
31:3:55:VAL:HG22	40:3:9444:HOH:O	2.15	0.47
1:0:475:G:C5'	6:C:73:LEU:HD23	2.45	0.47
1:0:1853:C:O2'	4:A:217:ARG:NH2	2.49	0.47
2:9:3091:C:H2'	2:9:3092:G:O4'	2.15	0.47
12:J:43:ARG:HG2	40:J:5361:HOH:O	2.15	0.47
16:N:37:ARG:NE	40:N:9330:HOH:O	2.47	0.47
29:1:28:HIS:CD2	29:1:30:LYS:HB2	2.50	0.47
1:0:1667:A:H5'	1:0:1667:A:C8	2.41	0.46
40:0:5274:HOH:O	16:N:21:HIS:HD2	1.97	0.46
4:A:36:ASP:HB2	4:A:85:SER:H	1.79	0.46
5:B:87:TYR:O	5:B:138:GLY:N	2.34	0.46
8:E:1:PRO:HG2	8:E:59:MET:SD	2.56	0.46
8:E:84:MET:HE1	8:E:148:ILE:HD12	1.97	0.46
8:E:126:ILE:HB	8:E:131:LEU:CD2	2.46	0.46
16:N:119:GLN:O	16:N:123:ILE:HG13	2.15	0.46
17:O:47:ARG:HH11	17:O:47:ARG:HG3	1.80	0.46
18:P:89:ASN:HB3	18:P:92:GLU:HB2	1.96	0.46
20:R:104:PHE:CB	20:R:109:MET:HE1	2.45	0.46
31:3:42:ARG:HH11	31:3:42:ARG:HG3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:447:A:OP1	22:T:2:LYS:HG2	2.15	0.46
1:0:1333:U:H2'	1:0:1334:C:H6	1.80	0.46
40:0:3549:HOH:O	6:C:78:ARG:HD3	2.15	0.46
2:9:3001:U:H5'	2:9:3121:C:O2	2.15	0.46
10:G:64:ASN:N	10:G:64:ASN:ND2	2.63	0.46
11:H:30:GLN:H	11:H:66:ARG:HH11	1.63	0.46
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.97	0.46
25:W:88:THR:CG2	25:W:89:ASP:H	2.28	0.46
26:X:85:VAL:HG12	26:X:86:GLU:N	2.30	0.46
32:I:139:ILE:CG2	32:I:140:GLU:N	2.78	0.46
1:0:57:C:H5'	24:V:46:ILE:HG21	1.98	0.46
2:9:3039:U:H1'	2:9:3044:A:N6	2.30	0.46
7:D:154:LYS:H	7:D:154:LYS:CD	2.24	0.46
16:N:167:ASP:O	16:N:168:LEU:HG	2.15	0.46
25:W:122:ARG:HG3	25:W:152:ALA:O	2.14	0.46
30:2:5:LYS:O	30:2:9:LYS:HG3	2.15	0.46
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.96	0.46
1:0:500:G:O2'	20:R:94:ASN:ND2	2.48	0.46
1:0:1211:G:O2'	1:0:1212:C:H5'	2.16	0.46
4:A:71:PRO:HD2	4:A:74:VAL:HG21	1.98	0.46
5:B:243:ASN:HA	5:B:244:PRO:C	2.36	0.46
5:B:305:ASP:O	5:B:306:LYS:CB	2.63	0.46
15:M:68:ARG:NH2	15:M:73:ARG:HD3	2.31	0.46
17:O:88:LYS:HD3	40:O:7061:HOH:O	2.15	0.46
20:R:119:VAL:O	20:R:119:VAL:CG1	2.63	0.46
23:U:20:MET:CE	23:U:30:HIS:NE2	2.79	0.46
1:0:399:C:H5'	15:M:179:GLY:O	2.15	0.46
2:9:3029:C:H2'	2:9:3030:C:C5'	2.42	0.46
3:4:76:DA:H5"	38:4:9701:SPS:C6	2.45	0.46
4:A:58:VAL:HG21	4:A:68:ILE:HD12	1.98	0.46
4:A:70:ALA:HA	4:A:71:PRO:HD3	1.76	0.46
4:A:132:ASP:OD1	4:A:133:ARG:N	2.49	0.46
9:F:21:GLU:O	9:F:24:ARG:HG3	2.15	0.46
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.46	0.46
20:R:33:ARG:NH1	40:R:9454:HOH:O	2.40	0.46
22:T:40:VAL:HG22	22:T:41:ARG:H	1.81	0.46
29:1:8:GLN:HE22	29:1:11:LYS:HZ1	1.62	0.46
1:0:462:A:H2'	40:0:5427:HOH:O	2.15	0.46
1:0:1717:A:H5"	18:P:54:LYS:HB2	1.97	0.46
1:0:2019:A:H5'	40:0:5087:HOH:O	2.16	0.46
14:L:120:LEU:HD12	14:L:133:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:143:THR:CG2	14:L:144:ASP:N	2.78	0.46
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.50	0.46
1:0:622:G:P	27:Y:148:GLY:HA3	2.55	0.46
1:0:1299:G:H5'	40:0:4642:HOH:O	2.15	0.46
4:A:96:LEU:HG	4:A:152:CYS:O	2.16	0.46
5:B:51:VAL:HG23	5:B:327:VAL:HG13	1.97	0.46
5:B:312:ARG:HD3	5:B:315:VAL:HG13	1.97	0.46
13:K:114:ALA:HB3	13:K:117:VAL:HG23	1.96	0.46
15:M:90:ARG:HB2	31:3:46:ILE:HD11	1.98	0.46
23:U:17:THR:CG2	23:U:18:GLY:H	2.27	0.46
25:W:29:VAL:O	25:W:30:ASN:HB2	2.16	0.46
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.15	0.46
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.15	0.46
1:0:57:C:H5'	24:V:46:ILE:CG2	2.46	0.46
1:0:951:A:O2'	1:0:952:G:H5'	2.16	0.46
1:0:2837:U:H2'	40:0:7315:HOH:O	2.14	0.46
4:A:66:ARG:HH11	4:A:66:ARG:HB2	1.80	0.46
11:H:18:GLU:HG3	11:H:19:TYR:CE1	2.51	0.46
15:M:95:LYS:HA	15:M:170:ASN:HD21	1.81	0.46
25:W:88:THR:CG2	25:W:90:TYR:HD1	2.27	0.46
31:3:69:TYR:O	31:3:77:ALA:HA	2.16	0.46
1:0:204:A:C2'	1:0:205:U:H5'	2.46	0.46
1:0:432:G:O2'	1:0:433:C:H5'	2.16	0.46
1:0:451:C:O2'	1:0:452:G:H5'	2.15	0.46
1:0:834:G:H3'	1:0:835:U:H4'	1.98	0.46
1:0:1940:C:H4'	40:0:7797:HOH:O	2.14	0.46
2:9:3006:C:H4'	16:N:35:VAL:HG11	1.98	0.46
4:A:125:ASN:HB3	4:A:158:VAL:HG12	1.98	0.46
4:A:126:ALA:HB1	4:A:138:VAL:CG1	2.46	0.46
5:B:140:LEU:HD23	40:B:9578:HOH:O	2.16	0.46
17:O:25:VAL:HG23	40:O:3062:HOH:O	2.16	0.46
22:T:41:ARG:NH1	22:T:42:VAL:O	2.49	0.46
26:X:25:ARG:NH2	40:X:5740:HOH:O	2.48	0.46
27:Y:144:ARG:NH1	40:Y:9377:HOH:O	2.49	0.46
1:0:1202:A:H2'	1:0:1203:G:O4'	2.16	0.46
2:9:3028:U:H2'	2:9:3029:C:C6	2.51	0.46
38:4:9701:SPS:O1	38:4:9701:SPS:H91	2.16	0.46
11:H:73:LEU:HD21	11:H:146:VAL:HA	1.98	0.46
14:L:144:ASP:O	14:L:147:GLU:HB2	2.16	0.46
17:O:26:TRP:HA	17:O:26:TRP:HE3	1.80	0.46
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:664:U:O4	1:0:681:G:H5"	2.16	0.45
1:0:1086:A:C6	25:W:11:VAL:HG11	2.51	0.45
1:0:1167:G:H2'	1:0:1168:C:O4'	2.16	0.45
1:0:1419:U:H2'	1:0:1685:A:C2	2.52	0.45
1:0:1730:G:H5'	1:0:1731:C:C6	2.50	0.45
1:0:2531:U:O2'	1:0:2532:A:H5'	2.16	0.45
1:0:2679:G:H2'	1:0:2681:A:OP2	2.15	0.45
5:B:41:PHE:CG	5:B:79:MET:HE2	2.51	0.45
5:B:71:VAL:CG1	5:B:296:LEU:HD22	2.46	0.45
5:B:138:GLY:O	5:B:139:ASP:O	2.34	0.45
7:D:159:PRO:O	7:D:163:VAL:HG23	2.17	0.45
8:E:81:GLU:HG2	8:E:134:SER:HB3	1.97	0.45
8:E:81:GLU:O	8:E:172:PRO:HD3	2.16	0.45
15:M:66:SER:HB3	15:M:128:TRP:NE1	2.31	0.45
18:P:135:ALA:HB1	18:P:139:ARG:NH1	2.31	0.45
20:R:82:GLU:OE1	20:R:86:LYS:HE3	2.16	0.45
23:U:52:THR:CG2	23:U:54:THR:HB	2.46	0.45
1:0:136:C:H2'	1:0:137:U:O4'	2.15	0.45
1:0:415:A:O2'	1:0:416:G:H5'	2.17	0.45
1:0:1165:G:O3'	1:0:1174:A:H4'	2.16	0.45
1:0:2825:C:H4'	1:0:2826:G:O5'	2.15	0.45
4:A:36:ASP:O	4:A:36:ASP:CG	2.54	0.45
9:F:26:THR:HG21	9:F:103:GLU:HG3	1.97	0.45
18:P:16:VAL:HG13	18:P:20:ARG:NH1	2.31	0.45
26:X:76:ARG:O	26:X:77:PHE:HB3	2.16	0.45
1:0:249:G:O2'	1:0:250:C:H5'	2.17	0.45
1:0:1135:G:H5'	40:0:6446:HOH:O	2.16	0.45
1:0:1829:A:H2'	1:0:1830:C:H5'	1.99	0.45
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.16	0.45
9:F:20:LEU:HB2	9:F:49:PHE:CZ	2.51	0.45
14:L:89:PHE:CD1	14:L:89:PHE:N	2.85	0.45
16:N:33:ARG:NH2	40:N:9350:HOH:O	2.50	0.45
23:U:14:GLU:OE1	23:U:15:PRO:HD2	2.17	0.45
25:W:88:THR:CG2	25:W:89:ASP:N	2.78	0.45
27:Y:106:THR:CG2	27:Y:107:PRO:HD2	2.47	0.45
1:0:289:G:H5'	40:0:5159:HOH:O	2.17	0.45
1:0:2619:UR3:H2'	1:0:2620:U:C6	2.51	0.45
2:9:3005:G:OP1	16:N:17:ARG:NH2	2.50	0.45
6:C:124:VAL:HA	6:C:230:GLY:O	2.16	0.45
8:E:16:ASP:O	8:E:17:HIS:HB2	2.15	0.45
8:E:101:GLU:HA	8:E:118:ILE:HG13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:54:VAL:HG11	12:J:138:THR:HG21	1.99	0.45
15:M:107:ARG:NH1	15:M:107:ARG:CG	2.78	0.45
22:T:12:ARG:NH1	40:T:3035:HOH:O	2.49	0.45
23:U:20:MET:CG	23:U:28:THR:HG23	2.47	0.45
1:0:734:U:H1'	1:0:737:A:N6	2.32	0.45
40:0:9834:HOH:O	4:A:11:ARG:HD3	2.17	0.45
7:D:51:ARG:HD3	40:D:7636:HOH:O	2.16	0.45
9:F:102:GLY:O	9:F:103:GLU:HB2	2.16	0.45
12:J:103:VAL:HG12	40:J:5907:HOH:O	2.16	0.45
13:K:109:LEU:CD1	13:K:113:ILE:HD11	2.46	0.45
15:M:164:THR:CG2	15:M:166:ALA:H	2.27	0.45
17:O:59:VAL:CG2	17:O:111:VAL:CG2	2.95	0.45
23:U:6:CYS:C	23:U:8:TYR:H	2.19	0.45
24:V:25:THR:HG22	24:V:29:ASN:ND2	2.32	0.45
1:0:371:U:H2'	1:0:372:A:H8	1.80	0.45
1:0:1130:U:H2'	1:0:1131:G:O4'	2.17	0.45
1:0:1624:A:H4'	1:0:1625:U:H5'	1.99	0.45
1:0:2697:A:H2'	1:0:2698:G:O4'	2.17	0.45
5:B:217:ARG:HG3	5:B:257:THR:CG2	2.47	0.45
6:C:168:ARG:NH2	6:C:190:ALA:O	2.50	0.45
7:D:167:GLU:C	7:D:169:THR:H	2.20	0.45
14:L:66:VAL:HG23	14:L:67:ARG:N	2.31	0.45
16:N:86:LEU:O	16:N:90:LEU:HG	2.15	0.45
20:R:25:PHE:CZ	20:R:29:LYS:HE2	2.50	0.45
26:X:43:VAL:CG1	26:X:47:ALA:HB3	2.45	0.45
1:0:968:G:O2'	1:0:969:G:H5'	2.17	0.45
1:0:1149:U:H5"	1:0:1151:G:O4'	2.17	0.45
1:0:1745:G:H22	1:0:2033:G:H5'	1.82	0.45
1:0:2289:G:H21	1:0:2291:A:H2	1.62	0.45
1:0:2356:A:H2'	1:0:2357:G:O4'	2.16	0.45
1:0:2506:A:O2'	1:0:2507:G:O5'	2.35	0.45
40:0:5514:HOH:O	11:H:58:ARG:HG3	2.16	0.45
4:A:122:SER:O	4:A:124:VAL:HG13	2.17	0.45
9:F:68:ASP:C	9:F:70:LYS:H	2.20	0.45
15:M:81:ARG:HG2	15:M:85:ARG:O	2.16	0.45
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.25	0.45
25:W:3:ALA:O	25:W:54:PHE:HA	2.17	0.45
26:X:30:MET:HB2	26:X:30:MET:HE3	1.76	0.45
26:X:73:ARG:NH1	26:X:88:GLU:HG2	2.32	0.45
1:0:59:A:H5'	40:0:4886:HOH:O	2.15	0.45
1:0:497:A:H2'	1:0:498:A:C5'	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1741:U:H3'	40:0:3369:HOH:O	2.16	0.45
4:A:130:THR:HG22	4:A:131:HIS:O	2.17	0.45
5:B:80:ARG:HB2	5:B:145:HIS:CE1	2.52	0.45
6:C:233:THR:HG22	6:C:234:VAL:H	1.82	0.45
6:C:236:THR:O	6:C:237:GLU:C	2.54	0.45
8:E:69:ILE:HA	8:E:72:MET:HE3	1.97	0.45
23:U:9:CYS:CA	23:U:52:THR:HG23	2.47	0.45
24:V:38:GLY:C	24:V:40:PRO:HD2	2.36	0.45
1:0:1151:G:OP1	10:G:63:ARG:NH1	2.50	0.45
1:0:1180:U:H1'	40:0:3822:HOH:O	2.17	0.45
1:0:1654:U:H2'	4:A:47:HIS:HD2	1.82	0.45
4:A:66:ARG:HH11	4:A:66:ARG:CB	2.29	0.45
4:A:88:ILE:HD13	4:A:100:PRO:CD	2.46	0.45
5:B:254:GLN:NE2	40:B:9588:HOH:O	2.49	0.45
7:D:60:GLU:O	7:D:61:PHE:C	2.55	0.45
13:K:119:GLN:O	13:K:119:GLN:HG2	2.17	0.45
30:2:20:ARG:HG3	30:2:21:VAL:N	2.31	0.45
31:3:75:GLY:HA2	40:3:9510:HOH:O	2.16	0.45
1:0:120:A:H2'	1:0:120:A:N3	2.32	0.45
1:0:968:G:H1'	11:H:32:LYS:HD2	1.98	0.45
1:0:2073:G:H5"	40:0:4398:HOH:O	2.16	0.45
1:0:2329:C:O2'	1:0:2330:U:H5'	2.17	0.45
4:A:128:LEU:HD21	4:A:131:HIS:CE1	2.51	0.45
7:D:10:PHE:CD1	7:D:11:HIS:N	2.85	0.45
7:D:170:TYR:O	7:D:171:ASP:CB	2.65	0.45
31:3:38:ARG:CB	31:3:42:ARG:HH12	2.25	0.45
1:0:1056:U:H2'	1:0:1057:A:O4'	2.16	0.44
1:0:1603:A:C5'	1:0:1605:G:H5'	2.47	0.44
1:0:1942:A:H3'	40:0:7797:HOH:O	2.17	0.44
1:0:2415:A:H2'	1:0:2416:G:H5'	1.98	0.44
1:0:2591:C:H2'	1:0:2592:G:O4'	2.17	0.44
6:C:157:LEU:HD22	6:C:162:VAL:HG11	1.98	0.44
9:F:109:GLU:HG2	9:F:113:ASP:OD2	2.17	0.44
11:H:29:ALA:C	11:H:30:GLN:HG3	2.38	0.44
12:J:19:MET:HE2	12:J:132:LEU:HD11	1.98	0.44
13:K:87:ARG:NH1	40:K:4066:HOH:O	2.49	0.44
16:N:74:PRO:HG2	16:N:159:TYR:CE1	2.52	0.44
18:P:13:VAL:HG11	18:P:40:VAL:CG1	2.47	0.44
18:P:18:LYS:O	18:P:21:VAL:HG13	2.17	0.44
26:X:25:ARG:HD3	26:X:64:ALA:O	2.17	0.44
1:0:1250:C:O2'	1:0:1251:C:H5'	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1435:U:H5'	40:0:3201:HOH:O	2.16	0.44
1:0:1835:U:C5	1:0:1840:A:N7	2.69	0.44
2:9:3051:A:H5'	16:N:160:SER:HB2	1.99	0.44
2:9:3052:A:H2'	2:9:3053:G:O4'	2.17	0.44
2:9:3064:C:C2'	2:9:3065:A:H5'	2.48	0.44
5:B:60:SER:HA	5:B:61:PRO:HD3	1.86	0.44
5:B:168:GLY:O	5:B:169:GLY:O	2.36	0.44
5:B:277:GLU:N	5:B:278:PRO:HD2	2.32	0.44
6:C:49:ASP:HB3	6:C:52:ALA:HB2	1.99	0.44
6:C:142:ASP:OD1	6:C:236:THR:HG23	2.16	0.44
7:D:91:ALA:HB2	7:D:106:PHE:CD2	2.52	0.44
7:D:154:LYS:HD2	7:D:154:LYS:N	2.26	0.44
9:F:117:GLU:C	9:F:119:ARG:H	2.21	0.44
10:G:19:GLU:HG2	10:G:66:LEU:HD13	1.99	0.44
22:T:53:GLY:HA3	40:T:6384:HOH:O	2.17	0.44
26:X:12:ILE:HD12	26:X:36:HIS:CG	2.52	0.44
1:0:1166:A:N6	1:0:1180:U:H3	2.00	0.44
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.83	0.44
1:0:1768:C:H2'	1:0:1769:C:O4'	2.17	0.44
1:0:1972:U:H2'	1:0:1973:A:H5"	1.98	0.44
1:0:2456:A:H2'	1:0:2457:U:H6	1.83	0.44
2:9:3108:C:O2'	2:9:3109:G:H5'	2.16	0.44
6:C:246:ARG:NH1	6:C:246:ARG:HB3	2.32	0.44
8:E:116:THR:CG2	8:E:151:LEU:HD22	2.47	0.44
10:G:68:GLU:O	10:G:72:ASP:HB2	2.18	0.44
16:N:108:SER:HA	16:N:109:PRO:HD3	1.82	0.44
27:Y:107:PRO:HD3	27:Y:182:PHE:CE1	2.52	0.44
31:3:91:GLN:O	31:3:92:GLU:HB2	2.17	0.44
1:0:177:A:H2'	1:0:178:U:O4'	2.16	0.44
1:0:447:A:OP1	22:T:1:SER:HB2	2.17	0.44
1:0:2073:G:H3'	40:0:4398:HOH:O	2.18	0.44
1:0:2361:A:H2'	1:0:2362:A:C8	2.51	0.44
4:A:99:ILE:O	4:A:131:HIS:CE1	2.70	0.44
4:A:164:ARG:NE	40:A:9572:HOH:O	2.50	0.44
7:D:66:GLY:O	7:D:67:ASP:HB3	2.17	0.44
7:D:173:GLU:OE1	7:D:174:VAL:HG23	2.18	0.44
12:J:63:ILE:CG2	12:J:64:GLY:N	2.79	0.44
15:M:95:LYS:HD2	15:M:99:ARG:HG2	1.98	0.44
17:O:38:ARG:NH1	40:O:7674:HOH:O	2.50	0.44
18:P:115:SER:HG	18:P:118:GLN:HG3	1.81	0.44
1:0:794:U:H3	1:0:819:A:H61	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2364:A:H5"	19:Q:15:LYS:HD3	2.00	0.44
40:0:9644:HOH:O	14:L:30:ARG:HD2	2.16	0.44
8:E:101:GLU:HB3	8:E:117:THR:HA	2.00	0.44
15:M:86:GLN:O	15:M:88:VAL:HG23	2.16	0.44
16:N:112:GLY:HA2	16:N:137:ALA:N	2.32	0.44
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.83	0.44
1:0:602:A:O2'	1:0:605:C:H4'	2.17	0.44
2:9:3092:G:H2'	2:9:3093:A:C8	2.53	0.44
5:B:24:PRO:CG	5:B:204:GLY:HA2	2.48	0.44
5:B:36:PRO:HB3	5:B:174:ARG:CB	2.47	0.44
5:B:74:ILE:HD13	5:B:309:VAL:HG21	2.00	0.44
6:C:7:ASP:OD1	6:C:11:ASN:N	2.50	0.44
11:H:76:GLU:O	11:H:77:LEU:HD23	2.16	0.44
14:L:145:LEU:HD23	14:L:145:LEU:C	2.37	0.44
16:N:168:LEU:HA	16:N:169:PRO:HD3	1.77	0.44
23:U:4:ARG:HG2	23:U:4:ARG:NH1	2.31	0.44
25:W:119:HIS:HD2	25:W:120:PRO:O	2.00	0.44
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.53	0.44
32:I:93:GLN:HA	32:I:96:PHE:HE2	1.83	0.44
1:0:220:C:H1'	40:0:6282:HOH:O	2.17	0.44
1:0:236:A:H8	1:0:236:A:OP1	2.01	0.44
1:0:1025:C:H5'	25:W:23:MET:O	2.17	0.44
1:0:1098:A:O3'	25:W:129:LYS:HE2	2.18	0.44
1:0:1120:U:H5"	1:0:1120:U:C6	2.53	0.44
1:0:2791:U:H1'	1:0:2792:A:H5"	1.99	0.44
5:B:14:GLY:HA2	5:B:15:PRO:C	2.37	0.44
5:B:225:GLY:HA3	40:B:9567:HOH:O	2.18	0.44
11:H:66:ARG:HD3	40:H:9545:HOH:O	2.18	0.44
18:P:63:ARG:NH2	40:P:190:HOH:O	2.51	0.44
20:R:39:THR:CG2	20:R:107:GLU:O	2.66	0.44
21:S:57:THR:HG22	21:S:59:ASP:H	1.81	0.44
24:V:20:LEU:HD11	24:V:53:ILE:HG23	2.00	0.44
28:Z:30:GLU:HA	28:Z:33:MET:HE3	1.99	0.44
1:0:111:C:HO2'	29:1:20:ARG:HG2	1.76	0.44
1:0:1182:C:H1'	1:0:1192:A:C8	2.50	0.44
1:0:1476:A:O2'	1:0:1868:G:H5'	2.18	0.44
1:0:1751:G:C2'	1:0:1752:G:H5"	2.42	0.44
4:A:135:VAL:HG13	4:A:135:VAL:O	2.17	0.44
8:E:101:GLU:OE2	8:E:115:ARG:HD3	2.17	0.44
1:0:90:A:H2'	1:0:91:G:O4'	2.18	0.44
1:0:335:U:H4'	22:T:92:ASP:OD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:407:A:H5'	40:0:6540:HOH:O	2.17	0.44
1:0:926:A:O2'	14:L:41:HIS:CD2	2.71	0.44
1:0:1852:A:H5"	4:A:232:ARG:O	2.18	0.44
1:0:1926:G:H2'	1:0:1927:A:H8	1.82	0.44
1:0:2506:A:O2'	1:0:2507:G:P	2.76	0.44
40:0:5826:HOH:O	25:W:119:HIS:CG	2.71	0.44
11:H:96:ARG:NH2	40:H:9498:HOH:O	2.50	0.44
14:L:34:GLY:HA3	14:L:38:HIS:CE1	2.53	0.44
19:Q:75:ILE:HD13	19:Q:84:ILE:CD1	2.48	0.44
21:S:57:THR:HG23	40:S:9487:HOH:O	2.17	0.44
27:Y:209:VAL:HG12	27:Y:214:ARG:HG3	1.99	0.44
1:0:1203:G:O2'	1:0:1204:C:H5'	2.17	0.43
1:0:1252:A:H2'	1:0:1253:C:O4'	2.17	0.43
1:0:2254:G:O2'	1:0:2255:A:H5'	2.18	0.43
40:0:5006:HOH:O	30:2:39:ARG:HG2	2.18	0.43
4:A:26:ASP:OD1	4:A:26:ASP:O	2.36	0.43
5:B:162:MET:HG3	5:B:310:ARG:HD3	2.00	0.43
9:F:11:ASP:O	9:F:14:ASP:HB2	2.17	0.43
11:H:99:LYS:HD3	11:H:119:LYS:HD3	1.98	0.43
15:M:36:ALA:HB1	40:M:9353:HOH:O	2.17	0.43
20:R:18:LEU:HB2	20:R:143:VAL:HG13	1.98	0.43
20:R:95:ALA:HB2	20:R:145:LEU:HD23	2.00	0.43
24:V:12:THR:HG23	24:V:14:ALA:H	1.82	0.43
30:2:48:ASP:O	30:2:49:GLU:CB	2.65	0.43
1:0:262:A:OP2	9:F:91:VAL:HG11	2.18	0.43
1:0:263:U:C2	9:F:59:ILE:HD12	2.53	0.43
1:0:1163:G:H2'	1:0:1164:U:C5	2.52	0.43
1:0:1306:U:OP1	6:C:184:ARG:HD2	2.18	0.43
1:0:2491:G:H1'	40:0:7345:HOH:O	2.17	0.43
40:9:3472:HOH:O	16:N:41:LYS:HD3	2.17	0.43
6:C:46:TYR:CE2	6:C:98:ARG:NH1	2.86	0.43
7:D:51:ARG:NH1	7:D:68:PRO:HB3	2.32	0.43
12:J:132:LEU:HD23	12:J:132:LEU:HA	1.89	0.43
20:R:96:VAL:HG13	20:R:106:GLY:HA3	2.00	0.43
25:W:141:HIS:HB2	25:W:146:ILE:HG12	2.00	0.43
26:X:43:VAL:CG1	26:X:44:ASP:N	2.81	0.43
1:0:137:U:H2'	1:0:139:C:C5	2.53	0.43
1:0:196:G:H1'	1:0:198:A:N7	2.34	0.43
1:0:449:A:N7	6:C:43:LYS:HG2	2.33	0.43
1:0:699:C:H2'	1:0:744:G:O4'	2.18	0.43
1:0:1972:U:C2'	1:0:1973:A:H5"	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:205:VAL:O	5:B:307:ARG:NE	2.49	0.43
9:F:32:GLY:N	40:F:3111:HOH:O	2.50	0.43
9:F:49:PHE:HE1	9:F:98:VAL:HG23	1.84	0.43
1:0:371:U:H2'	1:0:372:A:C8	2.53	0.43
1:0:921:G:H4'	1:0:924:G:N1	2.33	0.43
1:0:1015:C:H2'	1:0:1016:U:C6	2.53	0.43
1:0:1132:A:N6	1:0:1229:C:H2'	2.33	0.43
1:0:1218:U:H2'	1:0:1219:U:H6	1.82	0.43
1:0:1342:C:O2'	1:0:1343:C:H5'	2.18	0.43
1:0:1406:A:H5'	1:0:1407:A:C8	2.54	0.43
1:0:2649:A:O4'	1:0:2650:U:H5	2.01	0.43
13:K:30:LYS:O	13:K:55:VAL:HG13	2.18	0.43
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.34	0.43
1:0:93:C:H5"	24:V:1:THR:CB	2.43	0.43
1:0:308:U:C2	22:T:52:ARG:NH2	2.87	0.43
1:0:830:G:O2'	1:0:831:U:H5'	2.18	0.43
1:0:1206:U:H5'	1:0:1206:U:C6	2.33	0.43
1:0:1211:G:H2'	1:0:1212:C:H6	1.83	0.43
1:0:1503:U:H2'	1:0:1504:A:O4'	2.19	0.43
1:0:1838:U:H1'	1:0:2644:C:O4'	2.18	0.43
1:0:2372:A:H2'	1:0:2373:U:C6	2.54	0.43
1:0:2515:C:C2'	1:0:2516:G:H5'	2.48	0.43
40:0:3297:HOH:O	15:M:82:ARG:HA	2.17	0.43
4:A:65:ARG:HG2	4:A:65:ARG:HH11	1.83	0.43
4:A:201:PHE:HB3	40:A:9617:HOH:O	2.18	0.43
12:J:54:VAL:O	12:J:58:GLU:HG3	2.18	0.43
14:L:94:ARG:NH1	14:L:143:THR:HG21	2.34	0.43
1:0:544:G:C3'	1:0:545:G:H5"	2.49	0.43
1:0:945:U:H2'	1:0:946:C:H6	1.83	0.43
1:0:1268:C:O2'	1:0:1269:G:H5'	2.18	0.43
1:0:2676:C:H4'	12:J:70:PHE:HD1	1.83	0.43
6:C:120:ASP:C	6:C:120:ASP:OD1	2.57	0.43
6:C:184:ARG:HB3	40:C:9167:HOH:O	2.18	0.43
11:H:56:GLN:NE2	11:H:93:GLN:HG2	2.31	0.43
16:N:156:GLU:O	16:N:157:PRO:C	2.57	0.43
23:U:35:LYS:HE2	23:U:51:TRP:CZ2	2.53	0.43
25:W:106:THR:OG1	25:W:109:GLU:HB2	2.19	0.43
1:0:1189:A:H1'	1:0:1209:C:H1'	1.99	0.43
1:0:1201:C:C2'	1:0:1202:A:H5'	2.44	0.43
1:0:1439:C:OP1	30:2:41:HIS:HE1	2.02	0.43
1:0:1482:A:O2'	1:0:1483:C:H5'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1603:A:H5'	1:0:1605:G:C4'	2.48	0.43
1:0:2645:U:OP2	1:0:2645:U:H6	2.00	0.43
2:9:3044:A:H2'	2:9:3045:A:O4'	2.19	0.43
5:B:51:VAL:HG21	5:B:327:VAL:HG13	1.99	0.43
5:B:132:HIS:CE1	5:B:171:VAL:HG21	2.54	0.43
5:B:248:ARG:NH2	40:B:9527:HOH:O	2.44	0.43
8:E:18:LEU:HD13	8:E:34:TRP:CG	2.53	0.43
12:J:43:ARG:NH1	40:J:5361:HOH:O	2.52	0.43
21:S:38:ALA:O	21:S:42:GLU:HG3	2.18	0.43
25:W:11:VAL:O	25:W:12:ASN:HB2	2.18	0.43
1:0:10:U:O4	1:0:532:A:OP2	2.37	0.43
1:0:271:C:H41	1:0:378:A:H2	1.62	0.43
1:0:559:U:H5'	1:0:559:U:C6	2.44	0.43
1:0:1213:C:O2'	1:0:1214:G:H5'	2.19	0.43
1:0:2250:G:OP1	4:A:31:LYS:HD3	2.19	0.43
1:0:2346:C:O3'	7:D:52:THR:HG23	2.19	0.43
40:0:7250:HOH:O	16:N:4:PRO:HD2	2.18	0.43
6:C:45:ASP:OD2	6:C:98:ARG:HD2	2.19	0.43
11:H:83:TYR:CD1	11:H:83:TYR:C	2.92	0.43
13:K:125:ALA:O	13:K:127:ALA:N	2.47	0.43
16:N:143:ARG:HE	16:N:143:ARG:HB3	1.65	0.43
19:Q:30:VAL:HG12	19:Q:30:VAL:O	2.18	0.43
24:V:8:ILE:CG2	24:V:59:ILE:HG13	2.49	0.43
25:W:26:ILE:O	25:W:26:ILE:HG12	2.17	0.43
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.53	0.43
1:0:329:A:OP2	6:C:206:ASN:HB2	2.19	0.43
1:0:812:A:H2'	1:0:813:C:C6	2.54	0.43
1:0:1175:G:H2'	1:0:1176:C:O4'	2.19	0.43
1:0:1206:U:H6	1:0:1206:U:C5'	2.21	0.43
1:0:2032:U:C2'	1:0:2033:G:H5"	2.49	0.43
40:0:4961:HOH:O	4:A:11:ARG:CZ	2.66	0.43
2:9:3006:C:OP1	16:N:37:ARG:CZ	2.67	0.43
4:A:66:ARG:CB	4:A:66:ARG:NH1	2.81	0.43
7:D:172:VAL:CG1	7:D:173:GLU:H	2.26	0.43
22:T:20:HIS:HB3	22:T:41:ARG:HD2	2.00	0.43
22:T:78:THR:HB	22:T:87:VAL:O	2.19	0.43
22:T:88:PRO:HB3	40:T:6320:HOH:O	2.19	0.43
1:0:1044:C:H3'	1:0:1045:G:H5"	2.01	0.43
1:0:1755:A:H2'	1:0:1756:G:O4'	2.19	0.43
4:A:217:ARG:CG	4:A:217:ARG:NH1	2.79	0.43
6:C:98:ARG:NH1	40:C:9161:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:105:GLU:HG2	8:E:113:PRO:HB3	2.01	0.43
12:J:39:VAL:CG1	12:J:40:ASN:N	2.82	0.43
13:K:13:GLU:OE1	13:K:44:LEU:HD12	2.19	0.43
14:L:92:ASP:OD1	14:L:94:ARG:HB2	2.18	0.43
15:M:61:ILE:HD12	15:M:61:ILE:N	2.33	0.43
16:N:43:VAL:HG13	16:N:118:ILE:HD11	2.01	0.43
22:T:49:GLU:HB3	22:T:59:GLU:CG	2.44	0.43
27:Y:151:SER:HB3	27:Y:154:ARG:CB	2.49	0.43
30:2:19:SER:O	30:2:36:ASN:ND2	2.43	0.43
1:0:603:A:H5"	1:0:604:G:OP1	2.18	0.42
1:0:793:A:C5'	18:P:83:LYS:HG2	2.49	0.42
1:0:1196:C:H2'	1:0:1197:G:O4'	2.18	0.42
1:0:1377:C:H1'	40:0:7728:HOH:O	2.18	0.42
1:0:2435:U:H1'	40:0:5968:HOH:O	2.19	0.42
2:9:3001:U:O3'	2:9:3003:A:H5"	2.19	0.42
5:B:101:TRP:HB2	5:B:119:HIS:CD2	2.54	0.42
12:J:130:VAL:HG12	12:J:131:THR:H	1.84	0.42
13:K:34:VAL:HG21	13:K:47:ALA:HB2	2.00	0.42
13:K:63:GLU:HB2	40:K:6344:HOH:O	2.19	0.42
22:T:75:GLU:O	22:T:76:ASP:HB2	2.19	0.42
28:Z:75:GLY:O	28:Z:78:THR:HB	2.18	0.42
31:3:65:THR:HG23	31:3:88:LEU:HD22	2.00	0.42
32:I:80:LYS:HD3	32:I:86:GLU:O	2.18	0.42
1:0:565:A:OP2	1:0:592:G:N1	2.49	0.42
1:0:1186:C:H5"	32:I:119:TYR:CE1	2.54	0.42
1:0:1189:A:HO2'	1:0:1208:C:H2'	1.82	0.42
1:0:1226:G:H5'	40:0:5079:HOH:O	2.19	0.42
1:0:2428:G:N7	31:3:60:LYS:NZ	2.65	0.42
7:D:62:ASP:HA	40:D:4233:HOH:O	2.17	0.42
9:F:28:ALA:HB3	9:F:99:THR:O	2.19	0.42
9:F:40:ILE:HD11	9:F:48:VAL:HG11	2.00	0.42
11:H:3:ALA:HA	11:H:58:ARG:HH12	1.84	0.42
16:N:67:ALA:O	16:N:69:TYR:N	2.52	0.42
21:S:37:VAL:O	21:S:41:VAL:HG23	2.18	0.42
31:3:70:ARG:HG3	31:3:77:ALA:HB2	2.01	0.42
1:0:1174:A:C5	1:0:1201:C:H4'	2.54	0.42
1:0:2015:A:H2'	1:0:2016:U:O4'	2.19	0.42
1:0:2251:G:H2'	1:0:2252:A:C8	2.54	0.42
1:0:2353:A:H4'	1:0:2354:A:O5'	2.17	0.42
40:0:7872:HOH:O	22:T:9:LYS:HB2	2.18	0.42
4:A:192:VAL:HG12	4:A:207:GLN:CB	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:23:VAL:O	7:D:23:VAL:HG23	2.19	0.42
9:F:5:ASP:O	9:F:119:ARG:NH1	2.52	0.42
13:K:49:LEU:HD12	13:K:80:ILE:HD13	2.01	0.42
15:M:46:LEU:HD22	15:M:50:ARG:HG3	2.02	0.42
19:Q:75:ILE:CD1	19:Q:84:ILE:HD11	2.50	0.42
25:W:73:LEU:HD12	25:W:73:LEU:HA	1.89	0.42
26:X:7:GLU:HA	26:X:75:ALA:HA	2.01	0.42
27:Y:107:PRO:HB3	27:Y:182:PHE:CE2	2.54	0.42
1:0:362:G:H2'	1:0:363:A:C8	2.54	0.42
1:0:1925:G:O2'	1:0:1926:G:H5'	2.20	0.42
1:0:2478:U:O2'	1:0:2479:A:H5'	2.20	0.42
4:A:88:ILE:CD1	4:A:100:PRO:HD3	2.45	0.42
4:A:94:LEU:HG	4:A:99:ILE:HD11	2.00	0.42
14:L:143:THR:CG2	14:L:144:ASP:H	2.32	0.42
16:N:35:VAL:HG12	16:N:37:ARG:HD3	2.01	0.42
22:T:115:GLU:CG	22:T:116:ASP:N	2.79	0.42
25:W:48:VAL:O	25:W:48:VAL:CG1	2.67	0.42
26:X:74:ALA:HB2	26:X:85:VAL:HG22	2.02	0.42
1:0:137:U:OP1	1:0:259:G:O2'	2.37	0.42
1:0:1476:A:H1'	1:0:1867:G:O2'	2.19	0.42
1:0:2587:OMU:H2'	1:0:2589:U:H5"	2.01	0.42
7:D:52:THR:HB	7:D:70:GLY:C	2.39	0.42
7:D:67:ASP:O	7:D:69:ILE:HG13	2.20	0.42
12:J:45:VAL:CG2	12:J:129:PHE:CD1	3.03	0.42
14:L:12:THR:HG21	14:L:16:GLY:O	2.18	0.42
16:N:182:GLY:O	16:N:183:ASP:C	2.57	0.42
24:V:1:THR:OG1	24:V:2:VAL:N	2.52	0.42
24:V:16:ARG:NH2	24:V:63:GLU:HG3	2.35	0.42
30:2:19:SER:HB3	40:2:4479:HOH:O	2.20	0.42
31:3:20:HIS:HA	31:3:70:ARG:O	2.20	0.42
32:I:113:HIS:HE1	32:I:121:LEU:HD22	1.82	0.42
2:9:3107:C:H5	40:9:3167:HOH:O	2.02	0.42
7:D:10:PHE:CG	7:D:11:HIS:N	2.87	0.42
9:F:106:ALA:HB3	40:F:6617:HOH:O	2.18	0.42
17:O:18:ALA:HB2	17:O:26:TRP:HB2	2.01	0.42
17:O:49:GLU:OE1	17:O:70:LEU:HD12	2.19	0.42
20:R:114:VAL:HA	20:R:144:GLU:O	2.19	0.42
21:S:6:LYS:O	21:S:7:HIS:HB3	2.20	0.42
24:V:16:ARG:NH1	24:V:65:ASP:O	2.53	0.42
24:V:42:ASN:O	24:V:44:GLY:N	2.52	0.42
25:W:34:LEU:HD12	25:W:107:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:49:GLU:HB2	40:2:131:HOH:O	2.20	0.42
1:0:87:C:C2	30:2:30:ASP:OD2	2.73	0.42
1:0:204:A:H2'	1:0:205:U:H5'	2.01	0.42
1:0:646:G:H2'	1:0:647:U:C6	2.55	0.42
1:0:1159:G:H1	1:0:1208:C:N4	2.16	0.42
1:0:1185:U:H4'	32:I:123:ASN:HB3	2.01	0.42
1:0:1588:G:C6	1:0:1589:G:N1	2.88	0.42
1:0:1654:U:H2'	4:A:47:HIS:CD2	2.55	0.42
1:0:2577:A:H5'	40:0:8264:HOH:O	2.18	0.42
1:0:2667:G:H1'	1:0:2914:A:N3	2.34	0.42
1:0:2809:G:H2'	1:0:2810:G:O4'	2.19	0.42
5:B:16:ARG:NE	40:B:9557:HOH:O	2.28	0.42
8:E:22:VAL:O	8:E:28:SER:HA	2.20	0.42
18:P:55:LYS:HG2	18:P:56:GLY:N	2.34	0.42
25:W:38:THR:HG22	25:W:39:ASP:H	1.84	0.42
1:0:171:C:OP2	15:M:84:LYS:HG3	2.19	0.42
1:0:1185:U:H5'	40:0:7910:HOH:O	2.20	0.42
1:0:1603:A:H5"	1:0:1604:G:H3'	2.02	0.42
1:0:2324:G:N2	1:0:2377:U:H1'	2.35	0.42
1:0:2780:C:C1'	8:E:143:GLN:HE21	2.25	0.42
40:0:6241:HOH:O	13:K:87:ARG:CZ	2.68	0.42
4:A:81:GLN:N	4:A:92:ASN:OD1	2.42	0.42
5:B:234:ARG:NH1	40:B:9612:HOH:O	2.52	0.42
15:M:76:ARG:HG3	15:M:88:VAL:HG21	2.02	0.42
15:M:164:THR:HG22	15:M:167:GLY:H	1.85	0.42
18:P:89:ASN:OD1	18:P:92:GLU:HB2	2.19	0.42
26:X:43:VAL:HG12	26:X:47:ALA:HB3	2.00	0.42
27:Y:122:ARG:NH2	40:Y:9336:HOH:O	2.52	0.42
30:2:18:ASN:ND2	30:2:40:ARG:H	2.17	0.42
31:3:6:ARG:HA	31:3:20:HIS:O	2.20	0.42
1:0:1573:A:H2'	1:0:1574:C:O4'	2.19	0.42
1:0:1759:A:N3	1:0:1818:C:H2'	2.35	0.42
1:0:2011:A:H4'	1:0:2012:U:O5'	2.20	0.42
40:0:3426:HOH:O	5:B:252:PRO:HD3	2.20	0.42
2:9:3039:U:H3'	2:9:3040:C:H5"	2.01	0.42
11:H:88:ARG:HG2	11:H:133:LEU:O	2.20	0.42
13:K:74:VAL:O	13:K:74:VAL:HG12	2.18	0.42
13:K:118:ALA:HB1	13:K:125:ALA:CB	2.50	0.42
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.85	0.42
23:U:20:MET:HE3	23:U:30:HIS:NE2	2.35	0.42
26:X:30:MET:CE	26:X:58:ALA:HB3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:295:C:H2'	1:0:296:G:O4'	2.19	0.42
1:0:737:A:C8	1:0:737:A:H3'	2.55	0.42
1:0:879:C:H5	40:0:3763:HOH:O	2.03	0.42
1:0:2034:U:H4'	40:0:6439:HOH:O	2.20	0.42
4:A:95:PRO:HA	4:A:153:ARG:HA	2.02	0.42
4:A:207:GLN:O	4:A:208:HIS:HB3	2.20	0.42
4:A:223:ARG:NE	40:A:9559:HOH:O	2.52	0.42
7:D:99:ASP:HB3	7:D:103:ASN:H	1.85	0.42
9:F:70:LYS:C	9:F:72:VAL:H	2.23	0.42
11:H:28:ILE:HA	11:H:63:GLU:OE1	2.20	0.42
16:N:154:LEU:CG	16:N:155:GLU:H	2.25	0.42
23:U:44:ARG:HB3	40:U:3805:HOH:O	2.19	0.42
27:Y:133:HIS:HD2	40:Y:9384:HOH:O	2.03	0.42
29:1:28:HIS:O	29:1:32:LYS:N	2.45	0.42
1:0:1174:A:C6	1:0:1201:C:H4'	2.55	0.41
1:0:2089:A:O2'	1:0:2090:G:H5'	2.20	0.41
1:0:2523:U:O2'	1:0:2524:G:H5'	2.20	0.41
5:B:1:PRO:O	5:B:2:GLN:HB2	2.20	0.41
7:D:15:GLU:HA	7:D:16:PRO:HD3	1.83	0.41
11:H:146:VAL:HG22	40:H:9542:HOH:O	2.20	0.41
15:M:120:VAL:HG11	15:M:130:GLU:HG3	2.01	0.41
21:S:11:THR:H	21:S:14:ALA:HB3	1.83	0.41
22:T:102:ASP:OD1	22:T:104:GLU:HG3	2.20	0.41
1:0:304:G:H1'	1:0:347:A:N6	2.34	0.41
1:0:941:G:C5	1:0:942:U:C4	3.09	0.41
1:0:1257:C:H2'	1:0:1258:G:O4'	2.20	0.41
1:0:1507:C:H4'	40:0:4185:HOH:O	2.20	0.41
1:0:1748:U:H4'	40:0:7963:HOH:O	2.19	0.41
1:0:2768:A:O2'	1:0:2769:C:O4'	2.33	0.41
1:0:2869:G:H2'	1:0:2870:C:O4'	2.20	0.41
40:0:4417:HOH:O	11:H:11:LYS:HE2	2.20	0.41
4:A:112:PRO:HD3	4:A:152:CYS:SG	2.60	0.41
8:E:20:ILE:O	8:E:30:THR:HA	2.20	0.41
12:J:143:LYS:HG3	12:J:145:TRP:CE2	2.55	0.41
16:N:152:GLU:C	16:N:154:LEU:N	2.74	0.41
18:P:14:LEU:O	18:P:16:VAL:HG23	2.20	0.41
20:R:61:GLN:NE2	40:R:9451:HOH:O	2.53	0.41
20:R:114:VAL:HG13	20:R:114:VAL:O	2.20	0.41
24:V:59:ILE:O	24:V:63:GLU:HG2	2.20	0.41
1:0:271:C:O2	1:0:273:G:H5"	2.19	0.41
1:0:380:A:H2'	40:0:7686:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2363:G:O2'	19:Q:11:ARG:HG3	2.20	0.41
1:0:2637:A:H5"	38:4:9701:SPS:O3	2.19	0.41
2:9:3004:G:O2'	16:N:44:ARG:NH2	2.53	0.41
2:9:3056:A:C3'	2:9:3057:A:H5"	2.50	0.41
4:A:43:VAL:O	4:A:44:ASP:HB2	2.20	0.41
6:C:27:ARG:HD2	17:O:5:PRO:HD2	2.02	0.41
7:D:167:GLU:OE2	7:D:173:GLU:HB3	2.20	0.41
8:E:1:PRO:HD2	8:E:53:GLU:O	2.20	0.41
11:H:51:VAL:CG1	11:H:53:GLU:O	2.68	0.41
18:P:55:LYS:CG	18:P:56:GLY:N	2.82	0.41
22:T:79:LEU:HG	22:T:89:ARG:HB2	2.02	0.41
23:U:19:THR:HG22	23:U:20:MET:N	2.35	0.41
26:X:72:VAL:CG1	26:X:85:VAL:CG1	2.98	0.41
29:1:28:HIS:HD2	29:1:30:LYS:H	1.68	0.41
1:0:447:A:O2'	1:0:448:G:H5'	2.20	0.41
1:0:522:U:O2'	1:0:1366:C:H5'	2.19	0.41
1:0:1236:A:H2'	1:0:1237:U:O4'	2.20	0.41
1:0:1524:U:HO2'	1:0:1525:G:P	2.44	0.41
1:0:1741:U:O2'	1:0:2723:G:H4'	2.20	0.41
1:0:1849:G:H1'	1:0:2011:A:N1	2.35	0.41
1:0:2338:G:OP1	7:D:97:GLN:HG2	2.20	0.41
1:0:2453:G:H4'	14:L:50:GLY:C	2.40	0.41
1:0:2580:G:N3	1:0:2600:A:H2	2.18	0.41
1:0:2769:C:C2'	1:0:2770:G:C5'	2.98	0.41
1:0:2784:A:H1'	8:E:60:SER:OG	2.20	0.41
7:D:27:ILE:HB	40:D:5858:HOH:O	2.19	0.41
8:E:81:GLU:HA	8:E:133:VAL:O	2.20	0.41
15:M:183:THR:CG2	15:M:194:ALA:HB1	2.46	0.41
16:N:62:HIS:HB3	16:N:65:ASP:OD1	2.20	0.41
16:N:67:ALA:C	16:N:69:TYR:H	2.23	0.41
18:P:15:ASP:OD1	18:P:15:ASP:O	2.39	0.41
18:P:98:ILE:CD1	18:P:102:ARG:NE	2.84	0.41
1:0:162:C:H2'	1:0:163:U:H5'	2.02	0.41
1:0:697:G:H4'	1:0:730:G:O3'	2.21	0.41
1:0:899:C:H5'	40:0:3789:HOH:O	2.21	0.41
1:0:1020:A:H2'	1:0:1021:G:C8	2.56	0.41
1:0:1565:C:O4'	1:0:2738:G:H1'	2.20	0.41
1:0:1657:A:H2'	1:0:1658:A:C8	2.55	0.41
1:0:1666:C:C2'	1:0:1667:A:H5"	2.50	0.41
1:0:1675:C:H5"	30:2:5:LYS:HD2	2.03	0.41
1:0:1773:G:C8	28:Z:16:ALA:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:30:ARG:HE	4:A:30:ARG:HB3	1.69	0.41
4:A:43:VAL:HG21	4:A:59:GLU:HG3	2.01	0.41
5:B:154:VAL:HA	5:B:155:PRO:HD3	1.88	0.41
10:G:12:ILE:HG22	10:G:17:GLN:NE2	2.36	0.41
11:H:140:VAL:O	11:H:140:VAL:HG12	2.21	0.41
12:J:39:VAL:HG11	12:J:107:ASN:CG	2.41	0.41
15:M:74:LYS:HE3	15:M:75:ARG:O	2.20	0.41
21:S:10:VAL:HG11	24:V:36:ALA:CA	2.49	0.41
26:X:76:ARG:HG3	26:X:76:ARG:NH1	2.35	0.41
28:Z:10:ARG:C	28:Z:12:GLY:H	2.23	0.41
1:0:290:C:O2'	1:0:291:C:H5'	2.20	0.41
1:0:625:U:H5"	1:0:1044:C:H41	1.86	0.41
1:0:1318:A:H4'	1:0:1343:C:H4'	2.02	0.41
1:0:2253:G:O2'	1:0:2254:G:H5'	2.21	0.41
1:0:2351:C:H2'	1:0:2352:G:O4'	2.20	0.41
1:0:2428:G:H5'	40:0:7132:HOH:O	2.21	0.41
40:0:6789:HOH:O	27:Y:158:LYS:HD3	2.19	0.41
12:J:42:GLU:O	12:J:131:THR:HG23	2.20	0.41
16:N:24:LEU:HD13	19:Q:26:PRO:HB3	2.03	0.41
22:T:115:GLU:HG3	22:T:116:ASP:H	1.81	0.41
27:Y:102:LEU:HD11	27:Y:225:GLY:HA2	2.02	0.41
27:Y:213:LYS:HE3	27:Y:213:LYS:HB2	1.85	0.41
31:3:7:PHE:CE1	31:3:9:THR:HB	2.56	0.41
1:0:695:C:H2'	1:0:696:C:C6	2.55	0.41
1:0:1299:G:N2	40:0:5231:HOH:O	2.53	0.41
1:0:2299:G:O6	19:Q:1:PRO:HA	2.21	0.41
1:0:2388:C:H2'	1:0:2389:U:O4'	2.21	0.41
1:0:2517:A:H2'	1:0:2518:C:O4'	2.21	0.41
40:0:5826:HOH:O	25:W:69:ARG:NH2	2.54	0.41
40:0:9728:HOH:O	5:B:229:ARG:HD2	2.20	0.41
5:B:276:ASP:O	5:B:279:THR:HG22	2.20	0.41
5:B:280:VAL:HG13	5:B:333:GLU:O	2.21	0.41
7:D:60:GLU:O	7:D:60:GLU:HG3	2.21	0.41
7:D:135:VAL:HG22	7:D:136:ARG:H	1.86	0.41
7:D:166:ILE:O	7:D:169:THR:N	2.54	0.41
9:F:48:VAL:CG2	9:F:74:PHE:HB3	2.51	0.41
11:H:17:ARG:HD3	11:H:23:ILE:HD12	2.03	0.41
11:H:36:LYS:HA	11:H:84:LYS:NZ	2.36	0.41
15:M:82:ARG:O	15:M:84:LYS:N	2.53	0.41
19:Q:22:GLY:O	19:Q:23:THR:C	2.58	0.41
23:U:39:ASN:ND2	23:U:44:ARG:HH11	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:1:THR:O	24:V:2:VAL:C	2.59	0.41
26:X:73:ARG:NH1	26:X:73:ARG:HB2	2.35	0.41
1:0:359:U:H3'	40:0:6290:HOH:O	2.20	0.41
1:0:1173:A:H4'	1:0:1174:A:C8	2.56	0.41
1:0:1505:U:H1'	40:0:8100:HOH:O	2.20	0.41
1:0:1556:G:O2'	1:0:1557:G:H5'	2.21	0.41
1:0:1636:G:O2'	1:0:1637:A:H5'	2.20	0.41
1:0:2515:C:H2'	1:0:2516:G:C5'	2.51	0.41
4:A:223:ARG:CZ	40:A:9559:HOH:O	2.69	0.41
5:B:146:THR:C	5:B:148:PRO:HD3	2.41	0.41
8:E:20:ILE:HD12	8:E:33:LEU:CD1	2.49	0.41
12:J:95:ARG:HG2	12:J:99:GLU:OE2	2.21	0.41
13:K:7:ASP:OD2	13:K:81:ARG:NH2	2.54	0.41
13:K:82:ARG:NH2	13:K:115:ARG:HG2	2.36	0.41
14:L:80:ASP:HB3	14:L:90:ARG:HB3	2.02	0.41
15:M:82:ARG:O	15:M:83:SER:C	2.59	0.41
16:N:71:TRP:HB2	40:N:9335:HOH:O	2.19	0.41
21:S:57:THR:HG22	21:S:59:ASP:N	2.34	0.41
27:Y:148:GLY:O	27:Y:154:ARG:HD3	2.21	0.41
28:Z:49:ARG:HB2	28:Z:55:TRP:CZ3	2.56	0.41
31:3:38:ARG:HB3	31:3:42:ARG:NH1	2.31	0.41
1:0:255:A:H2'	1:0:256:C:C6	2.56	0.41
1:0:721:A:H4'	17:O:51:TYR:CD1	2.55	0.41
1:0:1095:U:O2	25:W:120:PRO:HG2	2.21	0.41
1:0:2281:C:C2'	1:0:2282:U:H5'	2.50	0.41
2:9:3118:C:H4'	16:N:56:ASP:OD1	2.21	0.41
3:4:76:DA:H8	38:4:9701:SPS:H81	1.85	0.41
4:A:104:PRO:HG3	4:A:127:GLN:OE1	2.21	0.41
5:B:62:ARG:HA	5:B:65:MET:HE3	2.03	0.41
5:B:75:GLU:C	5:B:77:PRO:HD3	2.40	0.41
5:B:141:ARG:HD2	5:B:163:GLU:OE2	2.21	0.41
5:B:171:VAL:HG23	5:B:172:SER:N	2.36	0.41
6:C:133:ARG:NH1	40:C:9214:HOH:O	2.53	0.41
6:C:162:VAL:HG13	6:C:192:ILE:HD11	2.02	0.41
9:F:57:GLU:O	9:F:61:MET:HG3	2.21	0.41
11:H:9:ILE:HD12	11:H:54:THR:HG22	2.03	0.41
11:H:54:THR:HG23	11:H:128:GLN:HA	2.03	0.41
11:H:167:PRO:O	11:H:168:ALA:HB2	2.21	0.41
13:K:118:ALA:HB1	13:K:125:ALA:HB2	2.03	0.41
14:L:59:GLU:HB3	40:L:9465:HOH:O	2.20	0.41
16:N:38:LYS:HD3	16:N:107:ASN:ND2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:66:LYS:HB2	19:Q:70:ALA:O	2.21	0.41
22:T:32:ARG:HH12	22:T:38:ARG:HH12	1.66	0.41
28:Z:39:CYS:HA	28:Z:40:PRO:HD3	1.95	0.41
30:2:11:LEU:HD23	30:2:11:LEU:HA	1.90	0.41
32:I:118:SER:CB	32:I:123:ASN:HB2	2.50	0.41
1:0:2016:U:H2'	1:0:2017:U:C6	2.55	0.41
1:0:2553:A:H2'	1:0:2553:A:N3	2.35	0.41
2:9:3011:A:P	19:Q:19:ARG:HH21	2.43	0.41
5:B:84:LEU:O	5:B:99:GLU:HA	2.21	0.41
7:D:88:LEU:N	7:D:89:PRO:CD	2.84	0.41
12:J:71:TYR:CD1	12:J:72:PRO:HD2	2.56	0.41
22:T:81:LYS:HD2	22:T:87:VAL:CG1	2.52	0.41
25:W:6:GLN:CB	25:W:26:ILE:HD11	2.27	0.41
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.51	0.41
1:0:526:U:H2'	1:0:527:U:C6	2.56	0.40
1:0:819:A:H5"	40:Z:9220:HOH:O	2.20	0.40
1:0:1132:A:N3	1:0:2521:A:O2'	2.49	0.40
1:0:1163:G:H5'	32:I:115:ASP:O	2.21	0.40
1:0:2094:G:O6	1:0:2649:A:H2	2.04	0.40
5:B:320:GLN:HA	5:B:321:PRO:HD3	1.95	0.40
7:D:28:GLY:O	7:D:29:HIS:HB3	2.21	0.40
7:D:40:ILE:HG13	7:D:41:LEU:N	2.36	0.40
17:O:15:LYS:HD3	17:O:19:ARG:NH2	2.36	0.40
27:Y:144:ARG:NH2	40:Y:9411:HOH:O	2.51	0.40
28:Z:39:CYS:O	28:Z:42:CYS:O	2.40	0.40
31:3:70:ARG:CG	31:3:77:ALA:HB2	2.51	0.40
32:I:78:LEU:CD1	32:I:112:LYS:HZ2	2.32	0.40
1:0:27:U:H2'	1:0:28:G:O4'	2.21	0.40
1:0:1176:C:H3'	40:0:5396:HOH:O	2.22	0.40
1:0:1797:A:H2'	1:0:1799:G:O5'	2.22	0.40
1:0:2421:G:H2'	40:0:4646:HOH:O	2.20	0.40
1:0:2515:C:H2'	1:0:2516:G:H5'	2.03	0.40
1:0:2821:C:H4'	5:B:116:PRO:HG3	2.03	0.40
1:0:2908:A:H2'	1:0:2909:G:C4'	2.51	0.40
2:9:3044:A:O4'	7:D:76:ARG:NE	2.55	0.40
5:B:24:PRO:HG3	5:B:204:GLY:HA2	2.03	0.40
11:H:54:THR:O	11:H:55:VAL:HG13	2.21	0.40
12:J:90:LYS:HB2	36:J:9302:CL:CL	2.57	0.40
16:N:23:ARG:HG2	16:N:23:ARG:NH1	2.34	0.40
17:O:23:GLY:C	40:O:3062:HOH:O	2.59	0.40
17:O:81:PHE:N	17:O:81:PHE:CD1	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:94:TRP:CZ2	18:P:98:ILE:HG13	2.56	0.40
32:I:108:ILE:C	32:I:110:GLU:H	2.24	0.40
1:0:338:C:H4'	6:C:174:ILE:HD11	2.02	0.40
1:0:432:G:H2'	1:0:433:C:H6	1.86	0.40
1:0:1077:G:H2'	1:0:1080:C:H42	1.86	0.40
1:0:1342:C:C2'	1:0:1343:C:H5'	2.51	0.40
1:0:2070:G:H2'	1:0:2072:G:OP1	2.22	0.40
1:0:2612:A:H4'	40:0:4260:HOH:O	2.21	0.40
2:9:3028:U:P	16:N:39:SER:OG	2.80	0.40
5:B:149:ASP:HB2	40:B:9579:HOH:O	2.21	0.40
6:C:123:LEU:HA	6:C:123:LEU:HD23	1.84	0.40
7:D:165:PHE:O	7:D:168:SER:HB3	2.22	0.40
11:H:165:SER:OG	11:H:168:ALA:HB3	2.21	0.40
12:J:107:ASN:C	12:J:107:ASN:ND2	2.73	0.40
24:V:12:THR:OG1	24:V:13:PRO:HD2	2.20	0.40
27:Y:170:SER:OG	27:Y:175:ARG:HG3	2.21	0.40
1:0:920:C:H5'	1:0:921:G:C4	2.56	0.40
1:0:956:G:H2'	1:0:957:A:O4'	2.21	0.40
1:0:1242:A:O3'	12:J:20:GLY:HA3	2.22	0.40
1:0:2326:U:H4'	1:0:2412:G:H4'	2.04	0.40
2:9:3095:C:O2'	2:9:3096:C:H5'	2.22	0.40
4:A:36:ASP:O	4:A:38:ILE:N	2.48	0.40
5:B:102:THR:CG2	5:B:182:VAL:HG12	2.51	0.40
8:E:7:ILE:HA	8:E:8:PRO:HD3	1.95	0.40
14:L:73:VAL:HG21	14:L:116:HIS:CD2	2.57	0.40
24:V:12:THR:HG23	24:V:14:ALA:N	2.36	0.40
25:W:126:ASP:HB3	25:W:135:GLY:O	2.21	0.40
31:3:17:HIS:O	31:3:18:GLN:HG3	2.22	0.40
1:0:401:C:O2'	15:M:92:THR:HB	2.22	0.40
1:0:559:U:H2'	1:0:560:C:O4'	2.22	0.40
1:0:816:G:C6	1:0:817:G:N1	2.90	0.40
1:0:1380:U:O4	1:0:2748:G:H1'	2.22	0.40
1:0:1504:A:H5'	40:0:4966:HOH:O	2.20	0.40
1:0:2896:A:N3	1:0:2896:A:C2'	2.84	0.40
40:0:4664:HOH:O	5:B:216:LYS:HE2	2.20	0.40
4:A:32:VAL:HG12	4:A:34:ASP:N	2.36	0.40
6:C:194:PHE:CE2	6:C:234:VAL:HG11	2.56	0.40
7:D:96:SER:C	7:D:98:PHE:H	2.24	0.40
11:H:70:ASN:O	11:H:74:ILE:HG13	2.21	0.40
19:Q:91:LEU:C	19:Q:92:ARG:HG2	2.41	0.40
23:U:52:THR:HG21	23:U:54:THR:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:3:48:ASN:ND2	31:3:50:GLY:H	2.20	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
4	A	235/240 (98%)	210 (89%)	21 (9%)	4 (2%)	9 6
5	B	335/338 (99%)	312 (93%)	19 (6%)	4 (1%)	13 10
6	C	244/246 (99%)	226 (93%)	18 (7%)	0	100 100
7	D	134/177 (76%)	103 (77%)	23 (17%)	8 (6%)	1 0
8	E	170/178 (96%)	163 (96%)	7 (4%)	0	100 100
9	F	117/120 (98%)	102 (87%)	13 (11%)	2 (2%)	9 6
10	G	25/348 (7%)	25 (100%)	0	0	100 100
11	H	156/171 (91%)	140 (90%)	13 (8%)	3 (2%)	8 5
12	J	140/145 (97%)	132 (94%)	6 (4%)	2 (1%)	11 8
13	K	130/132 (98%)	121 (93%)	8 (6%)	1 (1%)	19 19
14	L	141/165 (86%)	118 (84%)	21 (15%)	2 (1%)	11 8
15	M	192/194 (99%)	181 (94%)	9 (5%)	2 (1%)	15 14
16	N	184/187 (98%)	161 (88%)	13 (7%)	10 (5%)	2 0
17	O	113/116 (97%)	108 (96%)	5 (4%)	0	100 100
18	P	141/149 (95%)	134 (95%)	7 (5%)	0	100 100
19	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100 100
20	R	148/155 (96%)	141 (95%)	7 (5%)	0	100 100
21	S	79/85 (93%)	74 (94%)	5 (6%)	0	100 100
22	T	117/120 (98%)	111 (95%)	5 (4%)	1 (1%)	17 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
23	U	51/66 (77%)	48 (94%)	3 (6%)	0	100 100
24	V	63/71 (89%)	57 (90%)	3 (5%)	3 (5%)	2 1
25	W	152/154 (99%)	149 (98%)	3 (2%)	0	100 100
26	X	80/92 (87%)	72 (90%)	8 (10%)	0	100 100
27	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100 100
28	Z	71/83 (86%)	62 (87%)	6 (8%)	3 (4%)	3 1
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100 100
30	2	42/50 (84%)	41 (98%)	1 (2%)	0	100 100
31	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	14 12
32	I	68/162 (42%)	54 (79%)	11 (16%)	3 (4%)	2 1
All	All	3705/4430 (84%)	3410 (92%)	246 (7%)	49 (1%)	12 9

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	37	VAL
5	B	139	ASP
9	F	101	ALA
11	H	166	SER
11	H	168	ALA
14	L	80	ASP
16	N	154	LEU
16	N	167	ASP
16	N	183	ASP
16	N	184	ILE
28	Z	81	ARG
4	A	34	ASP
5	B	169	GLY
7	D	16	PRO
7	D	60	GLU
7	D	61	PHE
15	M	83	SER
16	N	155	GLU
16	N	162	ASP
28	Z	20	ARG
32	I	132	CYS
5	B	185	GLY
7	D	56	ARG

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Mol	Chain	Res	Type
7	D	137	PRO
7	D	164	ALA
7	D	171	ASP
12	J	143	LYS
16	N	65	ASP
16	N	68	GLU
24	V	43	PRO
28	Z	41	ASN
13	K	126	SER
14	L	82	ALA
31	3	56	PRO
32	I	114	PRO
4	A	132	ASP
4	A	205	GLY
12	J	5	GLU
22	T	53	GLY
7	D	69	ILE
9	F	71	GLY
24	V	40	PRO
32	I	129	VAL
5	B	182	VAL
16	N	157	PRO
16	N	161	GLY
11	H	167	PRO
15	M	88	VAL
24	V	2	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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
4	A	179/182 (98%)	166 (93%)	13 (7%)	14 15
5	B	282/283 (100%)	268 (95%)	14 (5%)	24 30
6	C	193/193 (100%)	176 (91%)	17 (9%)	10 10
7	D	117/148 (79%)	111 (95%)	6 (5%)	24 29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	E	152/156 (97%)	148 (97%)	4 (3%)	46 58
9	F	93/94 (99%)	89 (96%)	4 (4%)	29 36
10	G	27/283 (10%)	26 (96%)	1 (4%)	34 43
11	H	132/138 (96%)	127 (96%)	5 (4%)	33 42
12	J	118/121 (98%)	111 (94%)	7 (6%)	19 23
13	K	106/106 (100%)	100 (94%)	6 (6%)	20 24
14	L	113/127 (89%)	111 (98%)	2 (2%)	59 72
15	M	158/158 (100%)	153 (97%)	5 (3%)	39 50
16	N	149/150 (99%)	142 (95%)	7 (5%)	26 33
17	O	93/94 (99%)	89 (96%)	4 (4%)	29 36
18	P	113/117 (97%)	112 (99%)	1 (1%)	78 88
19	Q	79/80 (99%)	77 (98%)	2 (2%)	47 60
20	R	117/122 (96%)	116 (99%)	1 (1%)	78 88
21	S	71/74 (96%)	71 (100%)	0	100 100
22	T	105/106 (99%)	100 (95%)	5 (5%)	25 32
23	U	44/52 (85%)	44 (100%)	0	100 100
24	V	51/57 (90%)	50 (98%)	1 (2%)	55 69
25	W	130/130 (100%)	126 (97%)	4 (3%)	40 51
26	X	66/74 (89%)	59 (89%)	7 (11%)	6 6
27	Y	120/196 (61%)	108 (90%)	12 (10%)	7 7
28	Z	60/68 (88%)	59 (98%)	1 (2%)	60 74
29	1	46/47 (98%)	46 (100%)	0	100 100
30	2	42/46 (91%)	40 (95%)	2 (5%)	25 32
31	3	79/79 (100%)	76 (96%)	3 (4%)	33 42
32	I	58/130 (45%)	58 (100%)	0	100 100
All	All	3093/3611 (86%)	2959 (96%)	134 (4%)	29 36

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	ARG
4	A	26	ASP
4	A	33	GLU

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Mol	Chain	Res	Type
4	A	62	ASP
4	A	68	ILE
4	A	94	LEU
4	A	131	HIS
4	A	144	GLU
4	A	151	GLN
4	A	165	THR
4	A	179	MET
4	A	206	ARG
4	A	217	ARG
5	B	11	LEU
5	B	27	ASN
5	B	28	SER
5	B	82	VAL
5	B	98	THR
5	B	112	THR
5	B	149	ASP
5	B	162	MET
5	B	190	MET
5	B	251	VAL
5	B	254	GLN
5	B	264	GLU
5	B	265	LEU
5	B	312	ARG
6	C	2	GLN
6	C	16	VAL
6	C	27	ARG
6	C	76	ARG
6	C	91	PRO
6	C	94	THR
6	C	101	ASP
6	C	115	LEU
6	C	136	VAL
6	C	162	VAL
6	C	187	ARG
6	C	214	THR
6	C	223	LEU
6	C	234	VAL
6	C	236	THR
6	C	240	LEU
6	C	243	VAL
7	D	24	HIS

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Mol	Chain	Res	Type
7	D	47	GLN
7	D	50	VAL
7	D	61	PHE
7	D	100	ASP
7	D	133	ASN
8	E	15	GLN
8	E	86	VAL
8	E	155	ASN
8	E	164	ASP
9	F	12	LEU
9	F	46	GLU
9	F	99	THR
9	F	119	ARG
10	G	72	ASP
11	H	18	GLU
11	H	68	SER
11	H	84	LYS
11	H	154	TYR
11	H	159	PRO
12	J	70	PHE
12	J	74	ARG
12	J	79	PHE
12	J	107	ASN
12	J	112	ASP
12	J	127	ILE
12	J	131	THR
13	K	4	LEU
13	K	10	GLN
13	K	84	ASP
13	K	98	VAL
13	K	100	GLU
13	K	107	THR
14	L	35	ARG
14	L	43	HIS
15	M	46	LEU
15	M	68	ARG
15	M	93	ARG
15	M	99	ARG
15	M	116	ASN
16	N	14	ARG
16	N	26	LEU
16	N	37	ARG

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Mol	Chain	Res	Type
16	N	56	ASP
16	N	65	ASP
16	N	135	VAL
16	N	139	TRP
17	O	3	THR
17	O	25	VAL
17	O	96	VAL
17	O	115	ARG
18	P	98	ILE
19	Q	16	ASN
19	Q	57	ASP
20	R	13	THR
22	T	39	ASN
22	T	48	VAL
22	T	89	ARG
22	T	96	VAL
22	T	117	ASP
24	V	65	ASP
25	W	26	ILE
25	W	109	GLU
25	W	142	ASP
25	W	146	ILE
26	X	8	ARG
26	X	15	ARG
26	X	27	ASP
26	X	49	ARG
26	X	72	VAL
26	X	79	GLU
26	X	80	GLU
27	Y	103	THR
27	Y	108	ASP
27	Y	115	ARG
27	Y	141	THR
27	Y	144	ARG
27	Y	154	ARG
27	Y	189	ASN
27	Y	200	THR
27	Y	204	ARG
27	Y	220	GLU
27	Y	231	PRO
27	Y	235	GLU
28	Z	44	GLU

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Mol	Chain	Res	Type
30	2	18	ASN
30	2	46	ASP
31	3	15	ASN
31	3	56	PRO
31	3	65	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	5	GLN
4	A	199	HIS
5	B	2	GLN
5	B	27	ASN
5	B	145	HIS
5	B	191	ASN
5	B	221	GLN
5	B	238	ASN
5	B	256	GLN
5	B	260	HIS
5	B	320	GLN
5	B	332	ASN
6	C	11	ASN
6	C	39	GLN
6	C	129	HIS
6	C	163	HIS
7	D	47	GLN
7	D	103	ASN
7	D	133	ASN
8	E	106	ASN
8	E	143	GLN
10	G	17	GLN
10	G	64	ASN
11	H	56	GLN
11	H	59	HIS
11	H	70	ASN
11	H	132	GLN
11	H	170	ASN
12	J	25	GLN
12	J	107	ASN
12	J	126	ASN
13	K	10	GLN
14	L	18	HIS

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Mol	Chain	Res	Type
14	L	41	HIS
14	L	42	ASN
14	L	43	HIS
15	M	24	GLN
15	M	58	GLN
15	M	77	HIS
15	M	143	ASN
15	M	170	ASN
16	N	107	ASN
17	O	53	GLN
17	O	100	GLN
18	P	50	GLN
18	P	66	GLN
18	P	73	HIS
18	P	88	GLN
18	P	118	GLN
19	Q	16	ASN
19	Q	40	HIS
20	R	61	GLN
20	R	94	ASN
20	R	98	ASN
20	R	113	HIS
20	R	117	HIS
21	S	44	GLN
21	S	53	ASN
22	T	39	ASN
23	U	39	ASN
23	U	48	ASN
24	V	29	ASN
24	V	60	GLN
25	W	12	ASN
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	22	ASN
26	X	23	HIS
27	Y	133	HIS
27	Y	134	HIS
27	Y	149	GLN
27	Y	189	ASN
29	1	8	GLN

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Mol	Chain	Res	Type
29	1	16	HIS
29	1	28	HIS
30	2	16	ASN
30	2	18	ASN
30	2	41	HIS
30	2	45	ASN
31	3	30	GLN
31	3	48	ASN
32	I	93	GLN
32	I	113	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	237 (8%)	36 (1%)
2	9	121/122 (99%)	16 (13%)	2 (1%)
3	4	1/5 (20%)	0	0
All	All	2867/3049 (94%)	253 (8%)	38 (1%)

All (253) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	70	A
1	0	71	G
1	0	86	A
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	138	U
1	0	141	C
1	0	151	A
1	0	166	A
1	0	186	A
1	0	187	A
1	0	191	A
1	0	192	A

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Mol	Chain	Res	Type
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	308	U
1	0	309	C
1	0	318	C
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	457	U
1	0	461	C
1	0	473	A
1	0	487	G
1	0	498	A
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
1	0	559	U
1	0	581	G
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	698	A
1	0	701	U
1	0	702	G
1	0	759	C

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Mol	Chain	Res	Type
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	875	A
1	0	877	G
1	0	878	G
1	0	885	G
1	0	905	C
1	0	920	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
1	0	1087	G
1	0	1088	A
1	0	1100	G
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1151	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1193	A

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Mol	Chain	Res	Type
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1287	A
1	0	1289	C
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	1409	G
1	0	1474	C
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1528	A
1	0	1564	C
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	1732	A

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Mol	Chain	Res	Type
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2004	U
1	0	2006	C
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2063	U
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	2243	C
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

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Mol	Chain	Res	Type
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2476	C
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
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	2611	G
1	0	2613	G
1	0	2634	G
1	0	2637	A
1	0	2645	U
1	0	2646	G
1	0	2649	A
1	0	2650	U
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	2727	A
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

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Mol	Chain	Res	Type
1	0	2825	C
1	0	2852	A
1	0	2853	U
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	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3039	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

All (38) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	87	C
1	0	129	A
1	0	169	A
1	0	338	C
1	0	603	A
1	0	644	G
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1165	G
1	0	1232	A
1	0	1237	U

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Mol	Chain	Res	Type
1	0	1246	A
1	0	1352	A
1	0	1506	U
1	0	1563	G
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1730	G
1	0	1856	C
1	0	1942	A
1	0	1973	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2536	C
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2761	A
1	0	2791	U
1	0	2852	A
2	9	3055	U
2	9	3065	A

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	1MA	0	628	35,1	16,25,26	1.38	2 (12%)	18,37,40	1.17	3 (16%)
3	ACA	4	78	3	3,3,8	0.52	0	2,2,8	0.71	0
1	OMU	0	2587	1	19,22,23	0.23	0	26,31,34	0.43	0
1	PSU	0	2621	1	18,21,22	1.48	2 (11%)	22,30,33	1.28	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	UR3	0	2619	1	19,22,23	0.47	0	26,32,35	0.63	1 (3%)
1	OMG	0	2588	1	18,26,27	1.01	2 (11%)	19,38,41	0.72	1 (5%)

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
1	1MA	0	628	35,1	-	0/3/25/26	0/3/3/3
3	ACA	4	78	3	-	0/0/1/6	-
1	OMU	0	2587	1	-	0/9/27/28	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	4.87	1.43	1.36
1	0	628	1MA	C2-N3	3.76	1.33	1.29
1	0	2621	PSU	C6-C5	2.97	1.38	1.35
1	0	628	1MA	C6-N6	2.67	1.34	1.27
1	0	2588	OMG	C5-C6	-2.54	1.42	1.47
1	0	2588	OMG	C8-N7	-2.27	1.31	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	2621	PSU	C6-C5-C4	3.30	120.51	118.20
1	0	2621	PSU	C6-N1-C2	-2.97	119.65	122.68
1	0	628	1MA	N1-C2-N3	2.79	129.27	126.02
1	0	2621	PSU	O2-C2-N1	2.73	125.80	122.79
1	0	628	1MA	C5-C6-N1	2.59	117.76	113.90
1	0	2619	UR3	C4-N3-C2	2.31	126.74	124.56
1	0	2588	OMG	O6-C6-C5	2.21	128.68	124.37
1	0	628	1MA	CM1-N1-C6	2.05	123.37	120.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0
1	0	2619	UR3	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 313 ligands modelled in this entry, 312 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
38	SPS	4	9701	33	20,23,23	1.54	5 (25%)	18,30,30	2.80	3 (16%)

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
38	SPS	4	9701	33	-	5/15/18/18	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	4	9701	SPS	C6-C1	3.72	1.53	1.43
38	4	9701	SPS	C9-C10	-3.01	1.41	1.48
38	4	9701	SPS	C5-N4	2.44	1.38	1.34
38	4	9701	SPS	C1-N2	2.43	1.37	1.33
38	4	9701	SPS	O15-S15	-2.01	1.43	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	4	9701	SPS	C6-C1-N2	-8.45	118.51	124.40
38	4	9701	SPS	C3-N2-C1	7.35	121.34	115.14
38	4	9701	SPS	C6-C5-N4	-2.29	119.52	122.12

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	4	9701	SPS	C5-C6-C8-C9
38	4	9701	SPS	C12-C14-S15-O15
38	4	9701	SPS	C12-C14-S15-C16
38	4	9701	SPS	C14-C12-C13-O13
38	4	9701	SPS	N11-C12-C13-O13

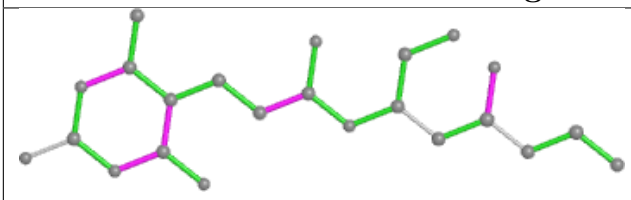
There are no ring outliers.

1 monomer is involved in 4 short contacts:

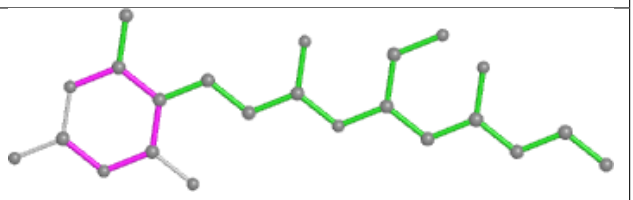
Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	4	9701	SPS	4	0

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

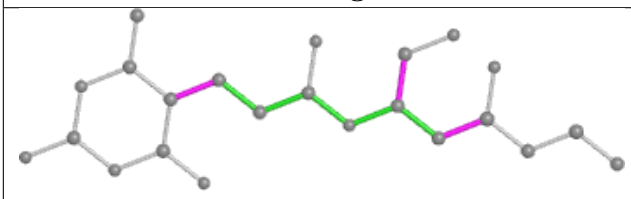
Ligand SPS 4 9701



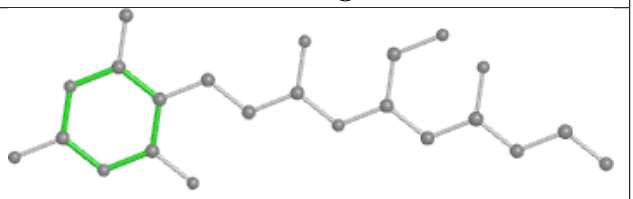
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	76:DA	O3'	77:PHE	C	1.60

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, 95^{th} 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	2749/2922 (94%)	-0.23	90 (3%) 46 44	19, 43, 76, 127	0
2	9	122/122 (100%)	0.03	6 (4%) 29 28	39, 58, 76, 127	0
3	4	4/5 (80%)	0.90	1 (25%) 0 0	52, 54, 55, 58	0
4	A	237/240 (98%)	0.43	14 (5%) 22 21	26, 45, 70, 85	0
5	B	337/338 (99%)	0.24	11 (3%) 46 44	27, 47, 65, 73	0
6	C	246/246 (100%)	-0.08	2 (0%) 86 85	26, 44, 61, 69	0
7	D	140/177 (79%)	2.07	61 (43%) 0 0	51, 74, 102, 109	0
8	E	172/178 (96%)	0.70	20 (11%) 4 4	40, 57, 69, 74	0
9	F	119/120 (99%)	1.00	31 (26%) 0 0	45, 62, 82, 87	0
10	G	29/348 (8%)	2.66	17 (58%) 0 0	59, 77, 83, 86	0
11	H	160/171 (93%)	0.72	27 (16%) 1 1	41, 54, 79, 83	0
12	J	142/145 (97%)	-0.03	3 (2%) 63 61	36, 45, 58, 71	0
13	K	132/132 (100%)	-0.10	2 (1%) 73 72	32, 43, 59, 64	0
14	L	145/165 (87%)	0.66	22 (15%) 2 2	26, 56, 90, 100	0
15	M	194/194 (100%)	0.49	20 (10%) 6 5	32, 42, 65, 70	0
16	N	186/187 (99%)	0.93	34 (18%) 1 1	42, 56, 89, 94	0
17	O	115/116 (99%)	0.06	3 (2%) 56 53	37, 50, 60, 65	0
18	P	143/149 (95%)	0.05	2 (1%) 75 73	35, 47, 57, 66	0
19	Q	95/96 (98%)	0.15	3 (3%) 47 45	39, 45, 56, 67	0
20	R	150/155 (96%)	-0.07	0 100 100	29, 41, 56, 64	0
21	S	81/85 (95%)	0.25	5 (6%) 20 19	39, 52, 66, 79	0
22	T	119/120 (99%)	0.54	7 (5%) 22 21	38, 50, 70, 92	0
23	U	53/66 (80%)	0.23	5 (9%) 8 7	38, 47, 61, 69	0
24	V	65/71 (91%)	1.77	18 (27%) 0 0	46, 64, 93, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	W	154/154 (100%)	0.01	1 (0%) 89 88	36, 47, 60, 68	0
26	X	82/92 (89%)	0.50	10 (12%) 4 3	39, 50, 69, 85	0
27	Y	142/241 (58%)	0.22	8 (5%) 24 23	28, 41, 59, 73	0
28	Z	73/83 (87%)	0.49	9 (12%) 4 3	43, 58, 70, 76	0
29	1	56/57 (98%)	-0.37	0 100 100	25, 32, 39, 48	0
30	2	46/50 (92%)	0.36	3 (6%) 18 17	31, 49, 62, 71	0
31	3	92/92 (100%)	0.26	4 (4%) 35 33	34, 51, 60, 70	0
32	I	70/162 (43%)	6.02	67 (95%) 0 0	90, 102, 117, 118	0
All	All	6650/7479 (88%)	0.21	506 (7%) 13 12	19, 47, 79, 127	0

All (506) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	71	GLY	18.3
7	D	63	ILE	17.6
16	N	166	ALA	15.7
24	V	1	THR	15.6
32	I	133	THR	14.1
32	I	79	ILE	12.7
32	I	76	ALA	11.9
32	I	118	SER	11.3
32	I	75	THR	10.8
32	I	85	PHE	10.3
7	D	57	THR	10.1
32	I	137	VAL	9.6
32	I	116	LEU	9.5
32	I	77	GLU	9.2
32	I	105	VAL	9.2
24	V	40	PRO	9.1
32	I	96	PHE	8.9
4	A	237	GLY	8.9
7	D	61	PHE	8.7
32	I	81	ASP	8.6
32	I	121	LEU	8.3
22	T	119	ALA	8.2
24	V	39	ALA	8.1
16	N	165	ALA	8.1
32	I	113	HIS	8.0
32	I	109	ALA	8.0

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Mol	Chain	Res	Type	RSRZ
32	I	91	GLU	7.9
2	9	3001	U	7.5
7	D	10	PHE	7.5
32	I	88	GLY	7.3
32	I	78	LEU	7.3
32	I	132	CYS	7.3
32	I	125	ALA	7.3
32	I	107	GLN	7.1
1	0	282	C	7.1
1	0	1951	G	7.0
32	I	126	LYS	7.0
32	I	87	THR	7.0
32	I	108	ILE	6.9
32	I	102	VAL	6.9
7	D	90	LEU	6.7
10	G	26	MET	6.6
15	M	70	GLY	6.6
32	I	104	GLN	6.6
10	G	23	ILE	6.4
4	A	37	VAL	6.3
32	I	93	GLN	6.2
32	I	86	GLU	6.2
32	I	129	VAL	6.2
32	I	114	PRO	6.2
26	X	80	GLU	5.9
7	D	170	TYR	5.9
22	T	118	SER	5.9
1	0	497	A	5.9
32	I	136	GLY	5.9
32	I	111	GLN	5.9
24	V	38	GLY	5.8
26	X	88	GLU	5.8
1	0	1199	A	5.8
32	I	138	THR	5.8
21	S	81	ILE	5.7
32	I	98	ALA	5.5
32	I	97	VAL	5.5
7	D	44	ILE	5.5
1	0	1202	A	5.4
2	9	3002	U	5.4
32	I	119	TYR	5.4
32	I	117	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
32	I	89	SER	5.4
2	9	3024	U	5.4
32	I	122	THR	5.3
30	2	49	GLU	5.3
16	N	68	GLU	5.2
7	D	93	LEU	5.2
16	N	180	LEU	5.2
1	0	1177	A	5.2
1	0	1173	A	5.1
32	I	74	PRO	5.0
8	E	45	ASP	5.0
10	G	27	ILE	4.9
32	I	134	SER	4.9
14	L	91	VAL	4.8
32	I	72	VAL	4.8
32	I	83	ALA	4.8
1	0	1172	G	4.7
7	D	166	ILE	4.7
22	T	117	ASP	4.7
24	V	37	GLY	4.6
22	T	116	ASP	4.6
1	0	1965	C	4.6
12	J	70	PHE	4.6
30	2	35	ARG	4.6
1	0	970	U	4.6
13	K	132	VAL	4.6
7	D	92	GLU	4.5
7	D	88	LEU	4.5
7	D	134	LEU	4.5
2	9	3023	U	4.5
1	0	514	G	4.5
4	A	36	ASP	4.5
7	D	11	HIS	4.5
1	0	280	C	4.4
7	D	66	GLY	4.4
10	G	71	LEU	4.4
9	F	22	VAL	4.4
32	I	84	GLY	4.4
13	K	118	ALA	4.4
17	O	22	GLY	4.3
1	0	1200	A	4.3
1	0	2508	C	4.3

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Mol	Chain	Res	Type	RSRZ
32	I	80	LYS	4.3
11	H	171	ALA	4.3
10	G	69	ARG	4.3
7	D	107	GLY	4.3
4	A	133	ARG	4.2
15	M	86	GLN	4.2
1	0	284	C	4.2
14	L	81	VAL	4.2
8	E	100	ASP	4.2
27	Y	235	GLU	4.1
32	I	99	ASP	4.1
11	H	146	VAL	4.1
24	V	36	ALA	4.1
1	0	1948	G	4.1
16	N	160	SER	4.1
7	D	135	VAL	4.1
1	0	1171	A	4.0
16	N	175	LEU	4.0
1	0	735	C	4.0
32	I	103	ASP	4.0
15	M	75	ARG	4.0
15	M	74	LYS	4.0
1	0	1192	A	4.0
7	D	62	ASP	4.0
14	L	80	ASP	4.0
1	0	1525	G	3.9
27	Y	95	THR	3.9
16	N	163	PHE	3.9
23	U	47	ARG	3.9
1	0	1950	G	3.9
28	Z	11	SER	3.9
9	F	99	THR	3.9
1	0	2237	G	3.9
32	I	106	LYS	3.9
7	D	91	ALA	3.9
1	0	283	U	3.8
1	0	2004	U	3.8
1	0	285	A	3.8
32	I	120	ASP	3.8
5	B	1	PRO	3.8
9	F	16	ALA	3.8
1	0	1168	C	3.8

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Mol	Chain	Res	Type	RSRZ
9	F	119	ARG	3.8
7	D	104	PHE	3.8
31	3	92	GLU	3.8
8	E	10	ASP	3.8
1	0	960	G	3.8
4	A	31	LYS	3.8
9	F	25	ASP	3.7
9	F	28	ALA	3.7
8	E	6	GLU	3.7
7	D	64	ARG	3.7
10	G	22	ALA	3.7
14	L	75	LEU	3.7
1	0	1198	U	3.7
7	D	69	ILE	3.7
4	A	35	GLY	3.7
27	Y	236	VAL	3.7
11	H	73	LEU	3.7
16	N	95	ALA	3.7
7	D	85	GLN	3.6
24	V	43	PRO	3.6
32	I	92	PRO	3.6
1	0	2769	C	3.6
22	T	82	THR	3.6
7	D	95	THR	3.6
32	I	110	GLU	3.6
7	D	27	ILE	3.6
32	I	123	ASN	3.6
16	N	184	ILE	3.6
14	L	76	LEU	3.6
19	Q	95	GLU	3.6
7	D	171	ASP	3.6
28	Z	20	ARG	3.6
2	9	3122	C	3.5
11	H	168	ALA	3.5
32	I	124	ALA	3.5
9	F	117	GLU	3.5
7	D	106	PHE	3.5
1	0	10	U	3.5
1	0	272	A	3.5
1	0	2511	A	3.5
4	A	236	GLY	3.5
32	I	90	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
7	D	172	VAL	3.5
7	D	81	GLU	3.5
1	0	2238	A	3.5
1	0	1966	U	3.5
1	0	1163	G	3.5
1	0	1164	U	3.5
7	D	40	ILE	3.4
22	T	115	GLU	3.4
1	0	1169	U	3.4
32	I	94	GLU	3.4
1	0	999	C	3.4
5	B	183	GLU	3.4
15	M	79	ALA	3.4
24	V	8	ILE	3.4
26	X	77	PHE	3.4
9	F	118	LEU	3.3
16	N	178	THR	3.3
16	N	181	ASP	3.3
1	0	288	A	3.3
28	Z	22	SER	3.3
14	L	97	VAL	3.3
1	0	2344	G	3.3
15	M	87	GLY	3.3
1	0	369	G	3.2
10	G	66	LEU	3.2
11	H	111	ASP	3.2
7	D	51	ARG	3.2
7	D	173	GLU	3.2
11	H	35	ARG	3.2
24	V	41	GLU	3.2
7	D	89	PRO	3.2
1	0	1181	A	3.2
7	D	56	ARG	3.2
15	M	71	SER	3.2
32	I	112	LYS	3.2
10	G	24	VAL	3.2
26	X	85	VAL	3.2
26	X	71	ARG	3.2
16	N	147	ILE	3.2
8	E	87	PHE	3.2
28	Z	21	VAL	3.2
16	N	159	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
11	H	138	CYS	3.2
1	0	138	U	3.2
1	0	1967	U	3.1
15	M	76	ARG	3.1
8	E	154	ILE	3.1
32	I	100	LEU	3.1
1	0	281	U	3.1
24	V	59	ILE	3.1
14	L	105	TYR	3.1
28	Z	24	ARG	3.1
16	N	134	ASP	3.1
32	I	115	ASP	3.1
9	F	12	LEU	3.1
26	X	10	VAL	3.0
4	A	85	SER	3.0
7	D	41	LEU	3.0
14	L	148	GLU	3.0
12	J	4	ALA	3.0
14	L	62	ALA	3.0
14	L	100	ALA	3.0
9	F	101	ALA	3.0
18	P	18	LYS	3.0
1	0	370	G	3.0
8	E	43	ASP	3.0
15	M	88	VAL	3.0
32	I	131	THR	3.0
10	G	12	ILE	2.9
16	N	155	GLU	2.9
9	F	105	ASP	2.9
6	C	61	PHE	2.9
14	L	145	LEU	2.9
9	F	106	ALA	2.9
11	H	83	TYR	2.9
16	N	161	GLY	2.9
7	D	73	VAL	2.9
7	D	130	VAL	2.9
9	F	100	ASP	2.9
9	F	107	ASP	2.9
32	I	135	LEU	2.9
5	B	2	GLN	2.9
14	L	79	ASP	2.9
16	N	185	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
8	E	126	ILE	2.9
4	A	97	ALA	2.9
14	L	147	GLU	2.9
1	0	358	G	2.8
1	0	1162	G	2.8
8	E	124	VAL	2.8
1	0	1170	U	2.8
11	H	149	ALA	2.8
1	0	1174	A	2.8
9	F	26	THR	2.8
7	D	67	ASP	2.8
28	Z	36	ASP	2.8
14	L	106	VAL	2.8
10	G	67	LEU	2.8
16	N	158	LEU	2.8
15	M	80	GLY	2.8
32	I	130	GLY	2.8
9	F	110	ASP	2.8
1	0	1180	U	2.8
27	Y	96	GLU	2.8
24	V	2	VAL	2.8
19	Q	18	PRO	2.8
1	0	362	G	2.8
27	Y	216	ARG	2.8
16	N	72	GLU	2.8
8	E	88	TYR	2.8
7	D	154	LYS	2.8
15	M	84	LYS	2.8
1	0	1165	G	2.8
11	H	47	ILE	2.8
10	G	15	TRP	2.8
11	H	82	ASP	2.7
1	0	279	C	2.7
21	S	20	PHE	2.7
16	N	183	ASP	2.7
11	H	78	GLY	2.7
1	0	361	C	2.7
8	E	94	GLN	2.7
24	V	5	VAL	2.7
1	0	1190	G	2.7
10	G	21	ASP	2.7
10	G	73	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
7	D	18	ILE	2.7
1	0	2345	A	2.7
1	0	1182	C	2.7
16	N	2	THR	2.7
11	H	37	GLN	2.7
11	H	162	ARG	2.7
7	D	26	GLY	2.7
14	L	60	GLU	2.7
1	0	1203	G	2.7
7	D	167	GLU	2.7
7	D	58	VAL	2.7
17	O	23	GLY	2.7
16	N	94	GLU	2.6
16	N	139	TRP	2.6
25	W	86	GLU	2.6
11	H	39	ASP	2.6
5	B	123	ALA	2.6
1	0	1175	G	2.6
7	D	68	PRO	2.6
11	H	141	GLU	2.6
15	M	77	HIS	2.6
30	2	39	ARG	2.6
1	0	969	G	2.6
1	0	1179	C	2.6
1	0	1184	C	2.6
11	H	139	ASN	2.6
5	B	57	GLU	2.6
7	D	157	LEU	2.6
7	D	23	VAL	2.6
9	F	98	VAL	2.6
19	Q	76	VAL	2.6
1	0	441	A	2.6
1	0	1947	G	2.6
5	B	117	GLU	2.6
14	L	99	GLU	2.6
10	G	65	THR	2.5
32	I	73	PRO	2.5
27	Y	234	VAL	2.5
24	V	10	ASP	2.5
1	0	295	C	2.5
11	H	74	ILE	2.5
1	0	372	A	2.5

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Mol	Chain	Res	Type	RSRZ
5	B	134	ALA	2.5
15	M	49	ALA	2.5
31	3	62	THR	2.5
5	B	180	ASP	2.5
14	L	102	ASP	2.5
16	N	182	GLY	2.5
9	F	19	ALA	2.5
9	F	23	ALA	2.5
1	0	1527	A	2.5
1	0	1625	U	2.5
1	0	2645	U	2.5
1	0	1161	A	2.5
31	3	56	PRO	2.5
9	F	21	GLU	2.5
11	H	67	LEU	2.5
24	V	3	LEU	2.5
7	D	160	ALA	2.5
4	A	65	ARG	2.5
1	0	736	A	2.5
1	0	1526	A	2.5
1	0	1929	G	2.5
9	F	11	ASP	2.5
9	F	15	ASP	2.5
21	S	78	ALA	2.4
15	M	78	LYS	2.4
17	O	1	SER	2.4
1	0	2748	G	2.4
7	D	75	LEU	2.4
9	F	49	PHE	2.4
9	F	103	GLU	2.4
14	L	149	ARG	2.4
26	X	7	GLU	2.4
32	I	128	VAL	2.4
1	0	1000	C	2.4
11	H	79	GLU	2.4
7	D	84	LEU	2.4
11	H	142	ASP	2.4
1	0	1167	G	2.4
1	0	2747	C	2.4
11	H	137	TYR	2.4
32	I	95	ASP	2.4
7	D	74	THR	2.4

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Mol	Chain	Res	Type	RSRZ
9	F	24	ARG	2.3
16	N	164	ASP	2.3
23	U	53	ASP	2.3
24	V	46	ILE	2.3
31	3	41	GLU	2.3
26	X	41	PHE	2.3
26	X	43	VAL	2.3
5	B	104	GLU	2.3
32	I	127	GLU	2.3
14	L	150	GLN	2.3
7	D	17	ARG	2.3
28	Z	25	ARG	2.3
5	B	176	ASP	2.3
7	D	77	ASP	2.3
8	E	127	ASP	2.3
11	H	166	SER	2.3
16	N	156	GLU	2.3
32	I	82	GLU	2.3
9	F	108	VAL	2.3
14	L	93	VAL	2.3
8	E	99	GLY	2.3
1	0	1208	C	2.3
15	M	81	ARG	2.3
14	L	104	ASP	2.3
1	0	1189	A	2.3
9	F	18	GLU	2.3
2	9	3072	C	2.3
16	N	138	ASP	2.3
7	D	53	LYS	2.3
24	V	14	ALA	2.3
23	U	54	THR	2.2
1	0	1964	U	2.2
7	D	165	PHE	2.2
8	E	86	VAL	2.2
16	N	74	PRO	2.2
7	D	65	GLU	2.2
9	F	109	GLU	2.2
10	G	25	GLU	2.2
11	H	76	GLU	2.2
12	J	5	GLU	2.2
1	0	716	G	2.2
28	Z	45	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
24	V	63	GLU	2.2
14	L	130	ARG	2.2
23	U	55	ALA	2.2
16	N	106	LEU	2.2
1	0	365	G	2.2
16	N	172	PHE	2.2
7	D	86	THR	2.2
27	Y	108	ASP	2.2
10	G	63	ARG	2.2
15	M	82	ARG	2.2
1	0	1279	U	2.2
7	D	70	GLY	2.2
7	D	38	GLU	2.2
1	0	363	A	2.2
4	A	86	ALA	2.2
9	F	90	GLU	2.2
16	N	177	GLU	2.2
8	E	103	VAL	2.2
7	D	45	THR	2.2
8	E	131	LEU	2.2
11	H	42	ASP	2.2
4	A	135	VAL	2.1
10	G	68	GLU	2.1
28	Z	12	GLY	2.1
9	F	115	VAL	2.1
4	A	38	ILE	2.1
15	M	73	ARG	2.1
6	C	1	MET	2.1
21	S	70	GLU	2.1
16	N	69	TYR	2.1
1	0	1178	G	2.1
15	M	83	SER	2.1
9	F	17	LEU	2.1
22	T	59	GLU	2.1
11	H	164	ASP	2.1
7	D	163	VAL	2.1
16	N	137	ALA	2.1
3	4	77	PHE	2.1
8	E	98	GLU	2.1
8	E	118	ILE	2.1
7	D	25	MET	2.1
11	H	44	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
27	Y	98	GLN	2.1
23	U	45	GLU	2.1
21	S	45	TYR	2.1
26	X	44	ASP	2.0
24	V	45	ARG	2.0
1	0	1201	C	2.0
8	E	169	THR	2.0
8	E	129	GLU	2.0
4	A	82	VAL	2.0
7	D	128	LEU	2.0
1	0	1195	G	2.0
1	0	1183	C	2.0
1	0	293	A	2.0
16	N	152	GLU	2.0
5	B	61	PRO	2.0
15	M	132	ILE	2.0
18	P	141	ILE	2.0
15	M	194	ALA	2.0

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

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, 95^{th} 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
3	ACA	4	78	4/9	0.84	0.31	57,57,58,58	0
1	UR3	0	2619	21/22	0.97	0.13	34,38,41,43	0
1	PSU	0	2621	20/21	0.97	0.13	31,33,38,38	0
1	OMG	0	2588	24/25	0.97	0.12	30,34,36,38	0
1	1MA	0	628	23/24	0.98	0.13	28,32,33,34	0
1	OMU	0	2587	21/22	0.98	0.12	30,35,36,37	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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, 95^{th} 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
33	MG	0	8094	1/1	0.14	0.47	83,83,83,83	0
33	MG	0	8047	1/1	0.18	0.37	85,85,85,85	0
37	SR	B	9521	1/1	0.19	0.89	185,185,185,185	0
37	SR	0	9547	1/1	0.26	0.35	166,166,166,166	0
37	SR	0	9501	1/1	0.26	0.21	196,196,196,196	0
39	CD	O	9205	1/1	0.43	0.47	197,197,197,197	0
35	NA	0	9122	1/1	0.48	0.40	77,77,77,77	0
33	MG	0	8050	1/1	0.50	0.23	88,88,88,88	0
35	NA	0	9129	1/1	0.52	0.24	74,74,74,74	0
35	NA	0	9184	1/1	0.57	0.23	73,73,73,73	0
35	NA	S	9112	1/1	0.60	0.61	75,75,75,75	0
35	NA	9	9183	1/1	0.62	0.34	77,77,77,77	0
33	MG	0	8065	1/1	0.63	0.52	93,93,93,93	0
35	NA	0	9164	1/1	0.64	0.32	60,60,60,60	0
35	NA	0	9172	1/1	0.66	0.46	76,76,76,76	0
33	MG	0	8082	1/1	0.67	0.26	82,82,82,82	0
33	MG	0	8092	1/1	0.70	0.74	80,80,80,80	0
33	MG	0	8014	1/1	0.71	0.24	67,67,67,67	0
37	SR	0	9468	1/1	0.71	0.07	97,97,97,97	0
35	NA	0	9185	1/1	0.72	0.41	52,52,52,52	0
37	SR	9	9588	1/1	0.73	0.12	118,118,118,118	0
33	MG	0	8093	1/1	0.76	0.12	45,45,45,45	0
33	MG	0	8113	1/1	0.77	0.12	49,49,49,49	0
37	SR	0	9537	1/1	0.77	0.11	136,136,136,136	0
35	NA	0	9120	1/1	0.78	0.15	55,55,55,55	0
33	MG	0	8042	1/1	0.79	0.08	57,57,57,57	0
33	MG	0	8054	1/1	0.79	0.12	55,55,55,55	0
35	NA	0	9111	1/1	0.81	0.21	59,59,59,59	0
35	NA	B	9161	1/1	0.81	0.28	62,62,62,62	0
35	NA	0	9179	1/1	0.82	0.55	89,89,89,89	0
37	SR	0	9484	1/1	0.82	0.11	134,134,134,134	0
35	NA	0	9141	1/1	0.82	0.13	70,70,70,70	0
37	SR	0	9459	1/1	0.82	0.06	95,95,95,95	0
35	NA	0	9152	1/1	0.83	0.36	64,64,64,64	0
37	SR	0	9581	1/1	0.83	0.07	110,110,110,110	0
35	NA	0	9163	1/1	0.83	0.19	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	MG	0	8052	1/1	0.83	0.20	74,74,74,74	0
35	NA	0	9169	1/1	0.83	0.64	90,90,90,90	0
33	MG	0	8108	1/1	0.84	0.18	81,81,81,81	0
37	SR	0	9530	1/1	0.84	0.11	102,102,102,102	0
35	NA	0	9127	1/1	0.85	0.16	57,57,57,57	0
33	MG	0	8045	1/1	0.85	0.18	84,84,84,84	0
33	MG	0	8101	1/1	0.85	0.10	59,59,59,59	0
33	MG	0	8103	1/1	0.85	0.19	62,62,62,62	0
33	MG	0	8061	1/1	0.85	0.15	75,75,75,75	0
35	NA	0	9173	1/1	0.86	0.24	59,59,59,59	0
33	MG	0	8055	1/1	0.86	0.16	83,83,83,83	0
35	NA	0	9101	1/1	0.86	0.22	45,45,45,45	0
35	NA	0	9166	1/1	0.86	0.10	68,68,68,68	0
33	MG	0	8040	1/1	0.86	0.18	69,69,69,69	0
35	NA	0	9154	1/1	0.86	0.18	57,57,57,57	0
35	NA	0	9114	1/1	0.87	0.15	56,56,56,56	0
34	K	0	9002	1/1	0.87	0.09	78,78,78,78	0
36	CL	0	9316	1/1	0.87	0.20	69,69,69,69	0
37	SR	0	9452	1/1	0.87	0.15	105,105,105,105	0
35	NA	0	9150	1/1	0.87	0.19	47,47,47,47	0
33	MG	A	8066	1/1	0.88	0.12	53,53,53,53	0
33	MG	0	8083	1/1	0.88	0.10	53,53,53,53	0
37	SR	0	9539	1/1	0.88	0.43	145,145,145,145	0
33	MG	0	8107	1/1	0.88	0.14	70,70,70,70	0
35	NA	0	9168	1/1	0.88	0.17	66,66,66,66	0
37	SR	0	9601	1/1	0.88	0.60	191,191,191,191	0
35	NA	0	9186	1/1	0.88	0.13	67,67,67,67	0
35	NA	0	9102	1/1	0.88	0.42	61,61,61,61	0
35	NA	0	9107	1/1	0.88	0.20	54,54,54,54	0
35	NA	0	9139	1/1	0.89	0.17	57,57,57,57	0
33	MG	0	8043	1/1	0.89	0.08	50,50,50,50	0
33	MG	0	8090	1/1	0.89	0.22	68,68,68,68	0
37	SR	0	9482	1/1	0.89	0.19	115,115,115,115	0
35	NA	D	9151	1/1	0.89	0.23	62,62,62,62	0
37	SR	0	9500	1/1	0.89	1.88	197,197,197,197	0
33	MG	0	8024	1/1	0.89	0.61	74,74,74,74	0
35	NA	0	9132	1/1	0.89	0.14	54,54,54,54	0
37	SR	0	9529	1/1	0.90	0.11	136,136,136,136	0
35	NA	0	9175	1/1	0.90	0.18	47,47,47,47	0
35	NA	0	9178	1/1	0.90	0.50	52,52,52,52	0
33	MG	4	8118	1/1	0.90	0.13	45,45,45,45	0
33	MG	0	8056	1/1	0.90	0.21	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	K	0	9001	1/1	0.90	0.30	84,84,84,84	0
33	MG	0	8102	1/1	0.90	0.09	66,66,66,66	0
35	NA	0	9158	1/1	0.90	0.34	55,55,55,55	0
33	MG	0	8114	1/1	0.90	0.28	71,71,71,71	0
38	SPS	4	9701	23/23	0.90	0.17	49,53,67,71	0
35	NA	0	9174	1/1	0.90	0.14	61,61,61,61	0
33	MG	0	8091	1/1	0.91	0.12	64,64,64,64	0
33	MG	0	8036	1/1	0.91	0.09	56,56,56,56	0
33	MG	0	8057	1/1	0.91	0.19	77,77,77,77	0
37	SR	0	9566	1/1	0.91	0.05	92,92,92,92	0
33	MG	0	8060	1/1	0.91	0.23	76,76,76,76	0
33	MG	0	8085	1/1	0.91	0.24	67,67,67,67	0
33	MG	0	8089	1/1	0.91	0.12	54,54,54,54	0
33	MG	0	8022	1/1	0.91	0.55	63,63,63,63	0
35	NA	0	9181	1/1	0.91	0.14	52,52,52,52	0
37	SR	0	9425	1/1	0.91	0.07	108,108,108,108	0
37	SR	0	9466	1/1	0.92	0.05	89,89,89,89	0
35	NA	0	9126	1/1	0.92	0.10	52,52,52,52	0
33	MG	0	8084	1/1	0.92	0.29	61,61,61,61	0
35	NA	R	9137	1/1	0.92	0.11	33,33,33,33	0
33	MG	0	8072	1/1	0.92	0.24	70,70,70,70	0
35	NA	0	9157	1/1	0.92	0.18	37,37,37,37	0
33	MG	0	8063	1/1	0.92	0.13	64,64,64,64	0
33	MG	9	8095	1/1	0.92	0.20	48,48,48,48	0
33	MG	0	8058	1/1	0.92	0.20	39,39,39,39	0
35	NA	0	9182	1/1	0.93	0.13	63,63,63,63	0
33	MG	0	8037	1/1	0.93	0.07	39,39,39,39	0
33	MG	0	8021	1/1	0.93	0.24	56,56,56,56	0
37	SR	0	9590	1/1	0.93	0.10	117,117,117,117	0
35	NA	0	9140	1/1	0.93	0.35	63,63,63,63	0
35	NA	0	9117	1/1	0.93	0.15	32,32,32,32	0
35	NA	0	9170	1/1	0.93	0.46	72,72,72,72	0
33	MG	0	8099	1/1	0.93	0.14	62,62,62,62	0
35	NA	M	9147	1/1	0.93	0.12	43,43,43,43	0
33	MG	0	8115	1/1	0.94	0.17	55,55,55,55	0
33	MG	0	8117	1/1	0.94	0.13	39,39,39,39	0
37	SR	0	9532	1/1	0.94	0.09	115,115,115,115	0
35	NA	0	9177	1/1	0.94	0.40	71,71,71,71	0
33	MG	0	8015	1/1	0.94	0.12	29,29,29,29	0
37	SR	0	9465	1/1	0.94	0.11	98,98,98,98	0
33	MG	0	8088	1/1	0.94	0.06	43,43,43,43	0
35	NA	J	9146	1/1	0.94	0.09	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
37	SR	0	9477	1/1	0.94	0.08	75,75,75,75	0
33	MG	0	8112	1/1	0.94	0.08	45,45,45,45	0
37	SR	0	9626	1/1	0.94	0.37	127,127,127,127	0
33	MG	0	8039	1/1	0.94	0.08	61,61,61,61	0
33	MG	0	8104	1/1	0.94	0.11	49,49,49,49	0
36	CL	0	9315	1/1	0.94	0.11	53,53,53,53	0
37	SR	0	9505	1/1	0.94	0.08	97,97,97,97	0
33	MG	0	8051	1/1	0.95	0.19	23,23,23,23	0
37	SR	0	9504	1/1	0.95	0.10	88,88,88,88	0
35	NA	0	9124	1/1	0.95	0.16	53,53,53,53	0
37	SR	0	9517	1/1	0.95	0.07	92,92,92,92	0
37	SR	0	9522	1/1	0.95	0.06	98,98,98,98	0
33	MG	0	8116	1/1	0.95	0.07	51,51,51,51	0
35	NA	0	9162	1/1	0.95	0.15	49,49,49,49	0
33	MG	0	8096	1/1	0.95	0.10	40,40,40,40	0
36	CL	J	9302	1/1	0.95	0.07	54,54,54,54	0
33	MG	0	8044	1/1	0.95	0.09	35,35,35,35	0
35	NA	0	9165	1/1	0.95	0.17	44,44,44,44	0
33	MG	0	8030	1/1	0.95	0.06	37,37,37,37	0
37	SR	0	9570	1/1	0.95	0.06	92,92,92,92	0
33	MG	0	8076	1/1	0.95	0.13	51,51,51,51	0
35	NA	0	9115	1/1	0.95	0.15	35,35,35,35	0
33	MG	T	8073	1/1	0.95	0.15	41,41,41,41	0
35	NA	0	9171	1/1	0.95	0.14	66,66,66,66	0
35	NA	C	9104	1/1	0.95	0.19	31,31,31,31	0
37	SR	0	9483	1/1	0.95	0.08	69,69,69,69	0
35	NA	0	9118	1/1	0.95	0.21	49,49,49,49	0
33	MG	0	8080	1/1	0.95	0.20	46,46,46,46	0
36	CL	3	9304	1/1	0.96	0.04	65,65,65,65	0
35	NA	0	9149	1/1	0.96	0.12	43,43,43,43	0
37	SR	0	9438	1/1	0.96	0.09	61,61,61,61	0
33	MG	0	8059	1/1	0.96	0.16	48,48,48,48	0
33	MG	0	8041	1/1	0.96	0.11	51,51,51,51	0
33	MG	0	8097	1/1	0.96	0.16	57,57,57,57	0
35	NA	0	9167	1/1	0.96	0.10	49,49,49,49	0
36	CL	0	9311	1/1	0.96	0.12	61,61,61,61	0
37	SR	0	9475	1/1	0.96	0.11	76,76,76,76	0
36	CL	0	9314	1/1	0.96	0.09	43,43,43,43	0
33	MG	0	8098	1/1	0.96	0.09	45,45,45,45	0
35	NA	0	9125	1/1	0.96	0.79	93,93,93,93	0
33	MG	0	8031	1/1	0.96	0.05	51,51,51,51	0
36	CL	J	9321	1/1	0.96	0.15	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	CL	L	9310	1/1	0.96	0.06	47,47,47,47	0
36	CL	M	9318	1/1	0.96	0.18	40,40,40,40	0
36	CL	N	9307	1/1	0.96	0.15	60,60,60,60	0
37	SR	0	9509	1/1	0.96	0.11	83,83,83,83	0
37	SR	0	9480	1/1	0.97	0.04	82,82,82,82	0
35	NA	0	9159	1/1	0.97	0.18	46,46,46,46	0
33	MG	0	8019	1/1	0.97	0.06	47,47,47,47	0
35	NA	0	9113	1/1	0.97	0.21	64,64,64,64	0
37	SR	0	9490	1/1	0.97	0.08	101,101,101,101	0
37	SR	0	9495	1/1	0.97	0.09	85,85,85,85	0
36	CL	B	9319	1/1	0.97	0.25	53,53,53,53	0
33	MG	0	8075	1/1	0.97	0.06	43,43,43,43	0
35	NA	0	9134	1/1	0.97	0.05	42,42,42,42	0
33	MG	0	8110	1/1	0.97	0.20	44,44,44,44	0
37	SR	0	9506	1/1	0.97	0.06	74,74,74,74	0
35	NA	0	9116	1/1	0.97	0.18	46,46,46,46	0
33	MG	0	8009	1/1	0.97	0.06	31,31,31,31	0
35	NA	0	9143	1/1	0.97	0.07	37,37,37,37	0
33	MG	0	8079	1/1	0.97	0.14	28,28,28,28	0
37	SR	0	9432	1/1	0.97	0.14	61,61,61,61	0
37	SR	0	9433	1/1	0.97	0.12	68,68,68,68	0
33	MG	0	8026	1/1	0.97	0.14	28,28,28,28	0
37	SR	0	9445	1/1	0.97	0.11	55,55,55,55	0
33	MG	0	8027	1/1	0.97	0.23	35,35,35,35	0
37	SR	0	9560	1/1	0.97	0.10	88,88,88,88	0
37	SR	0	9453	1/1	0.97	0.09	68,68,68,68	0
37	SR	0	9568	1/1	0.97	0.10	70,70,70,70	0
37	SR	0	9454	1/1	0.97	0.06	71,71,71,71	0
33	MG	0	8029	1/1	0.97	0.20	26,26,26,26	0
37	SR	0	9585	1/1	0.97	0.10	83,83,83,83	0
37	SR	0	9464	1/1	0.97	0.06	79,79,79,79	0
35	NA	Q	9148	1/1	0.97	0.17	51,51,51,51	0
35	NA	0	9155	1/1	0.97	0.23	52,52,52,52	0
37	SR	9	9503	1/1	0.97	0.05	102,102,102,102	0
37	SR	0	9467	1/1	0.97	0.12	71,71,71,71	0
35	NA	R	9138	1/1	0.97	0.08	58,58,58,58	0
37	SR	H	9486	1/1	0.97	0.14	107,107,107,107	0
35	NA	0	9106	1/1	0.97	0.14	35,35,35,35	0
33	MG	0	8067	1/1	0.97	0.10	33,33,33,33	0
35	NA	0	9160	1/1	0.98	0.12	36,36,36,36	0
37	SR	0	9469	1/1	0.98	0.05	83,83,83,83	0
36	CL	0	9317	1/1	0.98	0.06	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	CL	0	9322	1/1	0.98	0.12	51,51,51,51	0
36	CL	A	9309	1/1	0.98	0.07	56,56,56,56	0
35	NA	0	9131	1/1	0.98	0.07	45,45,45,45	0
36	CL	J	9301	1/1	0.98	0.07	46,46,46,46	0
33	MG	0	8032	1/1	0.98	0.09	33,33,33,33	0
37	SR	0	9488	1/1	0.98	0.11	72,72,72,72	0
37	SR	0	9489	1/1	0.98	0.06	85,85,85,85	0
33	MG	0	8013	1/1	0.98	0.39	14,14,14,14	0
35	NA	0	9135	1/1	0.98	0.09	39,39,39,39	0
35	NA	0	9136	1/1	0.98	0.10	30,30,30,30	0
33	MG	0	8046	1/1	0.98	0.08	37,37,37,37	0
36	CL	O	9308	1/1	0.98	0.09	59,59,59,59	0
36	CL	Y	9320	1/1	0.98	0.11	40,40,40,40	0
33	MG	0	8002	1/1	0.98	0.12	29,29,29,29	0
37	SR	0	9508	1/1	0.98	0.07	78,78,78,78	0
37	SR	0	9405	1/1	0.98	0.06	80,80,80,80	0
37	SR	0	9515	1/1	0.98	0.12	88,88,88,88	0
37	SR	0	9417	1/1	0.98	0.14	53,53,53,53	0
37	SR	0	9420	1/1	0.98	0.17	65,65,65,65	0
33	MG	0	8003	1/1	0.98	0.10	26,26,26,26	0
37	SR	0	9426	1/1	0.98	0.07	64,64,64,64	0
37	SR	0	9427	1/1	0.98	0.14	54,54,54,54	0
37	SR	0	9429	1/1	0.98	0.10	64,64,64,64	0
37	SR	0	9431	1/1	0.98	0.14	56,56,56,56	0
37	SR	0	9545	1/1	0.98	0.05	72,72,72,72	0
33	MG	0	8017	1/1	0.98	0.15	23,23,23,23	0
33	MG	0	8001	1/1	0.98	0.21	23,23,23,23	0
33	MG	0	8020	1/1	0.98	0.17	36,36,36,36	0
37	SR	0	9440	1/1	0.98	0.06	61,61,61,61	0
33	MG	0	8012	1/1	0.98	0.24	37,37,37,37	0
37	SR	0	9447	1/1	0.98	0.09	62,62,62,62	0
37	SR	0	9448	1/1	0.98	0.09	59,59,59,59	0
37	SR	0	9451	1/1	0.98	0.12	64,64,64,64	0
33	MG	0	8068	1/1	0.98	0.12	41,41,41,41	0
35	NA	0	9108	1/1	0.98	0.10	31,31,31,31	0
37	SR	9	9481	1/1	0.98	0.07	82,82,82,82	0
36	CL	0	9305	1/1	0.98	0.06	50,50,50,50	0
35	NA	0	9110	1/1	0.98	0.12	45,45,45,45	0
37	SR	A	9436	1/1	0.98	0.03	68,68,68,68	0
37	SR	A	9437	1/1	0.98	0.14	61,61,61,61	0
37	SR	A	9497	1/1	0.98	0.10	78,78,78,78	0
37	SR	B	9458	1/1	0.98	0.07	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	CL	0	9312	1/1	0.98	0.09	47,47,47,47	0
36	CL	0	9313	1/1	0.98	0.07	47,47,47,47	0
37	SR	S	9470	1/1	0.98	0.13	91,91,91,91	0
37	SR	1	9460	1/1	0.98	0.14	51,51,51,51	0
37	SR	3	9439	1/1	0.98	0.07	64,64,64,64	0
35	NA	0	9128	1/1	0.98	0.14	39,39,39,39	0
33	MG	0	8070	1/1	0.98	0.16	21,21,21,21	0
39	CD	Z	9203	1/1	0.98	0.14	59,59,59,59	0
39	CD	3	9204	1/1	0.98	0.08	59,59,59,59	0
37	SR	0	9441	1/1	0.99	0.09	57,57,57,57	0
37	SR	0	9442	1/1	0.99	0.12	59,59,59,59	0
37	SR	0	9443	1/1	0.99	0.11	54,54,54,54	0
37	SR	0	9444	1/1	0.99	0.13	50,50,50,50	0
33	MG	0	8005	1/1	0.99	0.08	29,29,29,29	0
37	SR	0	9446	1/1	0.99	0.09	78,78,78,78	0
33	MG	0	8038	1/1	0.99	0.26	18,18,18,18	0
35	NA	0	9130	1/1	0.99	0.12	47,47,47,47	0
37	SR	0	9449	1/1	0.99	0.10	57,57,57,57	0
37	SR	0	9450	1/1	0.99	0.09	60,60,60,60	0
37	SR	0	9407	1/1	0.99	0.17	46,46,46,46	0
37	SR	0	9410	1/1	0.99	0.20	45,45,45,45	0
37	SR	0	9534	1/1	0.99	0.09	95,95,95,95	0
37	SR	0	9412	1/1	0.99	0.16	48,48,48,48	0
37	SR	0	9414	1/1	0.99	0.15	54,54,54,54	0
37	SR	0	9455	1/1	0.99	0.10	61,61,61,61	0
37	SR	0	9456	1/1	0.99	0.07	64,64,64,64	0
37	SR	0	9457	1/1	0.99	0.12	49,49,49,49	0
37	SR	0	9415	1/1	0.99	0.12	54,54,54,54	0
37	SR	0	9461	1/1	0.99	0.04	71,71,71,71	0
37	SR	0	9462	1/1	0.99	0.13	64,64,64,64	0
33	MG	0	8025	1/1	0.99	0.33	24,24,24,24	0
33	MG	0	8008	1/1	0.99	0.23	16,16,16,16	0
37	SR	0	9421	1/1	0.99	0.10	65,65,65,65	0
37	SR	0	9422	1/1	0.99	0.13	55,55,55,55	0
37	SR	0	9423	1/1	0.99	0.12	51,51,51,51	0
37	SR	0	9629	1/1	0.99	0.10	68,68,68,68	0
33	MG	0	8074	1/1	0.99	0.21	20,20,20,20	0
37	SR	0	9473	1/1	0.99	0.06	69,69,69,69	0
37	SR	0	9474	1/1	0.99	0.07	71,71,71,71	0
35	NA	0	9156	1/1	0.99	0.15	55,55,55,55	0
36	CL	0	9303	1/1	0.99	0.09	43,43,43,43	0
37	SR	0	9478	1/1	0.99	0.07	69,69,69,69	0

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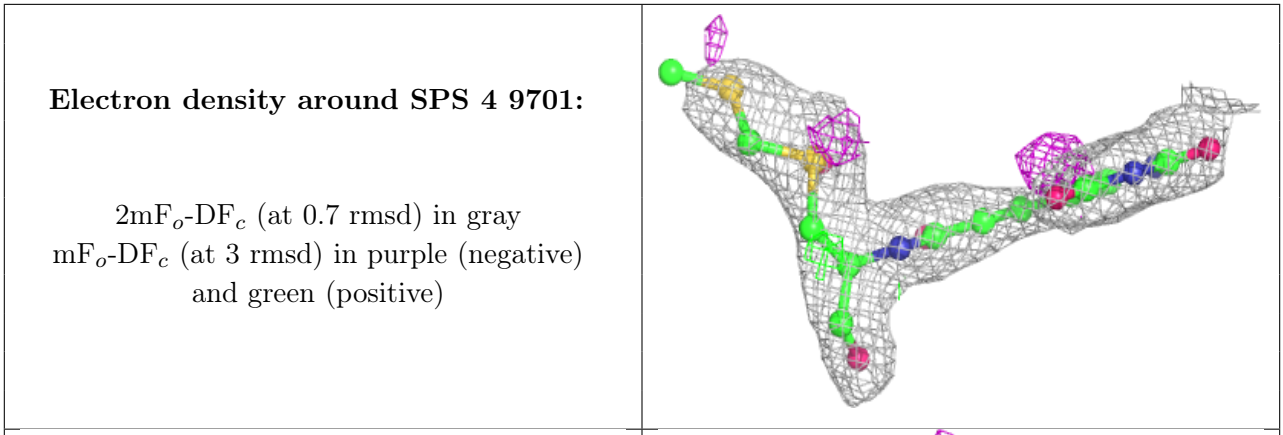
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
37	SR	0	9428	1/1	0.99	0.12	49,49,49,49	0
35	NA	0	9123	1/1	0.99	0.08	39,39,39,39	0
37	SR	F	9595	1/1	0.99	0.16	92,92,92,92	0
33	MG	Y	8109	1/1	0.99	0.04	35,35,35,35	0
37	SR	L	9409	1/1	0.99	0.21	49,49,49,49	0
37	SR	R	9418	1/1	0.99	0.16	54,54,54,54	0
33	MG	0	8004	1/1	0.99	0.11	26,26,26,26	0
37	SR	1	9419	1/1	0.99	0.15	43,43,43,43	0
33	MG	0	8028	1/1	0.99	0.12	31,31,31,31	0
37	SR	0	9434	1/1	0.99	0.12	59,59,59,59	0
37	SR	0	9435	1/1	0.99	0.08	68,68,68,68	0
33	MG	0	8106	1/1	0.99	0.06	47,47,47,47	0
39	CD	U	9201	1/1	0.99	0.13	59,59,59,59	0
37	SR	0	9498	1/1	0.99	0.06	61,61,61,61	0
39	CD	1	9202	1/1	0.99	0.07	55,55,55,55	0
36	CL	R	9306	1/1	0.99	0.11	43,43,43,43	0
37	SR	0	9406	1/1	1.00	0.22	43,43,43,43	0
37	SR	0	9430	1/1	1.00	0.17	46,46,46,46	0
37	SR	0	9413	1/1	1.00	0.14	49,49,49,49	0
35	NA	0	9105	1/1	1.00	0.04	33,33,33,33	0
37	SR	0	9424	1/1	1.00	0.17	46,46,46,46	0
37	SR	0	9408	1/1	1.00	0.21	45,45,45,45	0
37	SR	0	9416	1/1	1.00	0.16	47,47,47,47	0
33	MG	K	8069	1/1	1.00	0.23	24,24,24,24	0
37	SR	0	9411	1/1	1.00	0.19	46,46,46,46	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 SPS 4 9701:

$2mF_o$-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 (i)

There are no such residues in this entry.