



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:56 PM GMT

PDB ID : 1M90
Title : Co-crystal structure of CCA-Phe-caproic acid-biotin and sparsomycin bound to the 50S ribosomal subunit
Authors : Hansen, J.L.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.
Deposited on : 2002-07-26
Resolution : 2.80 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

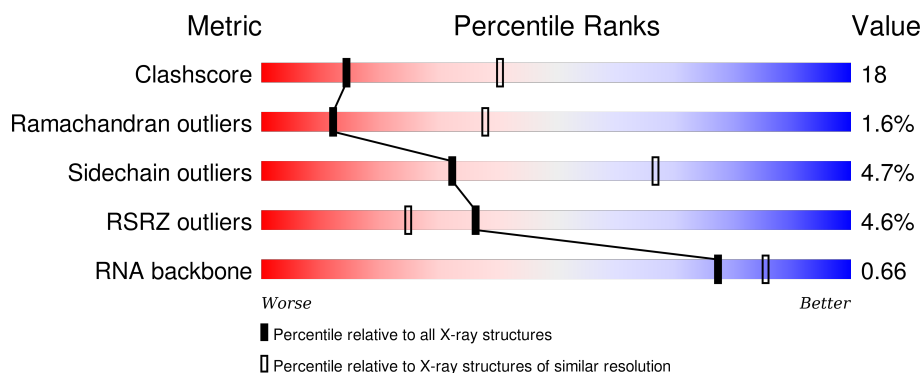
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)
RNA backbone	2183	1091 (3.20-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2922	<div> <div>2%</div> <div>59%</div> <div>30%</div> <div>5%</div> <div>6%</div> </div>
2	B	122	<div> <div>3%</div> <div>49%</div> <div>38%</div> <div>11%</div> <div>•</div> </div>
3	5	3	<div> <div>67%</div> <div>33%</div> </div>
4	C	239	<div> <div>5%</div> <div>60%</div> <div>32%</div> <div>7%</div> <div>•</div> </div>
5	D	337	<div> <div>%</div> <div>50%</div> <div>44%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
6	E	246	
7	F	176	
8	G	177	
9	H	119	
10	I	348	
11	J	167	
12	K	145	
13	L	132	
14	M	164	
15	N	194	
16	O	186	
17	P	115	
18	Q	148	
19	R	95	
20	S	154	
21	T	84	
22	U	119	
23	V	66	
24	W	70	
25	X	154	
26	Y	91	
27	Z	240	
28	1	73	
29	2	56	
30	3	48	

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Mol	Chain	Length	Quality of chain
31	4	92	 % 61% 35%

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
32	MG	A	8060	-	-	-	X
33	NA	A	8303	-	-	-	X
33	NA	A	8310	-	-	-	X
33	NA	A	8321	-	-	-	X
33	NA	A	8325	-	-	-	X
33	NA	A	8331	-	-	-	X
33	NA	A	8335	-	-	-	X
33	NA	A	8340	-	-	-	X
33	NA	A	8350	-	-	-	X
33	NA	A	8356	-	-	-	X
33	NA	A	8359	-	-	-	X
33	NA	A	8361	-	-	-	X
33	NA	A	8362	-	-	-	X
33	NA	A	8364	-	-	-	X
33	NA	A	8366	-	-	-	X
33	NA	A	8368	-	-	-	X
33	NA	A	8371	-	-	-	X
33	NA	A	8372	-	-	-	X
33	NA	A	8373	-	-	-	X
33	NA	A	8374	-	-	-	X
33	NA	A	8378	-	-	-	X
33	NA	B	8383	-	-	-	X
33	NA	M	8380	-	-	-	X
33	NA	S	8386	-	-	-	X
34	K	A	8390	-	-	-	X
34	K	A	8391	-	-	-	X
35	CL	A	8515	-	-	-	X
36	SPS	5	9080	-	-	-	X
37	PHA	5	9077	-	-	-	X
38	ACA	5	9078	-	-	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 98611 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S RRNA.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	560	C	U	CONFLICT	GB 3377779

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

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

- Molecule 3 is a RNA chain called CCA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	5	3	Total	C	N	O	P	0	0	0
			59	28	11	18	2			

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L2.

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

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L3.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	DELETION	UNP P20279
D	310	ARG	PHE	CONFLICT	UNP P20279

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L4.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L5.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L6.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L7AE.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10.

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

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L10E.

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

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L13.

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

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L14.

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

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	145	Total	C	N	O	S	0	0	0
			1114	668	222	224				

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L15E.

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

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18.

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

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L18E.

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

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L19E.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	71	LYS	TYR	CONFLICT	UNP P14119

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L21E.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L23.

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

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24.

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

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L24E.

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L29.

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

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L30.

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

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L31E.

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

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L32E.

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

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	?	-	ARG	DELETION	UNP P22452

- Molecule 31 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	1	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	5	1	Total	Mg	0	0
			1	1		
32	C	1	Total	Mg	0	0
			1	1		
32	Z	1	Total	Mg	0	0
			1	1		
32	A	111	Total	Mg	0	0
			111	111		
32	4	1	Total	Mg	0	0
			1	1		
32	U	1	Total	Mg	0	0
			1	1		
32	L	1	Total	Mg	0	0
			1	1		

- Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	J	1	Total	Na	0	0
			1	1		
33	K	1	Total	Na	0	0
			1	1		
33	E	1	Total	Na	0	0
			1	1		
33	B	2	Total	Na	0	0
			2	2		
33	C	1	Total	Na	0	0
			1	1		
33	A	73	Total	Na	0	0
			73	73		
33	T	1	Total	Na	0	0
			1	1		
33	N	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	U	1	Total 1	Na 1	0	0
33	R	1	Total 1	Na 1	0	0
33	S	2	Total 2	Na 2	0	0
33	M	1	Total 1	Na 1	0	0

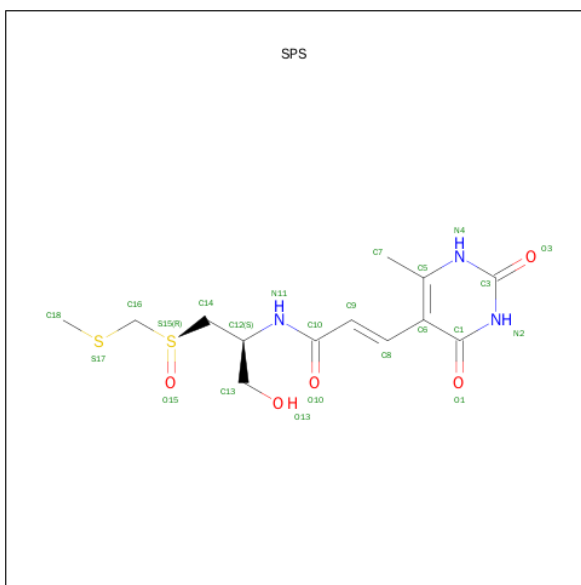
- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

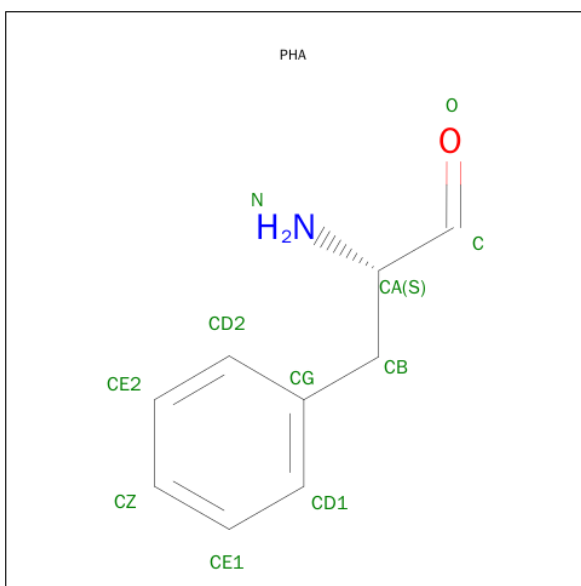
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	P	1	Total 1	Cl 1	0	0
35	D	1	Total 1	Cl 1	0	0
35	K	3	Total 3	Cl 3	0	0
35	C	1	Total 1	Cl 1	0	0
35	Z	1	Total 1	Cl 1	0	0
35	A	10	Total 10	Cl 10	0	0
35	4	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	O	1	Total 1	Cl 1	0	0
35	S	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

- Molecule 36 is SPARSOMYCIN (three-letter code: SPS) (formula: C₁₃H₁₉N₃O₅S₂).



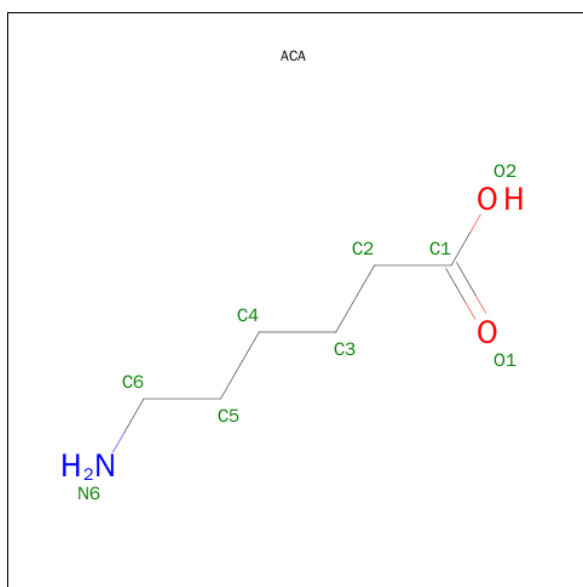
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
36	5	1	Total	C	N	O	S	0	0
			23	13	3	5	2		

- Molecule 37 is PHENYLALANINAL (three-letter code: PHA) (formula: $C_9H_{11}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	5	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 38 is 6-AMINOHEXANOIC ACID (three-letter code: ACA) (formula: $C_6H_{13}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	5	1	Total	C	N	O	0	0
			8	6	1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	P	1	Total	Cd	0	0
			1	1		
39	2	1	Total	Cd	0	0
			1	1		
39	1	1	Total	Cd	0	0
			1	1		
39	4	1	Total	Cd	0	0
			1	1		
39	V	1	Total	Cd	0	0
			1	1		

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	A	5920	Total	O	0	0
			5920	5920		
40	B	136	Total	O	0	0
			136	136		
40	5	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	C	119	Total 119	O 119	0	0
40	D	142	Total 142	O 142	0	0
40	E	172	Total 172	O 172	0	0
40	F	51	Total 51	O 51	0	0
40	G	44	Total 44	O 44	0	0
40	H	28	Total 28	O 28	0	0
40	I	21	Total 21	O 21	0	0
40	J	75	Total 75	O 75	0	0
40	K	56	Total 56	O 56	0	0
40	L	61	Total 61	O 61	0	0
40	M	86	Total 86	O 86	0	0
40	N	125	Total 125	O 125	0	0
40	O	69	Total 69	O 69	0	0
40	P	43	Total 43	O 43	0	0
40	Q	67	Total 67	O 67	0	0
40	R	49	Total 49	O 49	0	0
40	S	83	Total 83	O 83	0	0
40	T	35	Total 35	O 35	0	0
40	U	37	Total 37	O 37	0	0
40	V	24	Total 24	O 24	0	0
40	W	16	Total 16	O 16	0	0

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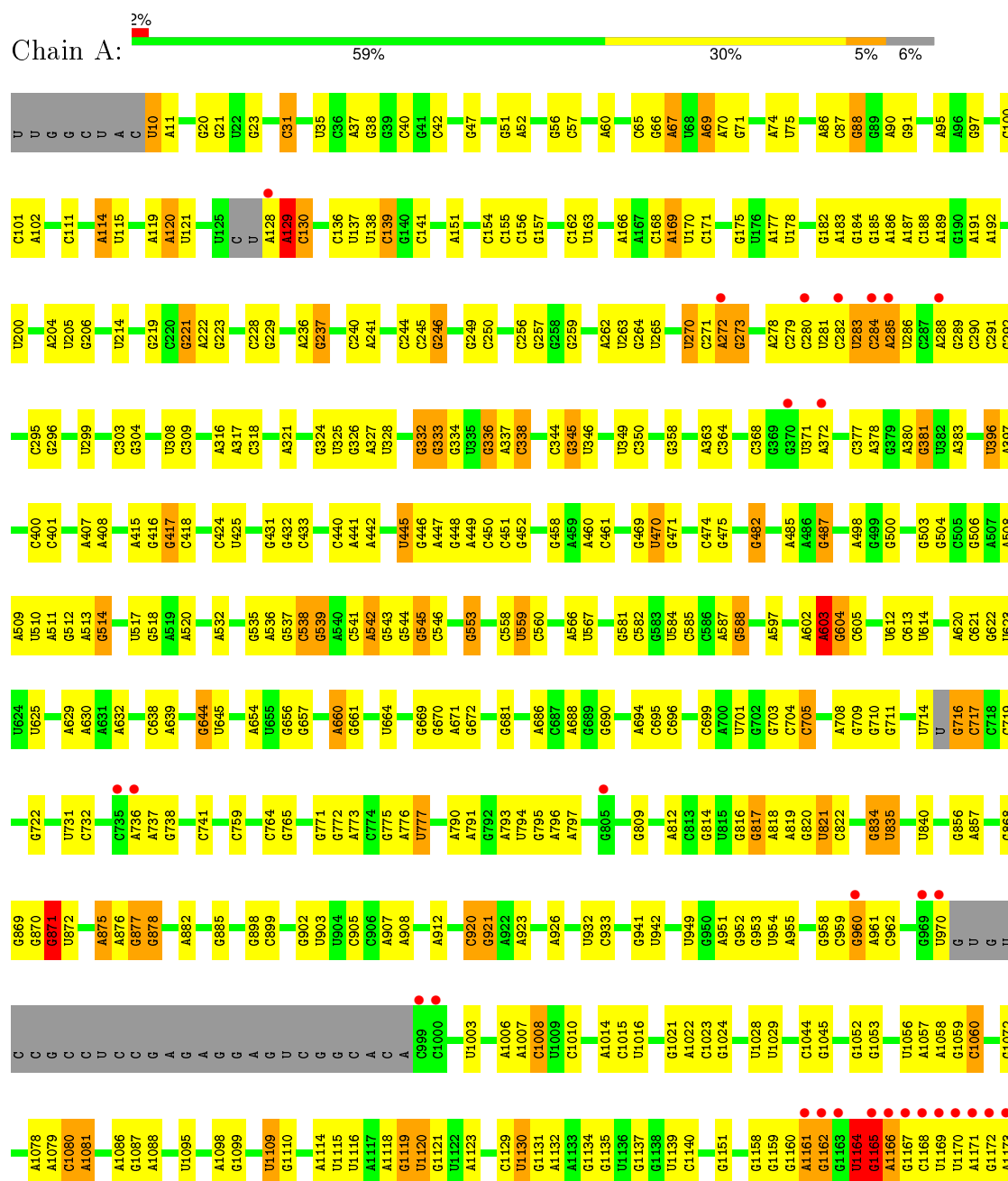
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	X	71	Total 71	O 71	0	0
40	Y	31	Total 31	O 31	0	0
40	Z	92	Total 92	O 92	0	0
40	1	36	Total 36	O 36	0	0
40	2	55	Total 55	O 55	0	0
40	3	40	Total 40	O 40	0	0
40	4	73	Total 73	O 73	0	0

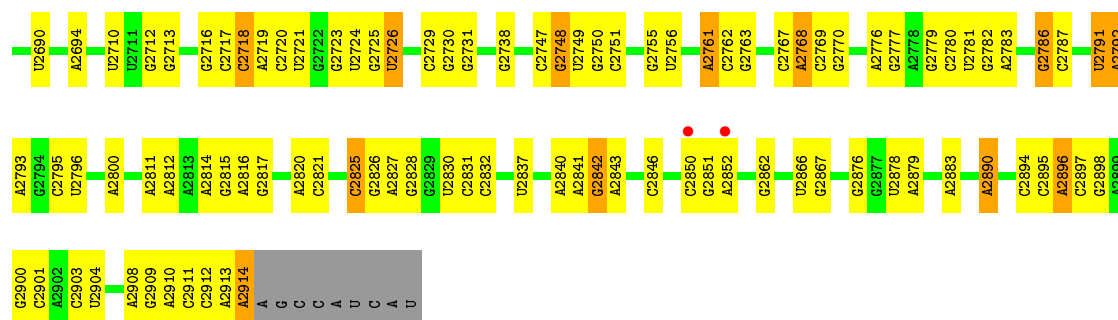
3 Residue-property plots

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

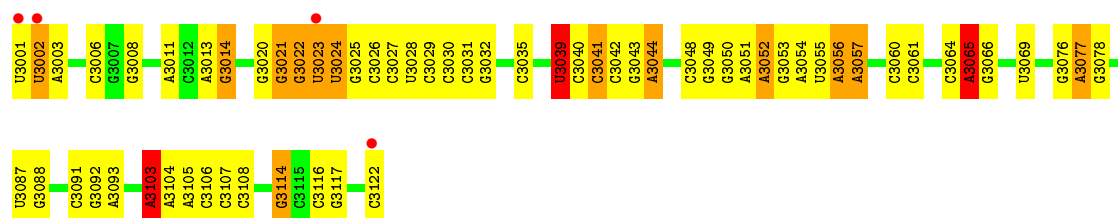
• Molecule 1: 23S rRNA



G2582	A2479	G2379	G2275	U2034	A1941	G1819	U1702	U1596	C1472	G1351	A1242	A1174
U2586	G2480	G2383	C2281	G2044	A1942	G1820	A1717	A1597	U1473	A1352	C1243	G1175
U2587	A2483	U2384	U2282	C	C1943	C	C	A1598	C1474	C1353	U1244	C1176
G2588	U2385	G2385	C	A2054	G1946	G1827	U1722	A1503	U1477	U1359	A1246	G1178
U2589	A2485	U2386	A2291	A2055	G1947	G1828	G1723	G1604	U1478	C1360	U1249	C1179
C2591	U2387	U2387	C	C2061	G1948	A1829	U1724	G1605	C	U1181	U1250	U1180
G2592	C2388	C2388	U	A2062	G1949	C1830	C1725	C1609	A1482	C1372	C1251	C1182
U2597	A2401	A2401	G	A2063	G1950	U1835	G1730	G1610	C1483	U1375	C1252	C1183
U2598	C2403	C2403	A	U2064	G1951	U1836	C1731	G1611	A1485	G1376	C1253	C1184
A2601	C2408	C2408	A	C	A	A1840	A1732	C1613	U1488	C1377	U1266	U1185
G2602	A2408	A	C	G2068	A	A1845	A1733	G1614	C	U1187	U1267	C1186
G2603	A2504	C	U	U2069	C	U1846	G1734	A1615	A1494	A1188	C1268	A1188
A2604	G2412	U	A	G2070	U	A1847	A1736	U1625	C	A1189	C1269	G1190
U2607	A2413	A	G	G2071	A	G1848	C	G1626	G1497	A1393	U1270	C1191
C2608	A2414	C	G	G2072	G	G1848	U1741	A1626	C1394	U1275	C1275	A1192
U2613	A2415	C	U	A2074	A	C1856	A1742	G1627	U1500	U1276	C1276	C1193
C2614	G2416	C	U	C	C	A1857	G1743	A1630	C	U1279	U1279	U1197
U2615	U2419	G	A	U2078	G	G1862	G1744	C1633	U1503	U1287	U1287	U1198
U2619	G2420	C	G	G2079	U1964	G1863	G1745	U1634	A1406	U1288	U1288	A1199
C2620	A2421	C	A	G2080	C	C1864	C	U1635	A1407	A1200	C1289	C1201
U2621	U2422	G	C	A2081	G1965	C1867	G1751	A1636	A1413	A1202	G1290	G1203
G2630	G2423	U	C	C2088	U1967	G1868	C1753	A1637	A1414	C1204	U1298	C1204
C2634	A2434	C	A	A2089	G	G1874	U1761	C1666	U1418	A1206	U1299	A1207
A2637	U2435	C	A	G2090	C	U1874	C1762	G1855	C1421	U1309	U1309	C1208
G2642	G2438	G	C	G2091	U1971	G1877	U1771	U1667	U1422	U1310	U1310	G1210
G2643	U2439	C	U	G2092	A1973	G1878	C1772	U1668	C1423	G1312	G1312	G1211
U2649	C2443	C	C	A2095	G1974	U1879	G1773	A1669	A1434	A1313	U1314	C1212
U2652	G2444	C	C	G2096	C1975	A1880	U1766	G1670	U1435	G1315	G1315	G1213
A2653	U2445	C	C	A2097	G1976	A1881	C	C1675	C1436	U1218	U1218	G1214
G2657	G2446	C	C	A2101	A1978	G1882	U1778	G1676	A1441	G1224	G1224	C1225
U2664	A2463	C	C	G2102	G1979	U1883	A1783	A1677	U	A1328	A1328	C1229
A	U2464	C	C	A2103	U1980	G1884	U1784	A1678	C1450	A1329	A1329	A1231
G2667	G2465	C	C	G2104	A1981	C	C1787	C1679	C1451	A1330	A1330	A1232
G2670	A2466	C	C	U2107	G1982	U1887	U1788	G1680	G1452	A1331	C1332	C1233
U2671	G2467	C	C	U2108	C1993	G1891	C1789	G1681	C1564	U1336	U1336	U1234
C2672	A2468	C	C	G2109	U1996	U1902	C1798	A1684	C1565	G1339	G1339	G1235
G2676	G2469	C	C	G2110	A1997	U1903	A1804	C1685	A1580	A1463	G1340	U1237
C2677	C2472	C	C	U2115	U2004	A1904	C1806	C1687	C	A1470	C1342	G1239
U2678	U2473	C	C	U2116	G2005	A1909	G1809	C1689	C1592	G1341	G1341	C1343
G2679	A2474	C	C	G2128	U2008	G1913	C1815	C1699	G1595	A1471	A1471	
A2680	C2475	C	C	G2136	G2009	A1919	C1920	C1700				
U2681	U2476	C	C	A	A2010	C1921	A1804	C1686				
C2682	G2477	C	C	C	U2012	A1921	C1806	C1687				
	C2478	C	C	G	G2013	A1922	G1806	C1687				
	U2478	C	C	U	G2014	A1922	G1806	C1687				
		C	C	G	A2015	G1926	G1809	C1687				
		C	C	U	U2016	A1927	C1815	C1687				
		C	C	C	G2033	C1940	C1815	C1687				



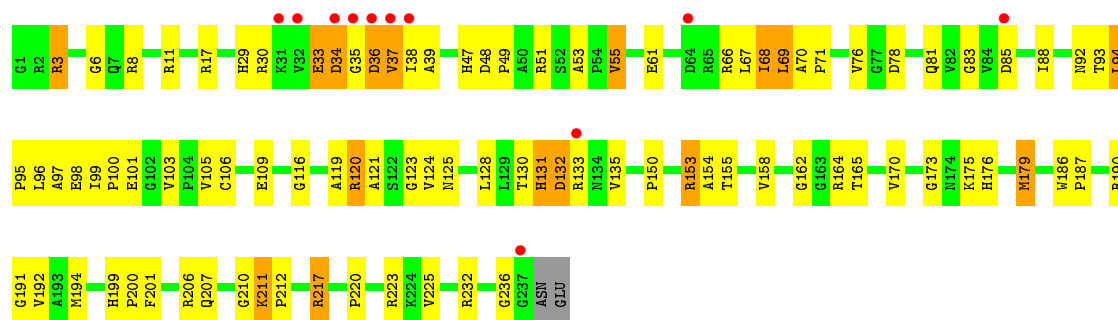
• Molecule 2: 5S rRNA



• Molecule 3: CCA

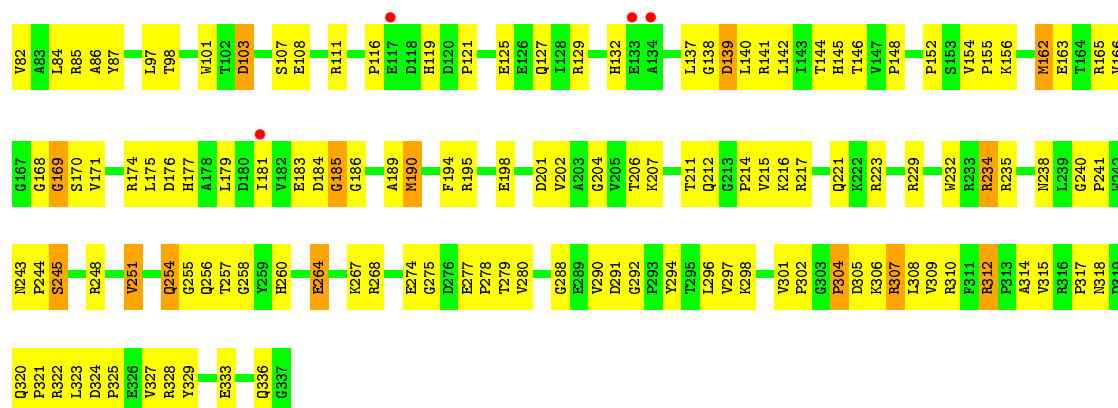


• Molecule 4: RIBOSOMAL PROTEIN L2



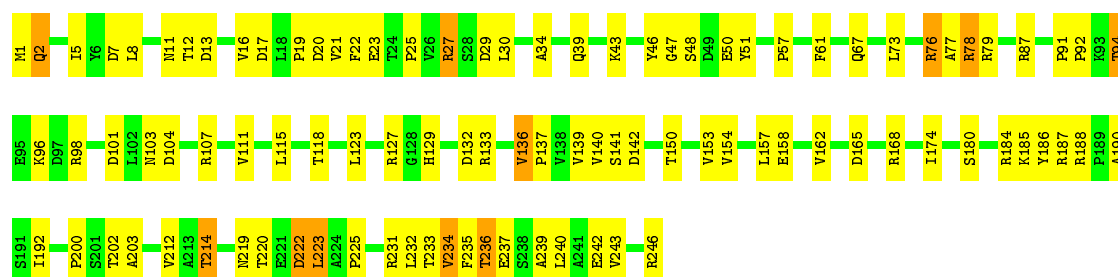
• Molecule 5: RIBOSOMAL PROTEIN L3





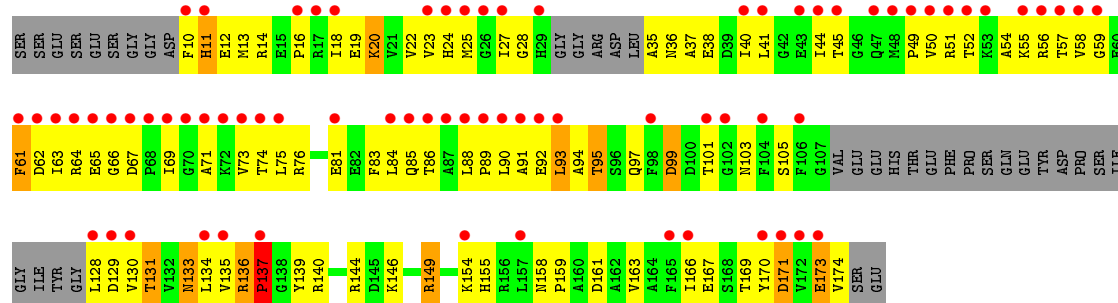
• Molecule 6: RIBOSOMAL PROTEIN L4

Chain E: 60% 35% .



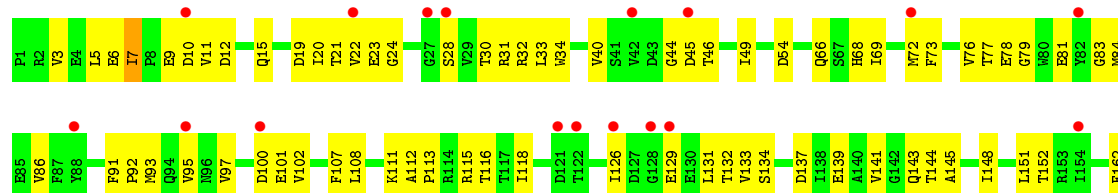
• Molecule 7: RIBOSOMAL PROTEIN L5

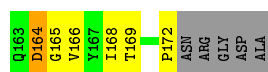
Chain F: 28% 41% 44% 7% 20% .



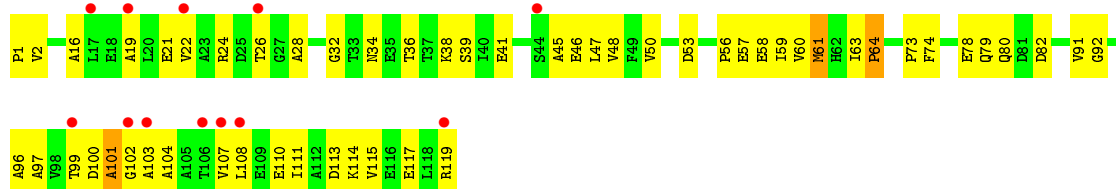
• Molecule 8: RIBOSOMAL PROTEIN L6

Chain G: 10% 53% 43% . .

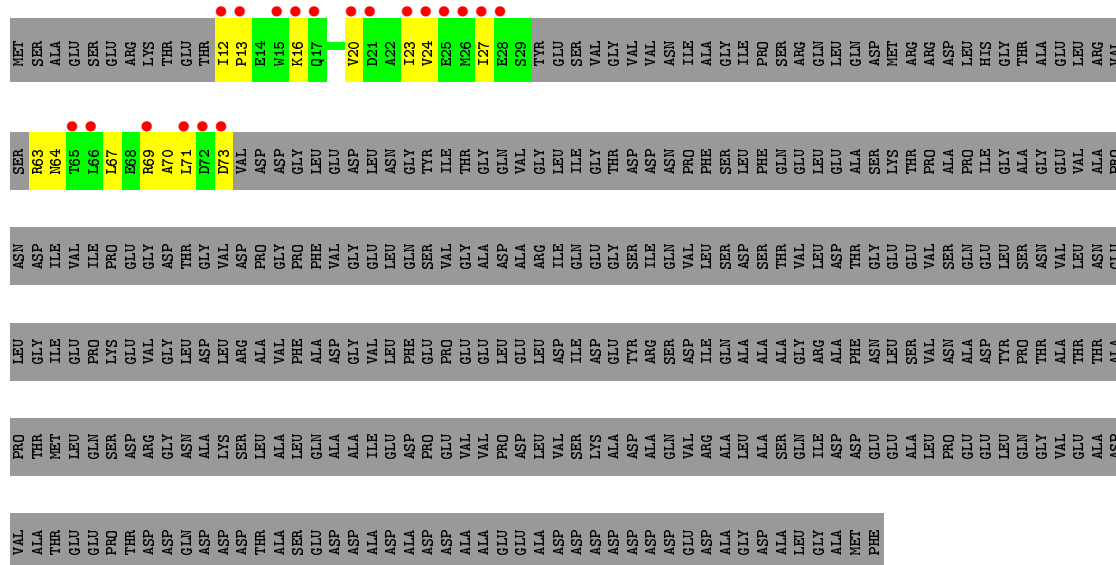




- Molecule 9: RIBOSOMAL PROTEIN L7AE



- Molecule 10: RIBOSOMAL PROTEIN L10

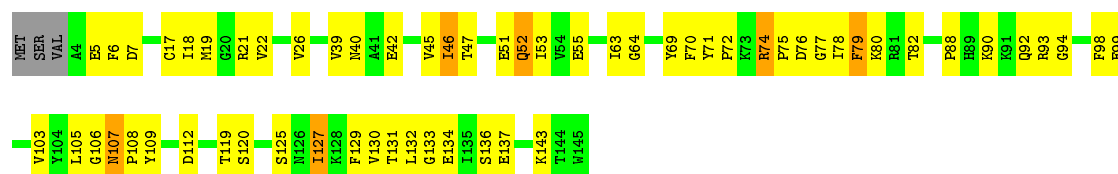


- Molecule 11: RIBOSOMAL PROTEIN L10E



- Molecule 12: RIBOSOMAL PROTEIN L13

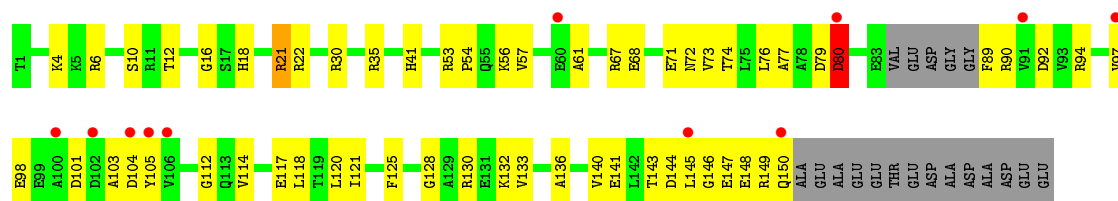




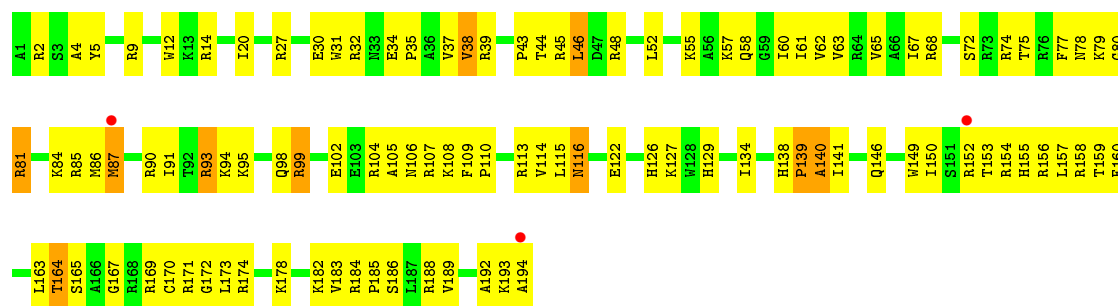
• Molecule 13: RIBOSOMAL PROTEIN L14



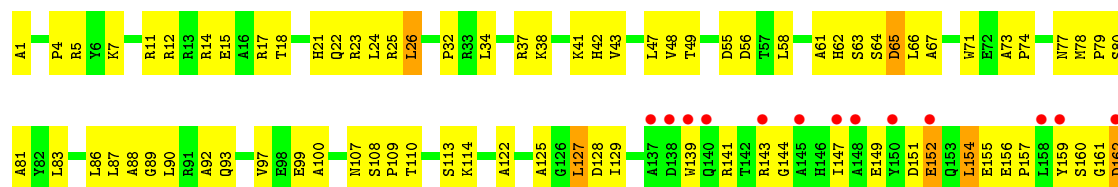
• Molecule 14: RIBOSOMAL PROTEIN L15

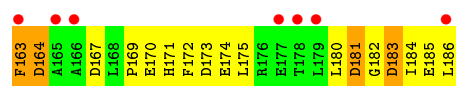


• Molecule 15: RIBOSOMAL PROTEIN L15E

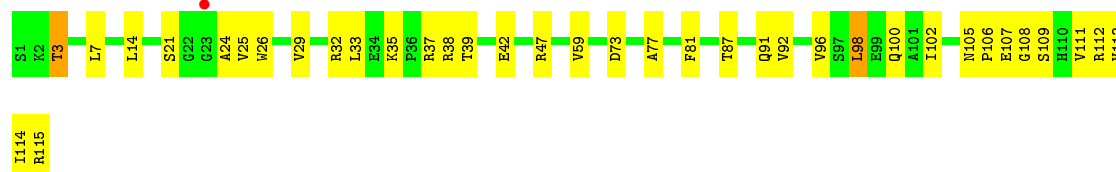


• Molecule 16: RIBOSOMAL PROTEIN L18

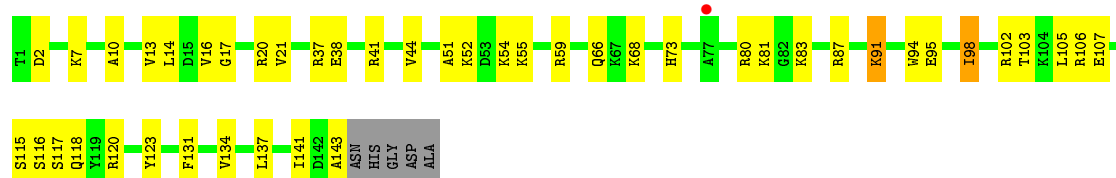




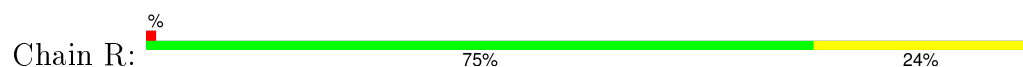
• Molecule 17: RIBOSOMAL PROTEIN L18E



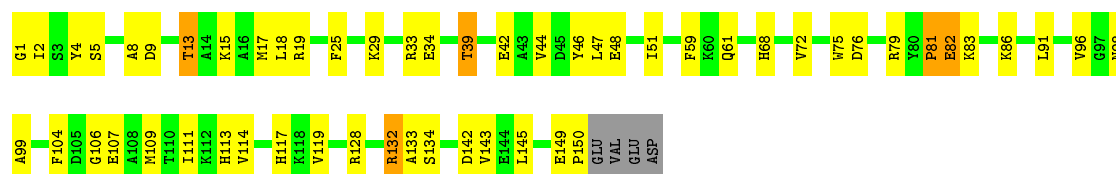
• Molecule 18: RIBOSOMAL PROTEIN L19E



• Molecule 19: RIBOSOMAL PROTEIN L21E



• Molecule 20: RIBOSOMAL PROTEIN L22



• Molecule 21: RIBOSOMAL PROTEIN L23

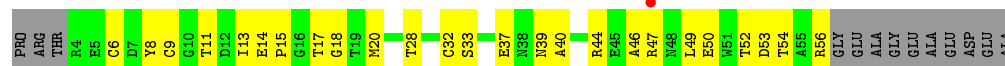
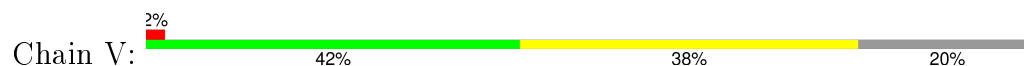


• Molecule 22: RIBOSOMAL PROTEIN L24

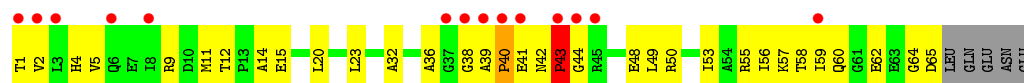




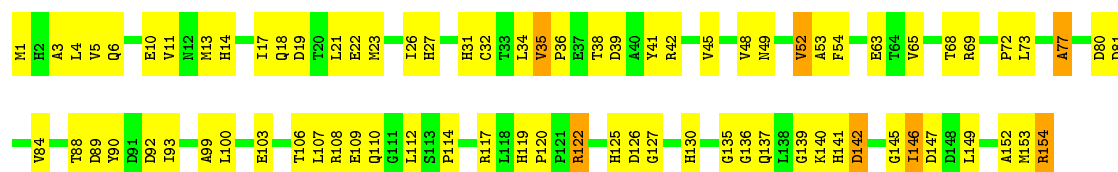
• Molecule 23: RIBOSOMAL PROTEIN L24E



• Molecule 24: RIBOSOMAL PROTEIN L29



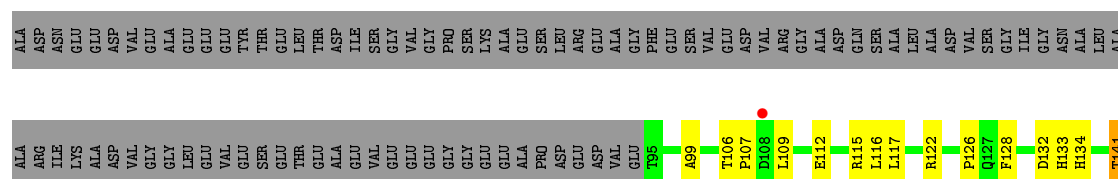
• Molecule 25: RIBOSOMAL PROTEIN L30

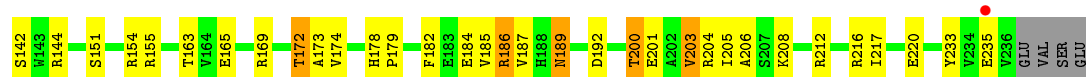


• Molecule 26: RIBOSOMAL PROTEIN L31E

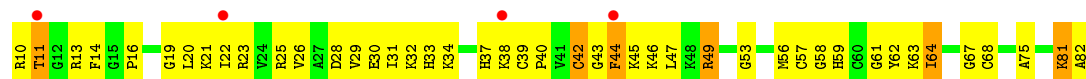


• Molecule 27: RIBOSOMAL PROTEIN L32E





• Molecule 28: RIBOSOMAL PROTEIN L37Ae



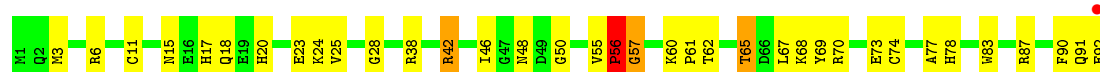
• Molecule 29: RIBOSOMAL PROTEIN L37E



• Molecule 30: RIBOSOMAL PROTEIN L39E



• Molecule 31: RIBOSOMAL PROTEIN L44E



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.66Å 299.77Å 573.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 49.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.3 (20.00-2.80) 94.4 (49.96-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.181 , 0.222 0.181 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 442473 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	98611	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.42	1/66076 (0.0%)	0.70	27/103052 (0.0%)
2	B	0.50	0/2905	0.79	4/4528 (0.1%)
3	5	0.74	0/65	1.17	1/99 (1.0%)
4	C	0.34	0/1787	0.66	0/2409
5	D	0.34	0/2689	0.65	0/3652
6	E	0.40	0/1883	0.66	0/2551
7	F	0.33	0/1111	0.60	0/1498
8	G	0.34	0/1382	0.59	0/1880
9	H	0.33	0/896	0.58	0/1219
10	I	0.27	0/241	0.47	0/324
11	J	0.39	0/1246	0.75	2/1686 (0.1%)
12	K	0.37	0/1135	0.61	0/1530
13	L	0.35	0/1003	0.67	0/1351
14	M	0.34	0/1126	0.67	0/1504
15	N	0.41	0/1633	0.70	1/2180 (0.0%)
16	O	0.31	0/1473	0.64	0/1999
17	P	0.38	0/873	0.63	0/1181
18	Q	0.37	0/1143	0.56	0/1521
19	R	0.38	0/748	0.67	0/1005
20	S	0.38	0/1172	0.67	0/1578
21	T	0.34	0/648	0.60	0/875
22	U	0.32	0/957	0.63	0/1289
23	V	0.35	0/417	0.57	0/562
24	W	0.32	0/502	0.56	0/675
25	X	0.36	0/1218	0.64	0/1655
26	Y	0.36	0/664	0.61	0/895
27	Z	0.39	0/1146	0.67	0/1536
28	1	0.39	0/575	0.71	0/763
29	2	0.44	0/437	0.67	0/578
30	3	0.34	0/398	0.56	0/527
31	4	0.40	0/771	0.62	0/1024
All	All	0.41	1/98320 (0.0%)	0.69	35/147126 (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	A	1	58
2	B	0	3
All	All	1	61

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2474	A	C5-C6	-5.43	1.36	1.41

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP1-P-O3'	-17.46	66.80	105.20
1	A	1164	U	OP2-P-O3'	-16.54	68.82	105.20
1	A	1563	G	C2'-C3'-O3'	9.62	130.67	109.50
1	A	1979	G	C2'-C3'-O3'	7.74	126.52	109.50
1	A	1942	A	C5'-C4'-C3'	7.39	127.82	116.00
2	B	3039	U	N1-C1'-C2'	7.36	123.57	114.00
3	5	9076	A	C2'-C3'-O3'	7.35	125.67	109.50
1	A	871	G	C5'-C4'-O4'	-7.05	100.64	109.10
1	A	2313	C	C5'-C4'-O4'	6.71	117.15	109.10
1	A	1504	A	C1'-O4'-C4'	-6.30	104.86	109.90
11	J	74	ASN	N-CA-C	-6.27	94.08	111.00
1	A	1819	G	C5'-C4'-C3'	6.09	125.75	116.00
1	A	1165	G	OP1-P-OP2	5.94	128.51	119.60
2	B	3103	A	C5'-C4'-O4'	5.90	116.17	109.10
1	A	1592	G	N9-C1'-C2'	5.88	121.64	114.00
1	A	2467	A	C1'-O4'-C4'	-5.68	105.36	109.90
1	A	1559	A	C2'-C3'-O3'	5.66	122.75	113.70
1	A	1504	A	N9-C1'-C2'	5.64	121.34	114.00
1	A	206	G	C5'-C4'-C3'	-5.54	107.13	116.00
1	A	1942	A	C5'-C4'-O4'	5.51	115.71	109.10
1	A	2316	G	C5'-C4'-C3'	-5.45	107.28	116.00
1	A	1942	A	C1'-O4'-C4'	-5.41	105.57	109.90
1	A	1120	U	C5'-C4'-C3'	-5.40	107.36	116.00
1	A	2726	U	N1-C1'-C2'	5.39	121.01	114.00
1	A	1942	A	C4'-C3'-C2'	-5.27	97.33	102.60
1	A	129	A	C2'-C3'-O3'	5.25	122.11	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3021	G	C5'-C4'-O4'	5.25	115.40	109.10
1	A	2291	A	N9-C1'-C2'	5.23	120.80	114.00
1	A	2475	C	O5'-P-OP1	5.17	116.91	110.70
1	A	2313	C	C5'-C4'-C3'	5.16	124.26	116.00
1	A	535	G	N9-C1'-C2'	5.15	120.70	114.00
2	B	3103	A	C4'-C3'-C2'	-5.07	97.53	102.60
15	N	139	PRO	N-CA-C	-5.07	98.92	112.10
11	J	110	GLY	N-CA-C	-5.03	100.53	113.10
1	A	603	A	N9-C1'-C2'	5.01	120.52	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'

All (61) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1078	A	Sidechain
1	A	1340	G	Sidechain
1	A	1342	C	Sidechain
1	A	1351	G	Sidechain
1	A	1359	U	Sidechain
1	A	1417	G	Sidechain
1	A	1430	G	Sidechain
1	A	1458	A	Sidechain
1	A	1682	A	Sidechain
1	A	1809	G	Sidechain
1	A	1819	G	Sidechain
1	A	1829	A	Sidechain
1	A	1848	G	Sidechain
1	A	1863	G	Sidechain
1	A	1867	G	Sidechain
1	A	1877	G	Sidechain
1	A	1878	G	Sidechain
1	A	1970	G	Sidechain
1	A	1972	U	Sidechain
1	A	1978	A	Sidechain
1	A	1979	G	Sidechain
1	A	1993	C	Sidechain
1	A	221	G	Sidechain
1	A	2316	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	246	G	Sidechain
1	A	2465	A	Sidechain
1	A	2493	C	Sidechain
1	A	2503	A	Sidechain
1	A	2506	A	Sidechain
1	A	2526	C	Sidechain
1	A	2541	U	Sidechain
1	A	2543	G	Sidechain
1	A	2551	C	Sidechain
1	A	2552	C	Sidechain
1	A	2557	U	Sidechain
1	A	2564	G	Sidechain
1	A	2582	G	Sidechain
1	A	2607	U	Sidechain
1	A	2615	U	Sidechain
1	A	2620	U	Sidechain
1	A	2630	G	Sidechain
1	A	2637	A	Sidechain
1	A	270	U	Sidechain
1	A	2793	A	Sidechain
1	A	2842	G	Sidechain
1	A	332	G	Sidechain
1	A	333	G	Sidechain
1	A	396	U	Sidechain
1	A	445	U	Sidechain
1	A	458	G	Sidechain
1	A	460	A	Sidechain
1	A	469	G	Sidechain
1	A	470	U	Sidechain
1	A	471	G	Sidechain
1	A	482	G	Sidechain
1	A	518	G	Sidechain
1	A	722	G	Sidechain
1	A	817	G	Sidechain
2	B	3039	U	Sidechain
2	B	3065	A	Sidechain
2	B	3087	U	Sidechain

5.2 Too-close contacts

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

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	59017	0	29805	894	0
2	B	2600	0	1326	73	0
3	5	59	0	34	2	0
4	C	1754	0	1763	129	0
5	D	2624	0	2533	176	0
6	E	1858	0	1816	114	0
7	F	1094	0	1085	127	0
8	G	1357	0	1266	77	0
9	H	885	0	854	62	0
10	I	240	0	231	21	0
11	J	1215	0	1215	152	0
12	K	1119	0	1098	67	0
13	L	993	0	1027	55	0
14	M	1114	0	1072	61	0
15	N	1605	0	1676	159	0
16	O	1444	0	1401	128	0
17	P	864	0	873	41	0
18	Q	1133	0	1127	49	0
19	R	734	0	728	21	0
20	S	1149	0	1122	65	0
21	T	641	0	605	19	0
22	U	949	0	923	48	0
23	V	410	0	364	32	0
24	W	499	0	511	34	0
25	X	1195	0	1137	101	0
26	Y	654	0	653	47	0
27	Z	1130	0	1133	61	0
28	1	563	0	597	59	0
29	2	430	0	426	24	0
30	3	393	0	406	28	0
31	4	755	0	728	36	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	5	1	0	0	0	0
32	A	111	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	73	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	B	2	0	0	0	0
33	C	1	0	0	0	0
33	E	1	0	0	0	0
33	J	1	0	0	0	0
33	K	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0
33	R	1	0	0	0	0
33	S	2	0	0	0	0
33	T	1	0	0	0	0
33	U	1	0	0	0	0
34	A	2	0	0	0	0
35	4	1	0	0	0	0
35	A	10	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	K	3	0	0	1	0
35	M	1	0	0	0	0
35	N	1	0	0	1	0
35	O	1	0	0	0	0
35	P	1	0	0	0	0
35	S	1	0	0	0	0
35	Z	1	0	0	0	0
36	5	23	0	19	4	0
37	5	11	0	8	0	0
38	5	8	0	12	0	0
39	1	1	0	0	0	0
39	2	1	0	0	0	0
39	4	1	0	0	0	0
39	P	1	0	0	0	0
39	V	1	0	0	0	0
40	1	36	0	0	8	0
40	2	55	0	0	3	0
40	3	40	0	0	4	0
40	4	73	0	0	10	0
40	5	1	0	0	0	0
40	A	5920	0	0	193	0
40	B	136	0	0	11	0
40	C	119	0	0	23	0
40	D	142	0	0	30	0
40	E	172	0	0	27	0
40	F	51	0	0	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	G	44	0	0	8	0
40	H	28	0	0	8	0
40	I	21	0	0	6	0
40	J	75	0	0	23	0
40	K	56	0	0	5	0
40	L	61	0	0	16	0
40	M	86	0	0	19	0
40	N	125	0	0	21	0
40	O	69	0	0	17	0
40	P	43	0	0	7	0
40	Q	67	0	0	1	0
40	R	49	0	0	3	0
40	S	83	0	0	11	0
40	T	35	0	0	5	0
40	U	37	0	0	4	0
40	V	24	0	0	5	0
40	W	16	0	0	2	0
40	X	71	0	0	12	0
40	Y	31	0	0	5	0
40	Z	92	0	0	14	0
All	All	98611	0	59574	2699	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 18.

All (2699) 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)
6:E:236:THR:HG22	6:E:239:ALA:H	1.04	1.16
1:A:1160:G:H5'	1:A:1161:A:H5'	1.22	1.15
11:J:86:ARG:NH1	11:J:133:ILE:HG13	1.63	1.13
11:J:45:GLN:HB3	11:J:163:PRO:HD2	1.30	1.12
24:W:12:THR:HG22	24:W:15:GLU:HG3	1.31	1.12
11:J:162:SER:HB2	11:J:163:PRO:HD3	1.31	1.10
1:A:1134:G:H4'	11:J:151:MET:HE1	1.33	1.09
1:A:156:C:H5''	15:N:171:ARG:HD3	1.36	1.08
1:A:1242:A:H5'	12:K:82:THR:HG23	1.39	1.04
26:Y:37:LEU:HD13	26:Y:85:VAL:HG21	1.35	1.03
7:F:134:LEU:HD11	7:F:166:ILE:HD11	1.38	1.02
2:B:3006:C:H5''	16:O:37:ARG:NH1	1.75	1.01
22:U:71:VAL:HG11	22:U:90:PRO:HB3	1.40	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:960:G:H4'	40:A:6940:HOH:O	1.60	0.99
13:L:10:GLN:NE2	13:L:10:GLN:H	1.60	0.99
11:J:86:ARG:HH11	11:J:133:ILE:HG13	0.83	0.99
11:J:29:ALA:HB3	11:J:65:ARG:HH12	1.26	0.98
11:J:26:LYS:HD2	11:J:28:ILE:HD12	1.44	0.98
1:A:542:A:H8	1:A:542:A:H5'	1.29	0.98
1:A:870:G:H2'	1:A:871:G:H5''	1.44	0.97
1:A:1751:G:H2'	1:A:1752:G:H5''	1.45	0.97
13:L:81:ARG:HB2	13:L:87:ARG:HH11	1.28	0.97
11:J:86:ARG:HH11	11:J:133:ILE:CG1	1.78	0.97
40:A:3981:HOH:O	15:N:146:GLN:HG2	1.61	0.97
5:D:140:LEU:HA	40:D:8574:HOH:O	1.63	0.97
20:S:99:ALA:HB1	20:S:109:MET:HE1	1.46	0.97
15:N:52:LEU:HD11	40:N:8617:HOH:O	1.64	0.96
16:O:83:LEU:HD13	16:O:175:LEU:HD23	1.45	0.95
13:L:29:LEU:HB3	13:L:55:VAL:HG11	1.47	0.95
2:B:3056:A:H2'	2:B:3057:A:H5''	1.48	0.95
6:E:5:ILE:HD11	6:E:16:VAL:HG23	1.48	0.95
28:1:10:ARG:HA	40:1:8415:HOH:O	1.67	0.95
2:B:3076:G:H3'	2:B:3077:A:H5''	1.47	0.94
15:N:164:THR:HG22	15:N:167:GLY:H	1.29	0.94
5:D:264:GLU:HG2	5:D:267:LYS:HE2	1.50	0.94
12:K:76:ASP:HA	40:K:5907:HOH:O	1.69	0.93
16:O:144:GLY:O	16:O:147:ILE:HG22	1.67	0.93
6:E:132:ASP:HB3	40:E:8363:HOH:O	1.66	0.93
6:E:115:LEU:HD13	6:E:223:LEU:HD21	1.49	0.93
1:A:856:G:H2'	40:A:4944:HOH:O	1.69	0.93
6:E:115:LEU:HD21	6:E:243:VAL:HG13	1.51	0.93
16:O:47:LEU:HD11	16:O:127:LEU:HD21	1.51	0.93
25:X:88:THR:HB	40:X:6679:HOH:O	1.69	0.93
4:C:211:LYS:HB3	4:C:212:PRO:HD2	1.51	0.91
18:Q:115:SER:H	18:Q:118:GLN:HE21	1.08	0.91
11:J:162:SER:HB2	11:J:163:PRO:CD	2.00	0.91
6:E:236:THR:HG22	6:E:239:ALA:N	1.84	0.91
1:A:1165:G:H4'	1:A:1174:A:O2'	1.71	0.91
1:A:1474:C:H5'	1:A:1474:C:H6	1.35	0.90
1:A:541:C:H2'	1:A:542:A:H5''	1.53	0.90
15:N:106:ASN:ND2	35:N:8518:CL:CL	2.41	0.90
7:F:25:MET:HE2	7:F:41:LEU:HG	1.53	0.90
13:L:10:GLN:HE21	13:L:10:GLN:N	1.68	0.90
25:X:6:GLN:HB2	25:X:26:ILE:HD12	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:137:GLN:HE21	25:X:141:HIS:HE1	1.15	0.90
1:A:871:G:C8	1:A:871:G:H5'	2.06	0.90
27:Z:200:THR:HG22	27:Z:201:GLU:HG3	1.54	0.90
11:J:55:GLN:HE21	11:J:124:ARG:HE	1.19	0.90
5:D:62:ARG:HA	5:D:65:MET:HE3	1.54	0.89
1:A:1667:A:H8	1:A:1667:A:H5'	1.36	0.89
25:X:88:THR:HG23	25:X:110:GLN:HE21	1.37	0.89
5:D:86:ALA:HA	40:D:8574:HOH:O	1.71	0.88
28:1:58:GLY:HA3	40:1:8437:HOH:O	1.72	0.88
25:X:88:THR:HG22	25:X:89:ASP:H	1.37	0.88
28:1:38:LYS:HE2	28:1:45:LYS:HE2	1.53	0.88
1:A:21:G:H5'	20:S:2:ILE:HA	1.56	0.88
7:F:64:ARG:HG2	7:F:67:ASP:HB3	1.56	0.88
1:A:2812:A:H2	1:A:2814:A:H62	1.21	0.87
25:X:21:LEU:HD13	25:X:26:ILE:HD11	1.54	0.87
1:A:1835:U:H5	1:A:1840:A:N7	1.72	0.87
1:A:2717:C:C2'	1:A:2718:C:H5''	2.05	0.87
8:G:20:ILE:HD11	8:G:40:VAL:HG11	1.57	0.87
6:E:2:GLN:HB3	40:E:8336:HOH:O	1.75	0.87
40:A:3296:HOH:O	15:N:189:VAL:HG21	1.73	0.86
28:1:38:LYS:HG2	28:1:45:LYS:HG2	1.55	0.86
15:N:106:ASN:HD22	15:N:114:VAL:HG23	1.39	0.86
1:A:2586:U:H3	1:A:2592:G:H22	1.23	0.86
1:A:871:G:H8	1:A:871:G:H5'	1.39	0.86
25:X:68:THR:HG23	25:X:69:ARG:HG2	1.57	0.86
18:Q:115:SER:OG	18:Q:118:GLN:HG3	1.75	0.86
13:L:10:GLN:HE21	13:L:10:GLN:H	0.90	0.86
16:O:87:LEU:HD12	16:O:186:LEU:HD21	1.55	0.86
40:A:5806:HOH:O	7:F:99:ASP:HA	1.75	0.86
7:F:105:SER:HB2	7:F:131:THR:HG23	1.56	0.85
16:O:113:SER:HB2	40:O:8561:HOH:O	1.75	0.85
20:S:8:ALA:HB1	20:S:13:THR:HG21	1.59	0.85
2:B:3006:C:H5''	16:O:37:ARG:HH12	1.41	0.85
21:T:43:GLU:HB3	40:T:8344:HOH:O	1.75	0.85
5:D:212:GLN:HB2	5:D:257:THR:HG21	1.58	0.85
15:N:102:GLU:OE1	15:N:164:THR:HG21	1.77	0.85
1:A:1166:A:H1'	1:A:1192:A:C2	2.12	0.85
13:L:81:ARG:HB2	13:L:87:ARG:NH1	1.92	0.84
20:S:18:LEU:HD12	20:S:143:VAL:HG11	1.58	0.84
7:F:154:LYS:H	7:F:154:LYS:HD2	1.41	0.84
15:N:35:PRO:HG2	15:N:38:VAL:HG23	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:4:62:THR:HB	40:4:8550:HOH:O	1.76	0.84
6:E:1:MET:HG2	6:E:2:GLN:H	1.41	0.84
5:D:321:PRO:HA	40:D:8652:HOH:O	1.78	0.84
1:A:2506:A:HO2'	1:A:2507:G:H8	0.87	0.84
1:A:645:U:OP2	14:M:4:LYS:HE2	1.77	0.84
14:M:133:VAL:HA	40:M:8574:HOH:O	1.76	0.84
14:M:79:ASP:HB3	40:M:8559:HOH:O	1.78	0.83
1:A:962:C:H1'	16:O:5:ARG:NH1	1.93	0.83
1:A:1625:U:H4'	40:A:4182:HOH:O	1.76	0.83
1:A:381:G:H5''	40:A:3830:HOH:O	1.77	0.83
1:A:1116:U:H3	1:A:1246:A:H62	1.26	0.83
1:A:1184:C:H1'	40:A:6979:HOH:O	1.77	0.83
21:T:57:THR:HG22	21:T:59:ASP:H	1.43	0.83
11:J:139:ASP:N	11:J:140:PRO:HD3	1.94	0.83
7:F:25:MET:HE1	7:F:37:ALA:HB1	1.59	0.83
1:A:1701:A:H5'	40:A:5794:HOH:O	1.80	0.82
5:D:238:ASN:HD22	5:D:240:GLY:H	1.23	0.82
14:M:68:GLU:HA	40:M:8542:HOH:O	1.79	0.82
1:A:2717:C:H2'	1:A:2718:C:H5''	1.60	0.82
1:A:1116:U:O2'	1:A:1118:A:H2	1.62	0.82
8:G:81:GLU:HG2	8:G:134:SER:HB3	1.61	0.82
11:J:27:LYS:H	11:J:58:HIS:HD2	1.27	0.82
7:F:146:LYS:NZ	16:O:107:ASN:HD21	1.77	0.82
6:E:242:GLU:HG3	40:E:8380:HOH:O	1.79	0.82
1:A:2780:C:H1'	8:G:143:GLN:HE21	1.44	0.81
31:4:25:VAL:HG22	31:4:68:LYS:HG3	1.60	0.81
1:A:1116:U:HO2'	1:A:1118:A:H2	0.81	0.81
1:A:2526:C:O2'	1:A:2527:U:H5'	1.80	0.81
13:L:39:GLY:HA2	40:L:4183:HOH:O	1.80	0.81
1:A:711:G:H1'	40:A:6602:HOH:O	1.80	0.81
1:A:2506:A:O2'	1:A:2507:G:H8	1.63	0.81
16:O:49:THR:HG22	16:O:56:ASP:HB2	1.63	0.81
11:J:59:ASN:H	11:J:59:ASN:HD22	1.27	0.81
11:J:4:ALA:HB3	40:J:8367:HOH:O	1.80	0.81
6:E:127:ARG:NH2	6:E:225:PRO:HG2	1.96	0.81
25:X:65:VAL:HA	25:X:68:THR:HG22	1.62	0.81
8:G:15:GLN:HG3	8:G:20:ILE:HG12	1.62	0.80
31:4:70:ARG:HG2	31:4:77:ALA:HB2	1.63	0.80
7:F:27:ILE:HG22	7:F:28:GLY:H	1.46	0.80
25:X:88:THR:HG23	25:X:110:GLN:NE2	1.96	0.80
1:A:506:G:H22	1:A:509:A:C5'	1.95	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:1:THR:HG23	24:W:2:VAL:H	1.46	0.80
13:L:62:PRO:HG3	13:L:65:ARG:HH21	1.47	0.80
6:E:236:THR:HG21	40:E:8372:HOH:O	1.82	0.80
4:C:88:ILE:HD13	4:C:100:PRO:HD3	1.64	0.80
6:E:78:ARG:HG3	6:E:78:ARG:HH11	1.47	0.80
11:J:165:GLY:HA3	40:J:8396:HOH:O	1.80	0.80
7:F:20:LYS:HA	7:F:75:LEU:O	1.82	0.80
4:C:100:PRO:HG2	4:C:103:VAL:HG21	1.63	0.80
2:B:3023:U:H5''	2:B:3024:U:OP2	1.81	0.80
40:A:6283:HOH:O	16:O:4:PRO:HD2	1.82	0.80
1:A:541:C:C2'	1:A:542:A:H5''	2.10	0.80
1:A:544:G:H2'	1:A:545:G:H5''	1.63	0.80
30:3:39:ARG:HG2	40:3:3143:HOH:O	1.81	0.79
1:A:545:G:H8	1:A:545:G:H5'	1.47	0.79
25:X:4:LEU:HD22	25:X:52:VAL:HG21	1.62	0.79
1:A:1701:A:H4'	1:A:1702:U:H5''	1.62	0.79
1:A:272:A:H3'	40:A:7046:HOH:O	1.81	0.79
17:P:96:VAL:HA	40:P:4258:HOH:O	1.81	0.79
1:A:870:G:C2'	1:A:871:G:H5''	2.12	0.79
1:A:2004:U:H4'	40:A:4823:HOH:O	1.80	0.79
1:A:2890:A:H1'	23:V:56:ARG:NH2	1.98	0.79
11:J:49:VAL:O	11:J:157:ILE:HG23	1.82	0.79
1:A:288:A:H61	1:A:364:C:H42	1.31	0.79
1:A:536:A:H3'	40:A:4563:HOH:O	1.82	0.79
4:C:35:GLY:O	4:C:36:ASP:HB3	1.82	0.79
25:X:72:PRO:HG2	25:X:77:ALA:HB3	1.65	0.79
11:J:150:LYS:HE2	40:J:8383:HOH:O	1.82	0.78
31:4:70:ARG:HD3	40:4:8539:HOH:O	1.83	0.78
8:G:97:VAL:HG12	40:G:4191:HOH:O	1.82	0.78
1:A:2716:G:H5''	5:D:206:THR:HG21	1.66	0.78
11:J:14:TYR:H	11:J:91:HIS:CE1	2.01	0.78
1:A:657:G:OP1	6:E:27:ARG:NH2	2.17	0.78
28:1:46:LYS:HD3	28:1:59:HIS:HB2	1.64	0.78
24:W:12:THR:HG22	24:W:15:GLU:CG	2.12	0.78
1:A:2533:C:H6	1:A:2533:C:H5'	1.47	0.78
1:A:1160:G:C5'	1:A:1161:A:H5'	2.11	0.78
11:J:55:GLN:NE2	11:J:124:ARG:HE	1.80	0.78
27:Z:185:VAL:HG12	40:Z:8565:HOH:O	1.84	0.78
11:J:59:ASN:N	11:J:59:ASN:HD22	1.81	0.78
15:N:35:PRO:CG	15:N:38:VAL:HG23	2.14	0.77
4:C:192:VAL:HB	40:C:8592:HOH:O	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:A:4376:HOH:O	15:N:14:ARG:HG2	1.84	0.77
6:E:139:VAL:HG13	40:E:8450:HOH:O	1.83	0.77
11:J:2:PRO:HB2	40:J:8367:HOH:O	1.84	0.77
5:D:201:ASP:HB2	5:D:312:ARG:HD2	1.65	0.77
6:E:236:THR:CG2	6:E:239:ALA:H	1.93	0.77
9:H:58:GLU:HA	9:H:61:MET:HE2	1.65	0.77
40:A:4465:HOH:O	2:B:3103:A:H4'	1.84	0.77
6:E:5:ILE:HD11	6:E:16:VAL:CG2	2.14	0.77
1:A:1372:A:H3'	40:A:6696:HOH:O	1.83	0.77
1:A:21:G:C5'	20:S:2:ILE:HA	2.14	0.77
29:2:8:GLN:HE22	29:2:11:LYS:NZ	1.82	0.77
20:S:39:THR:HG22	20:S:42:GLU:H	1.49	0.77
1:A:1450:C:H4'	1:A:1451:C:OP2	1.85	0.77
1:A:289:G:H22	1:A:363:A:H2	1.32	0.77
5:D:7:ARG:HG2	5:D:7:ARG:HH11	1.50	0.77
15:N:138:HIS:ND1	15:N:139:PRO:O	2.18	0.77
24:W:42:ASN:HB3	40:W:7247:HOH:O	1.84	0.77
28:1:61:GLY:HA3	40:1:8426:HOH:O	1.83	0.77
28:1:40:PRO:HD3	28:1:47:LEU:HD11	1.65	0.76
13:L:74:VAL:HG11	13:L:113:ILE:HG12	1.66	0.76
5:D:41:PHE:HB3	5:D:190:MET:HE3	1.67	0.76
7:F:64:ARG:CG	7:F:67:ASP:HB3	2.15	0.76
20:S:18:LEU:HG	20:S:91:LEU:HD13	1.65	0.76
16:O:7:LYS:HE3	19:R:21:ARG:O	1.84	0.76
18:Q:115:SER:H	18:Q:118:GLN:NE2	1.83	0.76
15:N:139:PRO:O	15:N:140:ALA:HB3	1.86	0.76
6:E:236:THR:HA	40:E:8453:HOH:O	1.86	0.76
11:J:162:SER:CB	11:J:163:PRO:HD3	2.14	0.76
17:P:47:ARG:HG3	17:P:47:ARG:HH11	1.50	0.76
9:H:96:ALA:HA	40:H:3111:HOH:O	1.84	0.76
6:E:104:ASP:HA	6:E:107:ARG:HH12	1.50	0.76
22:U:9:LYS:HE3	22:U:13:ARG:NH1	2.01	0.76
14:M:67:ARG:O	14:M:71:GLU:HG3	1.85	0.76
15:N:87:MET:HG2	31:4:46:ILE:HG21	1.68	0.76
1:A:2768:A:H2'	1:A:2769:C:O4'	1.86	0.76
1:A:2054:A:N3	20:S:128:ARG:NH2	2.34	0.76
1:A:1164:U:C4'	1:A:1165:G:OP1	2.33	0.76
1:A:1164:U:H3	1:A:1192:A:H2	1.30	0.76
6:E:236:THR:H	6:E:239:ALA:HB3	1.51	0.76
1:A:31:C:H2'	40:A:7207:HOH:O	1.86	0.75
4:C:69:LEU:HD21	4:C:120:ARG:HB3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:41:THR:HA	40:J:8394:HOH:O	1.83	0.75
1:A:1751:G:C2'	1:A:1752:G:H5''	2.16	0.75
1:A:1634:G:H3'	40:A:3404:HOH:O	1.85	0.75
1:A:1244:U:OP1	12:K:18:ILE:HD13	1.87	0.75
20:S:111:ILE:HG23	20:S:145:LEU:HD11	1.68	0.75
14:M:148:GLU:HA	40:M:8573:HOH:O	1.85	0.75
40:A:4057:HOH:O	11:J:151:MET:HE2	1.87	0.75
2:B:3006:C:OP1	16:O:37:ARG:NH1	2.20	0.75
27:Z:187:VAL:HG23	27:Z:192:ASP:HB2	1.66	0.75
28:1:37:HIS:HB2	28:1:47:LEU:HB2	1.69	0.74
1:A:284:C:H4'	1:A:285:A:O5'	1.85	0.74
24:W:39:ALA:N	24:W:40:PRO:HD2	2.03	0.74
15:N:172:GLY:O	15:N:183:VAL:HG11	1.87	0.74
40:A:3236:HOH:O	15:N:157:LEU:HD11	1.88	0.74
1:A:346:U:H4'	40:A:6357:HOH:O	1.86	0.74
16:O:23:ARG:HD3	40:O:8548:HOH:O	1.86	0.74
1:A:1118:A:H3'	1:A:1118:A:H8	1.52	0.74
1:A:1118:A:C8	1:A:1118:A:H3'	2.22	0.74
8:G:23:GLU:HG2	8:G:28:SER:HB3	1.69	0.74
1:A:560:C:H42	1:A:597:A:H61	1.35	0.74
12:K:45:VAL:HG23	12:K:130:VAL:O	1.87	0.74
26:Y:78:GLU:HG2	26:Y:79:GLU:H	1.53	0.74
25:X:137:GLN:HE21	25:X:141:HIS:CE1	2.03	0.74
2:B:3056:A:C2'	2:B:3057:A:H5''	2.18	0.74
1:A:1603:A:H5'	1:A:1605:G:O4'	1.88	0.74
18:Q:59:ARG:NH2	18:Q:66:GLN:HE22	1.85	0.74
11:J:137:ASN:O	11:J:139:ASP:N	2.21	0.73
1:A:2291:A:C8	1:A:2309:C:H5'	2.23	0.73
25:X:122:ARG:HH21	25:X:154:ARG:HD2	1.52	0.73
40:A:5309:HOH:O	15:N:170:CYS:SG	2.45	0.73
1:A:1329:A:H2	40:A:4198:HOH:O	1.70	0.73
1:A:1191:A:H3'	1:A:1192:A:H5''	1.69	0.73
7:F:146:LYS:HZ1	16:O:107:ASN:HD21	1.36	0.73
1:A:877:G:H5'	1:A:878:G:OP1	1.89	0.73
1:A:2710:U:H1'	40:A:7141:HOH:O	1.88	0.73
12:K:107:ASN:ND2	12:K:109:TYR:H	1.86	0.73
2:B:3029:C:H2'	2:B:3030:C:H5'	1.70	0.73
25:X:88:THR:HG22	25:X:89:ASP:N	2.04	0.73
6:E:214:THR:HG21	40:E:8400:HOH:O	1.89	0.73
8:G:166:VAL:HG12	40:G:3134:HOH:O	1.89	0.73
9:H:63:ILE:HB	9:H:64:PRO:HD3	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:99:ALA:HB1	20:S:109:MET:CE	2.18	0.73
1:A:871:G:C5'	1:A:871:G:H8	2.02	0.72
22:U:47:THR:HB	22:U:100:ASP:HB3	1.71	0.72
1:A:1666:C:O2'	1:A:1667:A:H5''	1.89	0.72
1:A:542:A:C8	1:A:542:A:H5'	2.19	0.72
31:4:73:GLU:HB3	40:4:8561:HOH:O	1.90	0.72
16:O:164:ASP:CG	16:O:167:ASP:HA	2.10	0.72
1:A:282:C:H1'	1:A:368:C:N4	2.04	0.72
26:Y:71:ARG:HB3	26:Y:88:GLU:OE1	1.90	0.72
15:N:34:GLU:HB3	15:N:35:PRO:HD2	1.71	0.72
15:N:87:MET:HB3	31:4:46:ILE:HD13	1.69	0.72
16:O:48:VAL:CG1	16:O:55:ASP:HB3	2.20	0.72
4:C:105:VAL:HG11	4:C:154:ALA:HB1	1.72	0.72
28:1:49:ARG:HD2	40:1:8428:HOH:O	1.89	0.72
1:A:2270:G:H4'	4:C:223:ARG:HH12	1.55	0.72
10:I:12:ILE:N	10:I:13:PRO:HD3	2.03	0.72
7:F:88:LEU:HB2	7:F:89:PRO:HD3	1.72	0.72
40:A:3066:HOH:O	15:N:152:ARG:HG3	1.89	0.72
8:G:69:ILE:HA	8:G:72:MET:CE	2.20	0.72
1:A:2908:A:H2'	1:A:2909:G:O4'	1.90	0.72
7:F:54:ALA:HB2	7:F:69:ILE:HD12	1.71	0.72
1:A:214:U:H5'	40:A:5654:HOH:O	1.89	0.71
22:U:32:ARG:NH1	22:U:38:ARG:HH12	1.88	0.71
14:M:143:THR:HG22	14:M:144:ASP:N	2.05	0.71
16:O:80:SER:HB2	40:O:8536:HOH:O	1.89	0.71
11:J:140:PRO:HB3	40:J:8381:HOH:O	1.90	0.71
1:A:1119:G:H2'	12:K:52:GLN:NE2	2.06	0.71
4:C:96:LEU:HD22	4:C:128:LEU:HD13	1.73	0.71
11:J:84:ARG:NH2	11:J:135:TRP:HH2	1.89	0.71
16:O:164:ASP:OD2	16:O:167:ASP:HA	1.90	0.71
4:C:170:VAL:HG22	28:1:22:ILE:HG23	1.71	0.71
1:A:2094:G:H4'	5:D:245:SER:HB3	1.71	0.71
1:A:1160:G:H5'	1:A:1161:A:C5'	2.11	0.71
25:X:122:ARG:HG2	25:X:122:ARG:HH11	1.55	0.71
9:H:91:VAL:HG12	9:H:92:GLY:N	2.06	0.71
27:Z:189:ASN:HA	27:Z:217:ILE:HD11	1.73	0.70
9:H:50:VAL:HG13	9:H:60:VAL:HG11	1.72	0.70
1:A:1679:C:H5'	40:A:8834:HOH:O	1.90	0.70
22:U:61:GLU:HG3	40:U:3851:HOH:O	1.91	0.70
5:D:62:ARG:HA	5:D:65:MET:CE	2.21	0.70
22:U:41:ARG:HG2	22:U:41:ARG:HH11	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:106:GLY:HA2	20:S:109:MET:HE3	1.73	0.70
1:A:1667:A:H5'	1:A:1667:A:C8	2.24	0.70
27:Z:187:VAL:HG23	27:Z:192:ASP:CB	2.21	0.70
9:H:53:ASP:OD1	9:H:80:GLN:HB2	1.92	0.70
30:3:41:HIS:H	30:3:45:ASN:HD22	1.37	0.70
11:J:141:ASN:HA	40:J:8369:HOH:O	1.90	0.70
11:J:130:HIS:CD2	11:J:133:ILE:HD11	2.26	0.70
1:A:1165:G:OP1	1:A:1165:G:H3'	1.90	0.70
20:S:18:LEU:HD12	20:S:143:VAL:CG1	2.20	0.70
1:A:506:G:H22	1:A:509:A:H5'	1.57	0.70
5:D:36:PRO:HA	5:D:168:GLY:CA	2.21	0.70
1:A:2414:A:H2'	1:A:2415:A:C8	2.26	0.70
5:D:307:ARG:HH11	5:D:307:ARG:HB2	1.55	0.70
1:A:1187:U:HO2'	1:A:1189:A:H2	1.39	0.70
20:S:18:LEU:HB2	20:S:143:VAL:HG12	1.72	0.70
25:X:149:LEU:HG	25:X:153:MET:HE2	1.72	0.70
1:A:1505:U:H6	1:A:1505:U:H5'	1.56	0.70
23:V:9:CYS:HA	23:V:52:THR:HG23	1.72	0.70
1:A:2426:G:H1'	40:A:5606:HOH:O	1.90	0.70
15:N:52:LEU:HD13	15:N:116:ASN:HB3	1.74	0.70
11:J:142:VAL:HG13	40:J:8381:HOH:O	1.91	0.70
13:L:74:VAL:CG1	13:L:113:ILE:HG12	2.22	0.70
40:A:6934:HOH:O	22:U:9:LYS:HB2	1.90	0.70
6:E:200:PRO:HB3	6:E:212:VAL:HG23	1.74	0.69
1:A:470:U:O2'	29:2:16:HIS:HD2	1.74	0.69
12:K:103:VAL:HG12	40:K:5907:HOH:O	1.91	0.69
1:A:1206:U:H5'	1:A:1206:U:H6	1.55	0.69
40:A:7100:HOH:O	28:1:31:ILE:HG13	1.92	0.69
5:D:162:MET:HE3	5:D:308:LEU:HD21	1.74	0.69
22:U:9:LYS:HE3	22:U:13:ARG:HH11	1.58	0.69
1:A:281:U:H2'	1:A:282:C:O4'	1.92	0.69
1:A:559:U:H6	1:A:559:U:H5'	1.57	0.69
5:D:329:TYR:CE2	23:V:15:PRO:HG2	2.27	0.69
1:A:182:G:H5'	40:A:4672:HOH:O	1.92	0.69
11:J:53:PRO:HG3	11:J:127:GLY:H	1.57	0.69
5:D:254:GLN:HG2	5:D:255:GLY:N	2.07	0.69
11:J:5:MET:HG3	40:J:8367:HOH:O	1.92	0.69
4:C:55:VAL:HG22	4:C:68:ILE:O	1.92	0.69
1:A:1119:G:H22	1:A:1246:A:H2	1.41	0.69
1:A:2896:A:H5''	40:A:5613:HOH:O	1.91	0.69
10:I:23:ILE:HD13	10:I:67:LEU:HD23	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:21:LEU:HD22	25:X:26:ILE:CD1	2.23	0.69
28:1:39:CYS:HA	28:1:47:LEU:HD11	1.75	0.69
9:H:91:VAL:HG12	9:H:92:GLY:H	1.58	0.69
13:L:14:LYS:HB2	13:L:45:PRO:HG2	1.74	0.69
11:J:33:MET:HB2	11:J:83:PHE:HB3	1.75	0.69
11:J:26:LYS:HG2	11:J:28:ILE:H	1.58	0.69
15:N:139:PRO:O	15:N:140:ALA:CB	2.39	0.69
40:A:4349:HOH:O	12:K:47:THR:HB	1.92	0.69
1:A:111:C:O2'	29:2:20:ARG:HG2	1.93	0.69
6:E:180:SER:HB2	40:E:8447:HOH:O	1.93	0.68
14:M:133:VAL:HB	40:M:8558:HOH:O	1.92	0.68
28:1:38:LYS:HE2	28:1:45:LYS:CE	2.22	0.68
27:Z:133:HIS:HD2	40:Z:8577:HOH:O	1.76	0.68
1:A:2346:C:O2'	7:F:52:THR:HG21	1.94	0.68
13:L:22:ASP:HB2	40:L:5264:HOH:O	1.92	0.68
12:K:74:ARG:HH11	12:K:74:ARG:HB3	1.56	0.68
5:D:238:ASN:HD22	5:D:240:GLY:N	1.91	0.68
15:N:87:MET:HB3	31:4:46:ILE:HG21	1.73	0.68
5:D:179:LEU:O	5:D:183:GLU:HG2	1.94	0.68
13:L:81:ARG:HD3	13:L:87:ARG:NH1	2.08	0.68
13:L:32:ILE:HD11	13:L:56:SER:HB3	1.76	0.68
15:N:164:THR:HG23	15:N:165:SER:N	2.08	0.68
20:S:39:THR:HG23	20:S:107:GLU:O	1.94	0.68
1:A:1209:C:H4'	40:A:4796:HOH:O	1.93	0.68
25:X:13:MET:HE3	25:X:17:ILE:HG22	1.76	0.68
40:B:4707:HOH:O	16:O:147:ILE:HB	1.94	0.68
8:G:69:ILE:HA	8:G:72:MET:HE3	1.76	0.68
2:B:3014:G:H8	2:B:3014:G:H5'	1.57	0.68
1:A:1185:U:H2'	1:A:1186:C:C6	2.28	0.68
4:C:131:HIS:O	4:C:132:ASP:HB2	1.93	0.68
1:A:1170:U:O2'	1:A:1172:G:N7	2.24	0.68
1:A:2676:C:H4'	12:K:70:PHE:CE1	2.29	0.68
1:A:541:C:H2'	1:A:542:A:C5'	2.24	0.68
4:C:199:HIS:HD2	4:C:201:PHE:H	1.42	0.68
1:A:871:G:C5'	1:A:871:G:C8	2.77	0.68
1:A:1209:C:H2'	1:A:1210:G:H8	1.57	0.68
12:K:93:ARG:HH11	12:K:93:ARG:HB3	1.57	0.68
1:A:338:C:H5''	40:E:8420:HOH:O	1.93	0.68
1:A:1641:A:H2'	1:A:1642:A:H5'	1.75	0.68
23:V:14:GLU:O	23:V:17:THR:HB	1.94	0.68
4:C:191:GLY:HA2	4:C:194:MET:CE	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1441:G:H1'	40:A:7283:HOH:O	1.92	0.68
26:Y:72:VAL:HG22	26:Y:85:VAL:HG12	1.75	0.67
16:O:71:TRP:CE3	16:O:175:LEU:HD22	2.29	0.67
8:G:68:HIS:O	8:G:72:MET:HG3	1.95	0.67
7:F:54:ALA:CB	7:F:69:ILE:HD12	2.24	0.67
1:A:962:C:H1'	16:O:5:ARG:HH12	1.58	0.67
11:J:57:ARG:HG3	40:J:8355:HOH:O	1.94	0.67
1:A:175:G:H2'	15:N:192:ALA:HB3	1.75	0.67
1:A:1119:G:N2	1:A:1246:A:C2	2.58	0.67
1:A:506:G:H22	1:A:509:A:H5''	1.60	0.67
40:A:3269:HOH:O	22:U:9:LYS:HD3	1.94	0.67
7:F:174:VAL:HG13	40:F:6555:HOH:O	1.93	0.67
1:A:553:G:P	27:Z:204:ARG:HH22	2.18	0.67
6:E:140:VAL:HB	40:E:8453:HOH:O	1.94	0.67
21:T:57:THR:HG22	21:T:59:ASP:N	2.08	0.67
40:A:3356:HOH:O	11:J:11:LYS:HE2	1.93	0.67
11:J:47:GLU:HB3	11:J:133:ILE:HD13	1.77	0.67
7:F:44:ILE:HG12	7:F:83:PHE:HE1	1.59	0.67
25:X:6:GLN:HB2	25:X:26:ILE:CD1	2.25	0.67
13:L:62:PRO:HG3	13:L:65:ARG:NH2	2.09	0.67
26:Y:15:ARG:HH11	26:Y:15:ARG:HB3	1.60	0.67
7:F:99:ASP:HB2	7:F:103:ASN:HB2	1.77	0.67
31:4:65:THR:HG23	31:4:67:LEU:HG	1.77	0.67
26:Y:12:ILE:HD12	26:Y:36:HIS:ND1	2.10	0.67
5:D:145:HIS:HD2	5:D:146:THR:O	1.75	0.67
1:A:183:A:H5'	15:N:157:LEU:HD12	1.76	0.66
5:D:51:VAL:CG2	5:D:327:VAL:HG13	2.25	0.66
23:V:14:GLU:OE1	23:V:15:PRO:HD2	1.95	0.66
29:2:21:ARG:HD2	29:2:37:CYS:SG	2.36	0.66
4:C:210:GLY:HA3	40:C:8585:HOH:O	1.93	0.66
40:A:7199:HOH:O	15:N:154:ARG:HB2	1.95	0.66
5:D:214:PRO:HD2	40:D:8521:HOH:O	1.96	0.66
31:4:60:LYS:HG3	31:4:61:PRO:HD2	1.76	0.66
1:A:200:U:H2'	40:A:9956:HOH:O	1.95	0.66
11:J:47:GLU:HB3	11:J:133:ILE:CD1	2.25	0.66
20:S:39:THR:HB	20:S:42:GLU:HG3	1.75	0.66
1:A:558:C:H2'	1:A:559:U:H5'	1.78	0.66
1:A:396:U:H1'	40:A:7149:HOH:O	1.95	0.66
15:N:164:THR:HG22	15:N:167:GLY:N	2.07	0.66
1:A:2878:U:H2'	1:A:2879:A:O4'	1.96	0.66
7:F:135:VAL:HG21	7:F:139:TYR:CD1	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:G:C2'	1:A:545:G:H5''	2.25	0.66
7:F:23:VAL:HG23	7:F:23:VAL:O	1.96	0.66
11:J:31:PHE:HE2	11:J:87:LYS:O	1.78	0.66
20:S:18:LEU:HB2	20:S:143:VAL:CG1	2.26	0.66
1:A:2840:A:OP1	5:D:211:THR:HG23	1.96	0.66
8:G:20:ILE:CD1	8:G:40:VAL:HG11	2.25	0.66
27:Z:141:THR:HG23	40:Z:8584:HOH:O	1.95	0.66
1:A:2748:G:H2'	40:A:7058:HOH:O	1.95	0.66
9:H:39:SER:HB3	9:H:45:ALA:HB2	1.77	0.66
2:B:3006:C:C5'	16:O:37:ARG:NH1	2.55	0.66
25:X:21:LEU:HD21	25:X:48:VAL:HG11	1.76	0.66
4:C:33:GLU:O	4:C:34:ASP:HB2	1.95	0.66
13:L:75:ARG:CZ	40:L:4172:HOH:O	2.43	0.66
40:A:3193:HOH:O	15:N:79:LYS:HD3	1.96	0.66
25:X:21:LEU:HD21	25:X:48:VAL:CG1	2.26	0.66
1:A:2241:C:O2'	1:A:2242:U:H5'	1.96	0.66
13:L:82:ARG:NH2	13:L:115:ARG:HG2	2.11	0.66
4:C:95:PRO:HG2	4:C:98:GLU:HG2	1.78	0.66
18:Q:115:SER:N	18:Q:118:GLN:HE21	1.89	0.65
11:J:3:GLY:HA2	11:J:57:ARG:HH12	1.59	0.65
7:F:57:THR:HG23	7:F:63:ILE:HG22	1.78	0.65
1:A:1741:U:H5'	1:A:1742:A:OP1	1.96	0.65
9:H:99:THR:HA	40:H:3461:HOH:O	1.96	0.65
1:A:1119:G:H8	12:K:52:GLN:HE22	1.42	0.65
24:W:55:ARG:O	24:W:59:ILE:HG12	1.96	0.65
6:E:12:THR:HB	40:E:8443:HOH:O	1.96	0.65
16:O:183:ASP:OD2	16:O:186:LEU:HD12	1.95	0.65
7:F:135:VAL:HG22	7:F:136:ARG:H	1.60	0.65
11:J:150:LYS:HB2	11:J:157:ILE:HD12	1.78	0.65
11:J:56:ILE:HG22	11:J:61:LEU:HD22	1.77	0.65
25:X:137:GLN:NE2	25:X:141:HIS:HE1	1.93	0.65
7:F:64:ARG:CD	7:F:67:ASP:HB3	2.27	0.65
1:A:1835:U:C5	1:A:1840:A:N7	2.62	0.65
4:C:121:ALA:O	4:C:124:VAL:HG22	1.96	0.65
6:E:237:GLU:HB2	40:E:8429:HOH:O	1.96	0.65
2:B:3055:U:H4'	2:B:3056:A:C8	2.31	0.65
1:A:31:C:H4'	40:A:6934:HOH:O	1.96	0.65
8:G:11:VAL:HG12	8:G:12:ASP:N	2.11	0.65
11:J:83:PHE:HZ	11:J:146:TRP:HE1	1.42	0.65
23:V:52:THR:HG22	23:V:54:THR:H	1.62	0.65
5:D:71:VAL:HG11	5:D:296:LEU:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:U:H5'	40:A:6846:HOH:O	1.97	0.65
17:P:32:ARG:O	17:P:32:ARG:HD3	1.96	0.65
15:N:114:VAL:HG21	15:N:159:THR:HG21	1.77	0.65
5:D:190:MET:HE1	5:D:194:PHE:CD1	2.32	0.65
8:G:132:THR:HB	40:G:2227:HOH:O	1.96	0.65
5:D:103:ASP:HB2	40:D:8587:HOH:O	1.96	0.65
2:B:3041:C:O4'	7:F:50:VAL:HG23	1.97	0.65
20:S:132:ARG:HG2	20:S:133:ALA:N	2.12	0.65
12:K:19:MET:HE3	12:K:132:LEU:HD11	1.78	0.65
18:Q:143:ALA:HA	40:Q:2178:HOH:O	1.97	0.65
1:A:236:A:H4'	1:A:237:G:H5'	1.79	0.65
7:F:35:ALA:N	40:F:5576:HOH:O	2.29	0.65
24:W:64:GLY:O	24:W:65:ASP:HB2	1.95	0.65
40:A:6388:HOH:O	15:N:178:LYS:HB2	1.96	0.65
4:C:223:ARG:HG3	40:C:8599:HOH:O	1.97	0.65
1:A:2630:G:O6	4:C:206:ARG:NH2	2.30	0.65
9:H:110:GLU:HG2	40:H:6926:HOH:O	1.97	0.65
6:E:115:LEU:O	6:E:118:THR:HB	1.97	0.64
16:O:47:LEU:HD13	16:O:97:VAL:HG11	1.78	0.64
1:A:2505:G:O2'	1:A:2506:A:H5'	1.98	0.64
6:E:76:ARG:HD2	40:E:8432:HOH:O	1.95	0.64
4:C:105:VAL:CG1	4:C:154:ALA:HB1	2.26	0.64
18:Q:10:ALA:HA	18:Q:13:VAL:HG12	1.79	0.64
6:E:47:GLY:HA2	6:E:92:PRO:HB2	1.78	0.64
5:D:204:GLY:HA3	40:D:8648:HOH:O	1.95	0.64
1:A:1474:C:H5'	1:A:1474:C:C6	2.25	0.64
1:A:603:A:H5''	1:A:604:G:OP1	1.97	0.64
1:A:2783:A:H3'	40:A:4748:HOH:O	1.96	0.64
7:F:37:ALA:O	7:F:40:ILE:HG12	1.97	0.64
15:N:186:SER:O	15:N:189:VAL:HG12	1.97	0.64
27:Z:189:ASN:HD22	27:Z:189:ASN:C	1.99	0.64
14:M:72:ASN:HB2	40:M:8584:HOH:O	1.97	0.64
4:C:200:PRO:HG2	4:C:225:VAL:HG21	1.80	0.64
5:D:18:ARG:HG3	5:D:256:GLN:HG3	1.80	0.64
1:A:1172:G:H1'	40:A:4487:HOH:O	1.95	0.64
31:4:17:HIS:O	31:4:18:GLN:HG3	1.97	0.64
4:C:81:GLN:HB2	4:C:92:ASN:ND2	2.12	0.64
1:A:450:C:OP1	6:E:184:ARG:NH2	2.22	0.64
1:A:1118:A:H8	1:A:1119:G:H5''	1.60	0.64
14:M:145:LEU:O	14:M:148:GLU:HG3	1.96	0.64
5:D:36:PRO:HA	5:D:168:GLY:HA3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:97:GLN:O	7:F:97:GLN:HG2	1.98	0.64
1:A:2827:A:H2'	1:A:2828:G:O4'	1.97	0.64
1:A:951:A:C2'	1:A:952:G:H5'	2.27	0.64
16:O:155:GLU:O	16:O:156:GLU:HG3	1.98	0.64
1:A:1766:U:O2	1:A:1778:A:H5'	1.97	0.64
16:O:86:LEU:HD12	16:O:125:ALA:HB2	1.80	0.64
25:X:4:LEU:HD22	25:X:52:VAL:CG2	2.28	0.64
24:W:49:LEU:O	24:W:53:ILE:HG13	1.98	0.64
9:H:50:VAL:CG1	9:H:60:VAL:HG11	2.26	0.64
13:L:34:VAL:HG22	13:L:47:ALA:HB2	1.77	0.64
15:N:12:TRP:CE2	15:N:20:ILE:HD11	2.33	0.64
6:E:78:ARG:NH1	6:E:78:ARG:HG3	2.13	0.64
7:F:19:GLU:HG3	40:F:6165:HOH:O	1.98	0.64
1:A:338:C:H4'	6:E:174:ILE:CD1	2.27	0.64
5:D:275:GLY:O	5:D:291:ASP:HA	1.97	0.64
1:A:2064:U:H4'	1:A:2653:A:OP1	1.98	0.64
11:J:26:LYS:HD2	11:J:28:ILE:CD1	2.25	0.64
1:A:820:G:O2'	1:A:856:G:H4'	1.98	0.64
5:D:62:ARG:CA	5:D:65:MET:HE3	2.25	0.64
4:C:37:VAL:HG22	40:C:8594:HOH:O	1.98	0.64
28:1:42:CYS:SG	28:1:44:PHE:HB2	2.37	0.64
27:Z:186:ARG:HH11	27:Z:186:ARG:HG2	1.63	0.64
1:A:2717:C:O2'	1:A:2718:C:H5''	1.96	0.64
6:E:1:MET:HG2	6:E:2:GLN:N	2.11	0.64
25:X:4:LEU:O	25:X:32:CYS:HA	1.98	0.64
22:U:9:LYS:CE	22:U:13:ARG:NH1	2.61	0.64
1:A:2346:C:O5'	1:A:2346:C:H6	1.80	0.64
24:W:12:THR:CG2	24:W:15:GLU:HG3	2.18	0.63
12:K:52:GLN:HG3	12:K:53:ILE:N	2.13	0.63
15:N:60:ILE:C	15:N:61:ILE:HD12	2.19	0.63
29:2:8:GLN:HE22	29:2:11:LYS:HZ2	1.44	0.63
30:3:35:ARG:HB2	40:3:2691:HOH:O	1.99	0.63
1:A:902:G:N7	14:M:18:HIS:HD2	1.96	0.63
1:A:1730:G:H5'	1:A:1731:C:C5	2.34	0.63
9:H:50:VAL:HG21	9:H:63:ILE:HG21	1.80	0.63
4:C:170:VAL:HG13	28:1:22:ILE:HG21	1.79	0.63
10:I:12:ILE:HD12	40:I:692:HOH:O	1.98	0.63
27:Z:220:GLU:HG2	40:Z:8547:HOH:O	1.97	0.63
5:D:141:ARG:HG2	5:D:165:ARG:HA	1.80	0.63
14:M:53:ARG:NH2	14:M:57:VAL:HG12	2.13	0.63
1:A:1234:U:N3	5:D:244:PRO:HB3	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:267:LYS:HD3	40:D:8524:HOH:O	1.98	0.63
1:A:282:C:O2'	1:A:283:U:H5'	1.98	0.63
1:A:285:A:H2'	1:A:286:U:O4'	1.99	0.63
1:A:1080:C:H4'	1:A:1081:A:OP1	1.98	0.63
40:A:3162:HOH:O	17:P:3:THR:HG21	1.98	0.63
6:E:104:ASP:HA	6:E:107:ARG:NH1	2.12	0.63
8:G:31:ARG:NH1	8:G:68:HIS:CG	2.67	0.63
1:A:1973:A:H5'	1:A:1973:A:H8	1.63	0.63
1:A:20:G:H21	20:S:117:HIS:HD2	1.47	0.63
21:T:51:GLN:HE21	21:T:53:ASN:HD21	1.45	0.63
11:J:48:LEU:HG	11:J:157:ILE:HG21	1.80	0.63
15:N:169:ARG:HD2	40:N:8590:HOH:O	1.99	0.63
7:F:51:ARG:HD3	40:F:7636:HOH:O	1.99	0.63
1:A:2533:C:C6	1:A:2533:C:H5'	2.32	0.63
11:J:3:GLY:HA2	11:J:57:ARG:NH1	2.13	0.63
8:G:172:PRO:HB3	40:G:6931:HOH:O	1.99	0.63
26:Y:76:ARG:HH11	26:Y:76:ARG:HG3	1.63	0.63
25:X:21:LEU:HB3	25:X:26:ILE:HG12	1.81	0.63
20:S:39:THR:HB	20:S:42:GLU:CG	2.28	0.63
12:K:107:ASN:HD21	12:K:109:TYR:HB2	1.64	0.63
4:C:105:VAL:HG13	4:C:155:THR:O	1.99	0.63
9:H:19:ALA:O	9:H:22:VAL:HG22	1.99	0.63
11:J:45:GLN:HG3	11:J:135:TRP:NE1	2.14	0.63
7:F:41:LEU:HA	7:F:44:ILE:HG22	1.80	0.63
4:C:192:VAL:HG13	40:C:8557:HOH:O	1.96	0.63
30:3:41:HIS:N	30:3:45:ASN:HD22	1.95	0.63
21:T:81:ILE:HG23	40:T:8336:HOH:O	1.99	0.63
1:A:738:G:H3'	40:A:6557:HOH:O	1.99	0.63
8:G:100:ASP:HB2	40:G:2789:HOH:O	1.99	0.63
7:F:99:ASP:CB	7:F:103:ASN:H	2.12	0.62
20:S:9:ASP:O	20:S:13:THR:HB	1.99	0.62
15:N:37:VAL:CG1	15:N:63:VAL:HG11	2.29	0.62
2:B:3069:U:OP1	16:O:4:PRO:HG3	1.99	0.62
2:B:3054:A:O2'	2:B:3055:U:H5'	1.99	0.62
11:J:139:ASP:H	11:J:140:PRO:HD3	1.63	0.62
26:Y:31:ILE:O	26:Y:35:GLU:HG3	1.99	0.62
1:A:2862:G:H4'	5:D:336:GLN:O	1.98	0.62
11:J:27:LYS:N	11:J:58:HIS:HD2	1.95	0.62
5:D:41:PHE:CD1	5:D:79:MET:HE2	2.34	0.62
16:O:154:LEU:O	16:O:155:GLU:HB3	2.00	0.62
1:A:2769:C:H2'	1:A:2770:G:O4'	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:148:GLU:HG2	40:M:8551:HOH:O	2.00	0.62
25:X:149:LEU:HG	25:X:153:MET:CE	2.29	0.62
10:I:64:ASN:HD22	10:I:64:ASN:N	1.96	0.62
11:J:69:ASN:O	11:J:72:VAL:HG12	1.98	0.62
1:A:1134:G:H4'	11:J:151:MET:CE	2.21	0.62
1:A:281:U:H3'	40:A:6714:HOH:O	2.00	0.62
1:A:1189:A:H3'	40:A:7200:HOH:O	1.99	0.62
1:A:2679:G:H2'	1:A:2681:A:OP2	2.00	0.62
1:A:1053:G:OP1	11:J:12:PRO:HG3	1.98	0.62
7:F:69:ILE:O	7:F:69:ILE:HG22	1.99	0.62
15:N:63:VAL:HG21	15:N:109:PHE:CE1	2.35	0.62
11:J:127:GLY:O	11:J:128:ALA:HB3	2.00	0.62
40:L:408:HOH:O	23:V:37:GLU:HB3	2.00	0.62
21:T:23:LYS:HE2	40:T:8330:HOH:O	1.98	0.62
4:C:199:HIS:CD2	4:C:201:PHE:H	2.17	0.62
1:A:1787:C:OP1	18:Q:68:LYS:HE2	2.00	0.62
8:G:84:MET:HE1	8:G:148:ILE:HD12	1.81	0.62
1:A:1819:G:H2'	1:A:1820:G:H4'	1.82	0.62
6:E:27:ARG:HG3	6:E:29:ASP:OD1	2.00	0.62
1:A:2830:U:H3'	40:A:4744:HOH:O	1.98	0.62
1:A:2508:C:H2'	40:A:6265:HOH:O	2.00	0.62
25:X:21:LEU:HD22	25:X:26:ILE:HD11	1.81	0.62
15:N:104:ARG:O	15:N:108:LYS:HE2	1.99	0.62
4:C:36:ASP:OD2	4:C:85:ASP:HB2	1.98	0.62
1:A:2503:A:OP1	11:J:147:ARG:NH2	2.33	0.61
1:A:558:C:O2'	1:A:559:U:H5''	1.99	0.61
4:C:153:ARG:HB2	4:C:153:ARG:HH11	1.64	0.61
1:A:1213:C:O2'	1:A:1214:G:H5'	2.00	0.61
23:V:52:THR:HG22	23:V:54:THR:N	2.15	0.61
40:A:6967:HOH:O	5:D:211:THR:HG21	1.98	0.61
15:N:61:ILE:HG13	40:N:8624:HOH:O	2.00	0.61
1:A:1377:C:H5'	1:A:1377:C:H6	1.65	0.61
1:A:2456:A:H5'	40:A:5213:HOH:O	2.00	0.61
1:A:2690:U:O2'	8:G:111:LYS:HE3	2.00	0.61
7:F:27:ILE:HG22	7:F:28:GLY:N	2.16	0.61
1:A:1666:C:H2'	1:A:1667:A:H5'	1.81	0.61
15:N:77:PHE:HD2	40:N:8527:HOH:O	1.83	0.61
1:A:2420:G:O2'	1:A:2421:G:H5'	2.00	0.61
11:J:85:ILE:HB	11:J:132:PHE:CE2	2.35	0.61
13:L:29:LEU:HB3	13:L:55:VAL:CG1	2.26	0.61
9:H:2:VAL:HG22	9:H:57:GLU:OE1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:42:GLU:HB2	40:P:2176:HOH:O	1.98	0.61
1:A:1058:A:H2'	1:A:1060:C:H5''	1.81	0.61
1:A:1771:U:H4'	28:1:20:LEU:HD21	1.81	0.61
11:J:44:ALA:HA	11:J:163:PRO:O	2.00	0.61
8:G:3:VAL:HG22	8:G:49:ILE:HB	1.83	0.61
1:A:1615:A:H4'	40:A:5402:HOH:O	2.01	0.61
40:A:8627:HOH:O	6:E:103:ASN:HB3	2.00	0.61
25:X:106:THR:OG1	25:X:109:GLU:HG3	2.00	0.61
21:T:33:SER:OG	21:T:36:GLU:HG3	2.01	0.61
14:M:136:ALA:HB3	40:M:8574:HOH:O	2.00	0.61
27:Z:187:VAL:CG2	27:Z:192:ASP:HB2	2.29	0.61
1:A:1329:A:C2	40:A:4198:HOH:O	2.50	0.61
7:F:38:GLU:HB3	7:F:49:PRO:HG2	1.82	0.61
10:I:12:ILE:HA	40:I:4499:HOH:O	1.99	0.61
1:A:2756:U:H3	1:A:2896:A:H2	1.48	0.61
1:A:2578:G:H8	1:A:2578:G:H5'	1.65	0.61
40:A:5046:HOH:O	15:N:58:GLN:HG3	2.00	0.61
27:Z:200:THR:HG22	27:Z:201:GLU:CG	2.30	0.61
40:A:4038:HOH:O	15:N:94:LYS:HE3	1.99	0.61
16:O:157:PRO:HA	40:O:8526:HOH:O	1.99	0.61
2:B:3048:C:H4'	16:O:141:ARG:HH21	1.65	0.61
20:S:111:ILE:HG23	20:S:145:LEU:CD1	2.31	0.61
7:F:136:ARG:HD2	7:F:155:HIS:O	2.00	0.61
1:A:2547:C:OP2	5:D:5:ARG:NH1	2.34	0.61
16:O:169:PRO:O	16:O:172:PHE:HB3	2.01	0.61
20:S:25:PHE:CE2	20:S:29:LYS:HE2	2.36	0.61
1:A:710:G:OP1	17:P:24:ALA:HB3	2.01	0.60
8:G:15:GLN:NE2	8:G:40:VAL:O	2.33	0.60
11:J:166:ASN:N	11:J:166:ASN:HD22	1.97	0.60
24:W:44:GLY:O	24:W:48:GLU:HG2	2.01	0.60
1:A:2256:G:H2'	1:A:2257:G:H5'	1.83	0.60
40:A:5644:HOH:O	30:3:20:ARG:HB3	2.00	0.60
2:B:3039:U:H1'	2:B:3044:A:H61	1.65	0.60
7:F:146:LYS:NZ	16:O:107:ASN:ND2	2.49	0.60
15:N:87:MET:CB	31:4:46:ILE:HG21	2.30	0.60
7:F:95:THR:O	7:F:97:GLN:N	2.30	0.60
1:A:1328:A:OP1	27:Z:169:ARG:HD2	2.02	0.60
1:A:1684:A:H1'	30:3:43:ARG:HH22	1.66	0.60
6:E:162:VAL:HG12	6:E:192:ILE:HD11	1.83	0.60
11:J:46:VAL:O	11:J:146:TRP:HH2	1.84	0.60
4:C:190:ARG:NH2	4:C:207:GLN:OE1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:C:H1'	1:A:368:C:H42	1.65	0.60
1:A:1187:U:O2'	1:A:1189:A:H2	1.85	0.60
4:C:191:GLY:HA2	4:C:194:MET:HE2	1.82	0.60
6:E:162:VAL:HG13	6:E:232:LEU:HD21	1.83	0.60
40:A:5036:HOH:O	5:D:298:LYS:HD3	2.01	0.60
17:P:113:VAL:O	17:P:114:ILE:HD13	2.01	0.60
8:G:6:GLU:HA	8:G:46:THR:HG22	1.84	0.60
22:U:24:ARG:HH21	22:U:39:ASN:HD22	1.49	0.60
40:L:1387:HOH:O	23:V:20:MET:HE3	2.00	0.60
1:A:289:G:N2	1:A:363:A:H2	1.97	0.60
15:N:57:LYS:HE2	15:N:140:ALA:O	2.00	0.60
10:I:12:ILE:N	10:I:13:PRO:CD	2.65	0.60
2:B:3026:C:H2'	2:B:3027:C:C6	2.36	0.60
11:J:84:ARG:CZ	11:J:135:TRP:HH2	2.14	0.60
16:O:71:TRP:HE3	16:O:175:LEU:HD22	1.66	0.60
2:B:3055:U:H4'	2:B:3056:A:H8	1.65	0.60
7:F:25:MET:CE	7:F:37:ALA:HB1	2.31	0.60
18:Q:13:VAL:HG21	18:Q:41:ARG:HG2	1.84	0.60
24:W:56:ILE:O	24:W:60:GLN:HG3	2.02	0.60
5:D:154:VAL:HG12	5:D:156:LYS:HG2	1.83	0.60
20:S:119:VAL:HG12	20:S:119:VAL:O	2.00	0.60
13:L:74:VAL:HG13	13:L:113:ILE:HG23	1.82	0.60
25:X:122:ARG:NH2	25:X:154:ARG:HD2	2.16	0.60
28:1:28:ASP:O	28:1:31:ILE:HG22	2.02	0.60
5:D:42:ALA:HB1	5:D:308:LEU:HD11	1.83	0.60
1:A:1615:A:H5'	40:A:3695:HOH:O	2.02	0.60
20:S:17:MET:HE1	20:S:19:ARG:NH2	2.16	0.60
1:A:2851:G:O2'	1:A:2852:A:H5'	2.01	0.60
4:C:93:THR:HG23	4:C:154:ALA:O	2.02	0.60
1:A:69:A:H5'	1:A:69:A:C8	2.37	0.60
4:C:211:LYS:HB3	4:C:212:PRO:CD	2.28	0.60
1:A:1119:G:H2'	12:K:52:GLN:HE22	1.66	0.60
11:J:136:VAL:HG22	11:J:137:ASN:O	2.01	0.60
11:J:59:ASN:H	11:J:59:ASN:ND2	2.00	0.60
1:A:1314:U:H2'	40:A:5390:HOH:O	2.02	0.60
1:A:1086:A:C6	25:X:11:VAL:HG11	2.36	0.60
1:A:793:A:H5''	18:Q:83:LYS:HG2	1.84	0.60
14:M:120:LEU:HD12	14:M:133:VAL:HG21	1.84	0.59
1:A:1701:A:H4'	1:A:1702:U:C5'	2.31	0.59
7:F:19:GLU:O	7:F:20:LYS:HG2	2.02	0.59
20:S:39:THR:HB	20:S:42:GLU:CD	2.22	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:C:H2'	1:A:559:U:C5'	2.32	0.59
13:L:115:ARG:HG3	13:L:116:GLU:N	2.15	0.59
1:A:1182:C:H1'	1:A:1192:A:H8	1.67	0.59
1:A:280:C:H2'	1:A:281:U:O4'	2.03	0.59
25:X:154:ARG:C	40:X:4276:HOH:O	2.39	0.59
11:J:75:SER:HB3	11:J:79:ALA:HB1	1.84	0.59
16:O:159:TYR:HB3	16:O:162:ASP:HB2	1.84	0.59
26:Y:25:ARG:HG2	40:Y:5356:HOH:O	2.03	0.59
15:N:52:LEU:HD21	40:N:8617:HOH:O	2.02	0.59
1:A:2815:G:OP2	12:K:99:GLU:HG2	2.03	0.59
18:Q:105:LEU:HD21	18:Q:137:LEU:HD21	1.85	0.59
1:A:2502:C:H4'	11:J:151:MET:HG2	1.85	0.59
11:J:139:ASP:HA	40:J:8373:HOH:O	2.02	0.59
1:A:1299:G:O6	14:M:6:ARG:HD3	2.03	0.59
40:A:3495:HOH:O	22:U:82:THR:HA	2.01	0.59
1:A:188:C:H5''	15:N:163:LEU:HD21	1.84	0.59
1:A:1594:C:OP2	18:Q:120:ARG:HD2	2.02	0.59
16:O:47:LEU:HD12	16:O:92:ALA:HB1	1.84	0.59
5:D:162:MET:CE	5:D:308:LEU:HD21	2.32	0.59
11:J:75:SER:O	11:J:79:ALA:HB2	2.02	0.59
26:Y:43:VAL:HG12	26:Y:44:ASP:N	2.16	0.59
1:A:681:G:N3	1:A:681:G:H5'	2.18	0.59
9:H:47:LEU:HB2	9:H:108:LEU:HD11	1.85	0.59
6:E:118:THR:O	6:E:136:VAL:HG13	2.02	0.59
8:G:23:GLU:HG2	8:G:28:SER:CB	2.33	0.59
4:C:132:ASP:OD1	4:C:133:ARG:N	2.34	0.59
20:S:132:ARG:CZ	40:S:8582:HOH:O	2.49	0.59
5:D:55:ASN:HB3	5:D:63:GLU:HA	1.84	0.59
17:P:39:THR:O	17:P:115:ARG:NH2	2.36	0.59
1:A:1654:U:H2'	4:C:47:HIS:HD2	1.67	0.59
1:A:371:U:H2'	1:A:372:A:H8	1.67	0.59
24:W:39:ALA:C	24:W:41:GLU:H	2.06	0.59
28:I:26:VAL:O	28:I:30:GLU:HG3	2.03	0.59
10:I:12:ILE:HG22	10:I:12:ILE:O	2.03	0.59
13:L:34:VAL:CG2	13:L:47:ALA:HB2	2.31	0.59
1:A:538:C:OP2	27:Z:134:HIS:HE1	1.86	0.59
4:C:232:ARG:NH2	4:C:236:GLY:O	2.29	0.59
11:J:55:GLN:HE22	11:J:91:HIS:CD2	2.20	0.59
11:J:136:VAL:HG23	40:J:8345:HOH:O	2.02	0.59
27:Z:189:ASN:ND2	27:Z:192:ASP:H	2.00	0.59
10:I:12:ILE:HG13	40:I:6833:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:106:GLY:HA3	40:L:5264:HOH:O	2.02	0.59
26:Y:25:ARG:HD2	40:Y:3861:HOH:O	2.03	0.59
26:Y:43:VAL:CG1	26:Y:47:ALA:HB3	2.32	0.59
1:A:1266:U:H4'	27:Z:115:ARG:HH21	1.66	0.59
6:E:168:ARG:NH2	6:E:190:ALA:O	2.35	0.59
25:X:38:THR:HG22	40:X:3580:HOH:O	2.02	0.59
2:B:3044:A:O4'	7:F:76:ARG:NE	2.36	0.58
6:E:76:ARG:HD3	40:E:8366:HOH:O	2.03	0.58
15:N:74:ARG:HH11	15:N:74:ARG:HG3	1.68	0.58
6:E:200:PRO:HB3	6:E:212:VAL:CG2	2.32	0.58
1:A:2256:G:H2'	1:A:2257:G:C5'	2.33	0.58
11:J:118:PRO:HD2	40:J:8341:HOH:O	2.01	0.58
24:W:58:THR:O	24:W:62:GLU:HG3	2.03	0.58
27:Z:117:LEU:HD12	27:Z:174:VAL:CG1	2.33	0.58
1:A:431:G:P	15:N:48:ARG:HH12	2.26	0.58
28:1:19:GLY:O	28:1:23:ARG:HG2	2.03	0.58
16:O:151:ASP:O	16:O:154:LEU:HB2	2.03	0.58
15:N:48:ARG:NH2	40:N:8563:HOH:O	2.33	0.58
1:A:119:A:H2'	1:A:120:A:H5''	1.84	0.58
16:O:62:HIS:HB3	16:O:65:ASP:OD1	2.03	0.58
2:B:3092:G:H2'	2:B:3093:A:C8	2.38	0.58
7:F:55:LYS:HA	40:F:6752:HOH:O	2.02	0.58
1:A:2694:A:H4'	8:G:91:PHE:CE1	2.37	0.58
5:D:195:ARG:HG2	5:D:323:LEU:HD22	1.84	0.58
1:A:2672:C:H1'	40:D:8629:HOH:O	2.04	0.58
7:F:166:ILE:HD12	40:F:6326:HOH:O	2.04	0.58
12:K:131:THR:HG22	12:K:133:GLY:N	2.18	0.58
30:3:40:ARG:HA	30:3:45:ASN:ND2	2.18	0.58
7:F:25:MET:CE	7:F:41:LEU:HG	2.28	0.58
5:D:217:ARG:HG3	5:D:257:THR:HG22	1.84	0.58
1:A:272:A:H5'	1:A:273:G:OP2	2.03	0.58
1:A:2548:C:OP2	5:D:5:ARG:NH2	2.36	0.58
1:A:69:A:H8	1:A:69:A:H5'	1.68	0.58
5:D:314:ALA:HB3	5:D:317:PRO:HG3	1.85	0.58
1:A:2320:U:H4'	1:A:2321:A:O4'	2.03	0.58
7:F:23:VAL:HG22	7:F:73:VAL:HB	1.86	0.58
7:F:86:THR:O	7:F:90:LEU:HG	2.04	0.58
23:V:46:ALA:HB1	23:V:52:THR:HG21	1.86	0.58
5:D:175:LEU:HD23	5:D:175:LEU:C	2.23	0.58
1:A:138:U:H5''	1:A:139:C:OP2	2.04	0.58
29:2:28:HIS:CD2	29:2:30:LYS:HB2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2081:A:H4'	12:K:69:TYR:CE1	2.39	0.58
18:Q:103:THR:HA	18:Q:106:ARG:NH1	2.18	0.58
15:N:79:LYS:HD2	40:N:8556:HOH:O	2.02	0.58
16:O:78:MET:HB2	16:O:79:PRO:HD3	1.85	0.58
1:A:447:A:O2'	1:A:448:G:H5'	2.04	0.58
8:G:137:ASP:OD1	8:G:139:GLU:HB2	2.04	0.58
28:1:30:GLU:HA	28:1:33:HIS:HB3	1.84	0.58
1:A:2604:A:H5'	40:A:5307:HOH:O	2.04	0.58
16:O:61:ALA:HB3	16:O:88:ALA:HB2	1.86	0.58
27:Z:151:SER:HB3	27:Z:154:ARG:HB3	1.85	0.58
11:J:71:TYR:C	11:J:73:GLN:H	2.07	0.58
1:A:1351:G:OP1	6:E:96:LYS:NZ	2.32	0.58
19:R:64:GLU:HG3	19:R:74:ASP:OD2	2.04	0.58
22:U:69:LYS:O	22:U:71:VAL:HG23	2.04	0.58
1:A:1118:A:H62	1:A:1244:U:H3	1.50	0.58
1:A:2780:C:H1'	8:G:143:GLN:NE2	2.17	0.58
9:H:58:GLU:OE1	15:N:27:ARG:NH2	2.32	0.58
25:X:141:HIS:HB2	25:X:146:ILE:HG12	1.85	0.57
15:N:87:MET:CG	31:4:46:ILE:HG21	2.33	0.57
15:N:87:MET:CB	31:4:46:ILE:HD13	2.33	0.57
15:N:61:ILE:HA	40:N:8624:HOH:O	2.04	0.57
1:A:2453:G:H5'	40:A:4206:HOH:O	2.04	0.57
5:D:258:GLY:H	5:D:260:HIS:CE1	2.22	0.57
1:A:709:G:O2'	17:P:25:VAL:HG12	2.03	0.57
1:A:2769:C:O2'	1:A:2770:G:H5'	2.04	0.57
1:A:1441:G:O2'	1:A:1442:A:H5'	2.04	0.57
1:A:1972:U:H2'	1:A:1973:A:H5'	1.86	0.57
15:N:45:ARG:CZ	15:N:48:ARG:HG3	2.34	0.57
1:A:1162:G:H2'	40:A:6094:HOH:O	2.05	0.57
5:D:108:GLU:HB3	5:D:111:ARG:HD2	1.86	0.57
14:M:143:THR:CG2	14:M:144:ASP:N	2.67	0.57
12:K:19:MET:CE	12:K:132:LEU:HD11	2.35	0.57
1:A:1123:A:C6	1:A:1238:C:H5'	2.39	0.57
1:A:1197:G:N2	40:A:5746:HOH:O	2.37	0.57
20:S:106:GLY:HA2	20:S:109:MET:CE	2.33	0.57
1:A:2270:G:H4'	4:C:223:ARG:NH1	2.20	0.57
25:X:13:MET:HE1	25:X:18:GLN:HA	1.86	0.57
2:B:3013:A:O2'	2:B:3014:G:H5''	2.04	0.57
2:B:3026:C:H2'	2:B:3027:C:H6	1.69	0.57
17:P:105:ASN:HD21	17:P:109:SER:H	1.52	0.57
1:A:2721:U:H4'	13:L:87:ARG:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1118:A:C8	1:A:1119:G:H5'	2.40	0.57
13:L:74:VAL:HG12	13:L:75:ARG:HG3	1.85	0.57
4:C:51:ARG:NH1	4:C:120:ARG:O	2.38	0.57
8:G:7:ILE:HD11	8:G:11:VAL:C	2.24	0.57
4:C:94:LEU:HG	4:C:99:ILE:HD11	1.86	0.57
13:L:45:PRO:HB2	40:L:7169:HOH:O	2.04	0.57
2:B:3041:C:C6	7:F:50:VAL:HG21	2.38	0.57
11:J:35:ASN:ND2	11:J:80:ASN:HA	2.18	0.57
1:A:1333:U:H2'	1:A:1334:C:C6	2.39	0.57
1:A:2769:C:C2'	1:A:2770:G:H5'	2.35	0.57
24:W:39:ALA:N	24:W:40:PRO:CD	2.67	0.57
12:K:130:VAL:HG12	12:K:131:THR:N	2.19	0.57
1:A:584:U:H3'	40:A:5609:HOH:O	2.03	0.57
30:3:22:PRO:HG2	30:3:25:VAL:HG23	1.87	0.57
25:X:108:ARG:HG3	40:X:3483:HOH:O	2.04	0.57
7:F:101:THR:HG22	40:F:7400:HOH:O	2.04	0.57
26:Y:74:ALA:HB2	26:Y:85:VAL:HG13	1.85	0.57
11:J:28:ILE:HA	11:J:62:GLU:OE1	2.05	0.57
16:O:86:LEU:O	16:O:90:LEU:HG	2.05	0.57
7:F:105:SER:CB	7:F:131:THR:HG23	2.31	0.57
15:N:38:VAL:C	15:N:63:VAL:HG13	2.25	0.57
8:G:31:ARG:HH12	8:G:68:HIS:CE1	2.23	0.57
11:J:46:VAL:HG12	11:J:146:TRP:HZ3	1.70	0.57
28:1:11:THR:OG1	28:1:23:ARG:HB2	2.04	0.57
14:M:114:VAL:HG11	40:M:8574:HOH:O	2.03	0.57
2:B:3029:C:C2'	2:B:3030:C:H5'	2.35	0.57
1:A:1189:A:H1'	1:A:1209:C:O4'	2.04	0.57
4:C:66:ARG:HB2	4:C:66:ARG:HH11	1.69	0.57
1:A:130:C:H2'	40:A:9668:HOH:O	2.05	0.57
1:A:621:C:H5'	27:Z:132:ASP:OD2	2.05	0.57
40:A:3488:HOH:O	31:4:57:GLY:HA2	2.04	0.57
1:A:1834:C:H2'	1:A:1840:A:N6	2.20	0.57
25:X:65:VAL:HA	25:X:68:THR:CG2	2.32	0.57
1:A:1119:G:H8	12:K:52:GLN:NE2	2.03	0.57
4:C:36:ASP:O	4:C:38:ILE:N	2.38	0.57
1:A:2815:G:N7	12:K:80:LYS:NZ	2.53	0.57
1:A:88:G:H8	1:A:88:G:H5'	1.70	0.57
7:F:44:ILE:HG23	7:F:45:THR:HG23	1.86	0.56
11:J:139:ASP:N	11:J:140:PRO:CD	2.67	0.56
28:1:30:GLU:HA	28:1:33:HIS:CB	2.35	0.56
1:A:2265:U:H2'	1:A:2266:A:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:21:SER:OG	17:P:106:PRO:HB2	2.05	0.56
15:N:134:ILE:HG23	15:N:141:ILE:HD13	1.87	0.56
6:E:142:ASP:OD1	6:E:237:GLU:HB3	2.04	0.56
1:A:1667:A:H2'	1:A:1668:U:C6	2.41	0.56
1:A:2718:C:H6	1:A:2718:C:H5'	1.70	0.56
1:A:1189:A:H1'	1:A:1209:C:C1'	2.34	0.56
2:B:3014:G:H5'	2:B:3014:G:C8	2.40	0.56
1:A:1500:U:P	18:Q:41:ARG:HH22	2.28	0.56
1:A:121:U:OP2	30:3:10:ARG:NH2	2.38	0.56
7:F:36:ASN:HA	40:F:7500:HOH:O	2.04	0.56
1:A:449:A:N7	6:E:43:LYS:HG2	2.20	0.56
15:N:98:GLN:O	15:N:102:GLU:HG3	2.05	0.56
6:E:127:ARG:HH11	6:E:127:ARG:HG2	1.70	0.56
15:N:157:LEU:HB3	15:N:160:PHE:HD1	1.70	0.56
8:G:31:ARG:HH12	8:G:68:HIS:CG	2.22	0.56
5:D:307:ARG:HH11	5:D:307:ARG:CB	2.17	0.56
1:A:1159:G:H21	1:A:1189:A:H8	1.52	0.56
1:A:1333:U:H2'	1:A:1334:C:H6	1.70	0.56
25:X:81:ASP:OD1	25:X:92:ASP:HB2	2.05	0.56
1:A:407:A:H5'	40:A:5538:HOH:O	2.06	0.56
1:A:2607:U:H4'	40:A:8949:HOH:O	2.05	0.56
8:G:79:GLY:HA3	40:G:7046:HOH:O	2.05	0.56
5:D:305:ASP:O	5:D:306:LYS:HB2	2.06	0.56
15:N:99:ARG:HD2	15:N:167:GLY:HA2	1.86	0.56
15:N:37:VAL:HG13	15:N:63:VAL:HG11	1.86	0.56
8:G:7:ILE:HG22	8:G:45:ASP:O	2.06	0.56
12:K:46:ILE:HA	40:K:1123:HOH:O	2.05	0.56
4:C:105:VAL:HG12	4:C:106:CYS:N	2.20	0.56
1:A:2729:C:O2'	1:A:2730:G:H5'	2.06	0.56
1:A:21:G:H4'	20:S:2:ILE:HG22	1.88	0.56
12:K:45:VAL:HG21	12:K:129:PHE:CD1	2.41	0.56
7:F:95:THR:C	7:F:97:GLN:H	2.09	0.56
7:F:135:VAL:HG22	7:F:136:ARG:N	2.20	0.56
3:5:9076:A:H5''	36:5:9080:SPS:C8	2.35	0.56
5:D:66:GLU:OE1	5:D:328:ARG:HD2	2.05	0.56
12:K:74:ARG:CB	12:K:74:ARG:HH11	2.18	0.56
40:B:4707:HOH:O	16:O:147:ILE:HD12	2.04	0.56
11:J:14:TYR:N	11:J:91:HIS:CE1	2.71	0.56
25:X:65:VAL:CA	25:X:68:THR:HG22	2.35	0.56
9:H:50:VAL:CG2	9:H:63:ILE:HG21	2.34	0.56
1:A:775:G:OP1	29:2:16:HIS:HE1	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:154:LEU:HG	16:O:155:GLU:H	1.69	0.56
12:K:99:GLU:HA	40:K:7377:HOH:O	2.05	0.56
1:A:694:A:N3	40:A:3329:HOH:O	2.33	0.56
16:O:32:PRO:HD2	16:O:99:GLU:O	2.06	0.56
13:L:55:VAL:HG12	13:L:56:SER:N	2.21	0.56
1:A:2890:A:H1'	23:V:56:ARG:HH21	1.70	0.56
4:C:192:VAL:HG12	4:C:207:GLN:HB3	1.87	0.56
26:Y:9:VAL:HG22	26:Y:88:GLU:OE2	2.05	0.56
1:A:1130:U:H2'	1:A:1131:G:O4'	2.06	0.56
9:H:21:GLU:O	9:H:24:ARG:HG3	2.04	0.56
1:A:1008:C:H5''	11:J:16:ARG:HH12	1.70	0.56
1:A:2502:C:C2'	1:A:2503:A:H5'	2.36	0.56
25:X:80:ASP:O	25:X:84:VAL:HG23	2.05	0.56
11:J:166:ASN:ND2	11:J:166:ASN:N	2.53	0.56
1:A:2676:C:H4'	12:K:70:PHE:HE1	1.69	0.56
1:A:1778:A:H2'	1:A:1779:A:H5'	1.88	0.56
1:A:500:G:H21	20:S:98:ASN:HD21	1.52	0.56
4:C:76:VAL:HG23	28:1:63:LYS:HB3	1.87	0.56
27:Z:107:PRO:HB3	27:Z:182:PHE:CD2	2.41	0.56
1:A:567:U:H5''	40:X:5817:HOH:O	2.05	0.56
30:3:18:ASN:HD21	30:3:40:ARG:H	1.52	0.56
27:Z:235:GLU:CD	27:Z:235:GLU:H	2.08	0.56
25:X:41:TYR:O	25:X:45:VAL:HG13	2.06	0.56
25:X:108:ARG:HE	25:X:114:PRO:HG3	1.71	0.56
1:A:2310:G:OP2	11:J:114:PRO:HD2	2.05	0.56
1:A:1636:G:O2'	1:A:1637:A:H5'	2.05	0.56
16:O:11:ARG:NH2	40:O:8520:HOH:O	2.38	0.56
22:U:53:GLY:HA3	40:U:6384:HOH:O	2.06	0.56
25:X:126:ASP:HB3	25:X:135:GLY:O	2.06	0.56
7:F:38:GLU:OE2	7:F:51:ARG:CZ	2.54	0.55
1:A:1118:A:C8	1:A:1118:A:C3'	2.86	0.55
16:O:38:LYS:HD2	16:O:114:LYS:HE3	1.88	0.55
1:A:545:G:H5'	1:A:545:G:C8	2.35	0.55
4:C:101:GLU:OE2	4:C:131:HIS:HB2	2.06	0.55
1:A:1209:C:H2'	1:A:1210:G:C8	2.41	0.55
7:F:93:LEU:HB3	7:F:97:GLN:OE1	2.06	0.55
25:X:90:TYR:N	25:X:90:TYR:CD1	2.74	0.55
7:F:99:ASP:HB3	7:F:103:ASN:H	1.71	0.55
15:N:183:VAL:HG12	15:N:184:ARG:N	2.21	0.55
40:A:5786:HOH:O	17:P:7:LEU:HD22	2.05	0.55
40:A:6970:HOH:O	6:E:188:ARG:CD	2.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:2:1:THR:HA	40:2:435:HOH:O	2.07	0.55
1:A:820:G:H5'	1:A:821:U:H5'	1.88	0.55
8:G:15:GLN:HG2	8:G:19:ASP:O	2.07	0.55
5:D:141:ARG:HD2	5:D:163:GLU:OE2	2.06	0.55
1:A:2363:G:O3'	19:R:11:ARG:NH1	2.40	0.55
2:B:3020:G:H3'	40:B:2984:HOH:O	2.06	0.55
1:A:2301:A:H5''	1:A:2302:A:H5'	1.87	0.55
1:A:2502:C:C4'	11:J:151:MET:HG2	2.36	0.55
1:A:157:G:H4'	15:N:95:LYS:HE3	1.89	0.55
28:1:38:LYS:HG3	40:1:8429:HOH:O	2.05	0.55
4:C:88:ILE:HD13	4:C:100:PRO:CD	2.36	0.55
1:A:95:A:H5''	1:A:97:G:O4'	2.06	0.55
1:A:899:C:H5'	40:A:9712:HOH:O	2.07	0.55
8:G:9:GLU:HG3	8:G:10:ASP:N	2.21	0.55
5:D:74:ILE:HD13	5:D:309:VAL:HG21	1.87	0.55
12:K:74:ARG:O	12:K:78:ILE:HG12	2.06	0.55
1:A:182:G:O3'	15:N:157:LEU:HD13	2.06	0.55
25:X:122:ARG:CZ	40:X:5817:HOH:O	2.55	0.55
3:5:9076:A:H5''	36:5:9080:SPS:C6	2.36	0.55
1:A:1120:U:H5'	1:A:1121:G:OP2	2.06	0.55
17:P:87:THR:O	17:P:91:GLN:HG3	2.05	0.55
11:J:27:LYS:H	11:J:58:HIS:CD2	2.16	0.55
1:A:797:A:C4'	28:1:10:ARG:N	2.70	0.55
4:C:100:PRO:HG2	4:C:103:VAL:CG2	2.35	0.55
6:E:246:ARG:NE	40:E:8423:HOH:O	2.40	0.55
6:E:246:ARG:NH2	40:E:8423:HOH:O	2.39	0.55
6:E:185:LYS:HD3	6:E:186:TYR:CE1	2.42	0.55
7:F:58:VAL:HG12	7:F:59:GLY:N	2.21	0.55
1:A:926:A:O2'	14:M:41:HIS:HD2	1.90	0.55
1:A:485:A:N3	1:A:487:G:H5''	2.22	0.55
7:F:163:VAL:HA	40:F:6326:HOH:O	2.06	0.55
2:B:3039:U:H1'	2:B:3044:A:N6	2.21	0.55
7:F:50:VAL:O	7:F:71:ALA:HA	2.06	0.55
1:A:400:C:O2'	1:A:401:C:H5'	2.06	0.55
1:A:1996:U:O2'	1:A:1997:A:H5'	2.06	0.55
40:A:9456:HOH:O	26:Y:23:HIS:HD2	1.90	0.55
24:W:4:HIS:HB3	40:W:6622:HOH:O	2.06	0.55
11:J:117:LYS:HB2	40:J:8341:HOH:O	2.07	0.55
4:C:8:ARG:HG2	40:C:8552:HOH:O	2.06	0.55
7:F:10:PHE:CG	7:F:11:HIS:N	2.74	0.55
16:O:100:ALA:O	16:O:129:ILE:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2468:A:H61	31:4:48:ASN:HD21	1.54	0.55
1:A:474:C:O3'	6:E:73:LEU:HD21	2.07	0.55
23:V:52:THR:CG2	23:V:54:THR:HB	2.37	0.55
4:C:191:GLY:HA2	4:C:194:MET:HE3	1.88	0.55
1:A:1972:U:H2'	1:A:1973:A:C5'	2.37	0.55
25:X:35:VAL:HG23	25:X:41:TYR:CD2	2.42	0.55
18:Q:16:VAL:HG12	18:Q:17:GLY:N	2.22	0.55
1:A:1132:A:N6	1:A:1229:C:H2'	2.22	0.55
1:A:2570:G:H5''	40:A:4427:HOH:O	2.07	0.55
6:E:107:ARG:NE	40:E:8459:HOH:O	2.11	0.55
5:D:36:PRO:HA	5:D:168:GLY:HA2	1.88	0.55
18:Q:38:GLU:HA	18:Q:41:ARG:NH1	2.22	0.55
18:Q:105:LEU:CD2	18:Q:137:LEU:HD21	2.37	0.55
28:1:53:GLY:HA2	28:1:67:GLY:O	2.07	0.55
25:X:88:THR:CG2	25:X:89:ASP:H	2.16	0.54
9:H:58:GLU:CD	15:N:27:ARG:HH22	2.09	0.54
11:J:75:SER:C	11:J:79:ALA:HB2	2.28	0.54
25:X:90:TYR:CE2	25:X:99:ALA:HB2	2.42	0.54
1:A:415:A:O2'	1:A:416:G:H5'	2.07	0.54
26:Y:18:ARG:NH1	40:Y:4132:HOH:O	2.40	0.54
1:A:316:A:H5'	22:U:54:ASP:OD2	2.06	0.54
1:A:1940:C:H4'	40:A:6857:HOH:O	2.07	0.54
1:A:2506:A:O2'	1:A:2507:G:O5'	2.25	0.54
14:M:143:THR:HG22	14:M:144:ASP:H	1.73	0.54
1:A:558:C:C2'	1:A:559:U:H5''	2.37	0.54
10:I:12:ILE:HB	40:I:4714:HOH:O	2.06	0.54
9:H:101:ALA:HB2	9:H:108:LEU:CD2	2.37	0.54
4:C:109:GLU:HG2	4:C:116:GLY:N	2.22	0.54
5:D:2:GLN:HA	40:D:8615:HOH:O	2.06	0.54
9:H:107:VAL:O	9:H:111:ILE:HG13	2.06	0.54
1:A:317:A:H5''	22:U:52:ARG:HD2	1.88	0.54
1:A:259:G:H21	15:N:58:GLN:NE2	2.05	0.54
28:1:62:TYR:CE2	28:1:64:ILE:HG23	2.42	0.54
27:Z:212:ARG:HD2	40:Z:8596:HOH:O	2.07	0.54
15:N:43:PRO:HG3	15:N:62:VAL:HG21	1.90	0.54
16:O:90:LEU:HB2	16:O:186:LEU:HD22	1.88	0.54
1:A:2064:U:H5'	1:A:2652:U:O3'	2.08	0.54
5:D:195:ARG:NH1	5:D:324:ASP:OD1	2.40	0.54
4:C:109:GLU:HG2	4:C:116:GLY:H	1.73	0.54
16:O:87:LEU:CD1	16:O:186:LEU:HD21	2.32	0.54
16:O:110:THR:HB	16:O:113:SER:OG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:4:LEU:HD23	25:X:54:PHE:HB3	1.88	0.54
1:A:470:U:O2'	29:2:16:HIS:CD2	2.59	0.54
1:A:2419:U:H5''	1:A:2420:G:H5'	1.90	0.54
1:A:244:C:OP2	9:H:38:LYS:HE3	2.08	0.54
1:A:2281:C:C2'	1:A:2282:U:H5'	2.36	0.54
1:A:1477:C:H5'	1:A:1868:G:C5'	2.37	0.54
1:A:1753:C:O2	5:D:229:ARG:NH2	2.39	0.54
25:X:110:GLN:HA	25:X:110:GLN:NE2	2.23	0.54
1:A:281:U:O2'	1:A:282:C:H5'	2.08	0.54
15:N:61:ILE:N	15:N:61:ILE:HD12	2.23	0.54
30:3:22:PRO:HG2	30:3:25:VAL:CG2	2.37	0.54
1:A:2300:A:H4'	1:A:2301:A:O5'	2.08	0.54
1:A:316:A:N3	1:A:336:G:O2'	2.40	0.54
1:A:1342:C:O2'	1:A:1343:C:H5'	2.07	0.54
1:A:960:G:N3	1:A:960:G:H2'	2.23	0.54
4:C:212:PRO:HB2	40:C:8561:HOH:O	2.06	0.54
1:A:1164:U:H4'	1:A:1165:G:OP1	2.07	0.54
1:A:1181:A:H2'	1:A:1182:C:O4'	2.07	0.54
4:C:88:ILE:O	4:C:88:ILE:HG22	2.08	0.54
2:B:3028:U:H2'	2:B:3029:C:C6	2.43	0.54
1:A:656:G:OP2	17:P:37:ARG:HD2	2.07	0.54
6:E:13:ASP:O	6:E:13:ASP:OD1	2.25	0.54
1:A:1878:G:H1'	40:A:5635:HOH:O	2.06	0.54
8:G:101:GLU:HB2	8:G:116:THR:O	2.08	0.54
11:J:84:ARG:CZ	11:J:135:TRP:CH2	2.91	0.54
9:H:16:ALA:HA	9:H:111:ILE:HD13	1.90	0.54
6:E:25:PRO:HG2	40:E:8324:HOH:O	2.08	0.54
15:N:84:LYS:HE2	40:N:8577:HOH:O	2.08	0.54
1:A:2587:U:H2'	1:A:2589:U:H5''	1.90	0.54
17:P:14:LEU:CD2	17:P:102:ILE:HD11	2.38	0.54
1:A:183:A:C5'	15:N:157:LEU:HD12	2.38	0.54
8:G:22:VAL:O	8:G:28:SER:HA	2.08	0.54
2:B:3002:U:H4'	2:B:3002:U:OP2	2.08	0.54
1:A:2438:G:H5'	40:A:5683:HOH:O	2.07	0.54
16:O:37:ARG:NE	40:O:8534:HOH:O	2.41	0.54
12:K:133:GLY:O	12:K:137:GLU:HG3	2.07	0.54
9:H:99:THR:O	9:H:99:THR:HG23	2.07	0.54
1:A:1528:A:H2'	1:A:1529:G:O4'	2.08	0.54
16:O:12:ARG:HD3	16:O:18:THR:OG1	2.08	0.54
1:A:2795:C:O2'	1:A:2796:U:H5'	2.07	0.54
11:J:31:PHE:CD2	11:J:85:ILE:HG23	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:39:ALA:O	24:W:41:GLU:N	2.41	0.53
1:A:175:G:C2'	15:N:192:ALA:HB3	2.38	0.53
27:Z:112:GLU:CD	27:Z:115:ARG:NH1	2.61	0.53
27:Z:117:LEU:HD12	27:Z:174:VAL:HG11	1.91	0.53
1:A:2361:A:H5'	1:A:2361:A:H8	1.73	0.53
31:4:11:CYS:HB2	31:4:20:HIS:CE1	2.43	0.53
22:U:73:HIS:CD2	22:U:88:PRO:HG3	2.42	0.53
1:A:2434:A:O3'	31:4:28:GLY:HA3	2.09	0.53
1:A:2473:U:O3'	1:A:2474:A:H3'	2.07	0.53
1:A:654:A:OP2	17:P:38:ARG:HD3	2.08	0.53
6:E:129:HIS:HD2	6:E:165:ASP:OD2	1.91	0.53
25:X:21:LEU:CD1	25:X:26:ILE:HD11	2.35	0.53
9:H:58:GLU:HG3	9:H:61:MET:HE1	1.91	0.53
22:U:32:ARG:NH1	22:U:38:ARG:NH1	2.56	0.53
4:C:94:LEU:HD23	4:C:94:LEU:N	2.23	0.53
7:F:94:ALA:O	7:F:95:THR:O	2.26	0.53
26:Y:75:ALA:O	26:Y:83:ALA:HA	2.08	0.53
14:M:125:PHE:CZ	14:M:140:VAL:HG13	2.44	0.53
15:N:81:ARG:O	15:N:86:MET:HE2	2.08	0.53
16:O:49:THR:CG2	16:O:56:ASP:HB2	2.36	0.53
8:G:31:ARG:HH12	8:G:68:HIS:CD2	2.26	0.53
5:D:185:GLY:HA2	40:D:8628:HOH:O	2.08	0.53
1:A:1596:U:H2'	1:A:1598:A:OP2	2.08	0.53
1:A:2897:C:H2'	1:A:2898:G:H8	1.72	0.53
5:D:248:ARG:O	5:D:251:VAL:CG1	2.57	0.53
26:Y:78:GLU:CG	26:Y:79:GLU:H	2.20	0.53
10:I:23:ILE:O	10:I:27:ILE:HG13	2.08	0.53
1:A:2694:A:H4'	8:G:91:PHE:HE1	1.74	0.53
40:A:6970:HOH:O	6:E:188:ARG:HD2	2.08	0.53
16:O:139:TRP:HA	16:O:139:TRP:CE3	2.43	0.53
40:A:9798:HOH:O	13:L:9:THR:HA	2.07	0.53
5:D:268:ARG:NE	40:D:8602:HOH:O	2.40	0.53
25:X:125:HIS:CD2	25:X:127:GLY:H	2.26	0.53
15:N:182:LYS:HB2	15:N:194:ALA:HB2	1.91	0.53
27:Z:184:GLU:OE1	27:Z:204:ARG:NH1	2.41	0.53
1:A:656:G:H5'	17:P:3:THR:CG2	2.38	0.53
5:D:314:ALA:CB	5:D:317:PRO:HG3	2.39	0.53
29:2:28:HIS:CE1	29:2:31:LYS:HE2	2.43	0.53
5:D:297:VAL:HB	40:D:8600:HOH:O	2.08	0.53
1:A:1167:G:O2'	1:A:1168:C:H5'	2.08	0.53
1:A:1887:U:OP1	28:1:21:LYS:HE3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:69:ILE:HA	8:G:72:MET:HE2	1.89	0.53
24:W:64:GLY:O	24:W:65:ASP:CB	2.57	0.53
5:D:82:VAL:O	5:D:82:VAL:HG12	2.08	0.53
9:H:113:ASP:O	9:H:117:GLU:HG3	2.08	0.53
13:L:87:ARG:CZ	40:L:4854:HOH:O	2.56	0.53
15:N:164:THR:CG2	15:N:165:SER:N	2.72	0.53
12:K:107:ASN:HD22	12:K:107:ASN:C	2.11	0.53
5:D:138:GLY:O	5:D:139:ASP:O	2.26	0.53
18:Q:131:PHE:CD1	18:Q:137:LEU:HD13	2.43	0.53
27:Z:112:GLU:OE2	27:Z:115:ARG:NH1	2.41	0.53
40:A:9693:HOH:O	15:N:9:ARG:HG3	2.08	0.53
8:G:145:ALA:HB1	8:G:168:ILE:CD1	2.39	0.53
25:X:19:ASP:O	25:X:23:MET:HG3	2.08	0.53
23:V:13:ILE:HG12	23:V:32:CYS:HB3	1.90	0.53
1:A:1559:A:H1'	40:A:5381:HOH:O	2.08	0.53
1:A:65:C:O2'	1:A:66:G:H5'	2.08	0.53
11:J:53:PRO:HA	11:J:125:VAL:O	2.09	0.53
1:A:263:U:O4'	9:H:59:ILE:HD13	2.09	0.53
15:N:72:SER:HB2	15:N:93:ARG:HG2	1.91	0.53
5:D:30:PRO:HB2	5:D:39:GLN:NE2	2.23	0.53
8:G:93:MET:HE1	8:G:165:GLY:N	2.24	0.53
14:M:6:ARG:NH2	40:M:8547:HOH:O	2.41	0.53
8:G:49:ILE:HD11	8:G:69:ILE:HD12	1.91	0.53
6:E:235:PHE:HE2	6:E:243:VAL:HG21	1.74	0.53
2:B:3039:U:H3'	2:B:3040:C:H5''	1.91	0.53
14:M:143:THR:HG22	14:M:145:LEU:H	1.74	0.53
16:O:171:HIS:CE1	40:O:8568:HOH:O	2.62	0.53
4:C:128:LEU:HG	40:C:8574:HOH:O	2.09	0.53
5:D:329:TYR:HE2	23:V:15:PRO:HG2	1.73	0.53
1:A:1377:C:C6	1:A:1377:C:H5'	2.44	0.53
16:O:64:SER:C	16:O:66:LEU:H	2.13	0.53
31:4:55:VAL:HB	31:4:56:PRO:HD2	1.90	0.53
1:A:1393:A:H2'	1:A:1394:C:C6	2.44	0.53
11:J:31:PHE:HA	11:J:85:ILE:CG2	2.39	0.52
11:J:58:HIS:HA	11:J:61:LEU:HD23	1.92	0.52
12:K:52:GLN:HG3	12:K:53:ILE:H	1.73	0.52
1:A:2781:U:H1'	8:G:139:GLU:OE2	2.08	0.52
6:E:107:ARG:NH2	40:E:8459:HOH:O	2.42	0.52
12:K:107:ASN:HD22	12:K:109:TYR:H	1.57	0.52
1:A:1741:U:O2'	1:A:2723:G:H4'	2.09	0.52
16:O:154:LEU:HG	16:O:155:GLU:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:120:ARG:NH2	18:Q:123:TYR:CD2	2.77	0.52
23:V:47:ARG:HG3	40:V:4381:HOH:O	2.08	0.52
1:A:2608:C:H2'	40:A:3086:HOH:O	2.08	0.52
4:C:123:GLY:HA3	4:C:162:GLY:HA2	1.91	0.52
40:A:4082:HOH:O	6:E:50:GLU:HG2	2.07	0.52
1:A:1677:U:OP2	30:3:8:LYS:NZ	2.42	0.52
6:E:233:THR:HG22	6:E:234:VAL:N	2.23	0.52
27:Z:106:THR:HG23	27:Z:107:PRO:HD2	1.91	0.52
5:D:27:ASN:HD22	5:D:27:ASN:H	1.55	0.52
6:E:219:ASN:O	6:E:222:ASP:OD1	2.26	0.52
1:A:1847:A:OP1	4:C:175:LYS:HG3	2.09	0.52
6:E:111:VAL:HB	40:E:8323:HOH:O	2.09	0.52
14:M:148:GLU:HB2	40:M:8593:HOH:O	2.09	0.52
5:D:307:ARG:HH11	5:D:307:ARG:CG	2.22	0.52
1:A:2837:U:H1'	5:D:307:ARG:HH12	1.73	0.52
1:A:396:U:O2'	1:A:418:C:H4'	2.10	0.52
26:Y:76:ARG:O	26:Y:77:PHE:HB3	2.09	0.52
40:A:8909:HOH:O	15:N:94:LYS:HE2	2.09	0.52
1:A:1086:A:N6	25:X:11:VAL:HG11	2.25	0.52
26:Y:30:MET:HE1	26:Y:58:ALA:HB3	1.91	0.52
18:Q:80:ARG:HG2	18:Q:87:ARG:CZ	2.39	0.52
18:Q:91:LYS:O	18:Q:95:GLU:HG3	2.08	0.52
2:B:3049:G:H5''	40:B:4707:HOH:O	2.09	0.52
8:G:81:GLU:HG2	8:G:134:SER:CB	2.34	0.52
15:N:173:LEU:HD23	15:N:183:VAL:HG12	1.91	0.52
23:V:9:CYS:CA	23:V:52:THR:HG23	2.39	0.52
8:G:77:THR:OG1	8:G:78:GLU:N	2.42	0.52
8:G:21:THR:HG23	8:G:30:THR:OG1	2.10	0.52
21:T:29:ASP:OD1	21:T:31:ARG:HG3	2.08	0.52
1:A:660:A:H4'	1:A:661:G:O5'	2.10	0.52
28:I:11:THR:CG2	28:I:23:ARG:HB2	2.39	0.52
15:N:114:VAL:HG21	15:N:159:THR:CG2	2.39	0.52
16:O:152:GLU:C	16:O:154:LEU:H	2.11	0.52
1:A:2256:G:C2'	1:A:2257:G:H5'	2.39	0.52
1:A:1168:C:H2'	1:A:1169:U:O4'	2.09	0.52
40:A:9479:HOH:O	25:X:10:GLU:HG2	2.08	0.52
18:Q:98:ILE:HD12	18:Q:102:ARG:NE	2.25	0.52
1:A:1593:C:OP1	18:Q:117:SER:HB3	2.10	0.52
11:J:13:ALA:HA	11:J:91:HIS:CE1	2.45	0.52
4:C:192:VAL:CG1	4:C:207:GLN:HB3	2.40	0.52
1:A:1299:G:N2	40:A:4198:HOH:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1189:A:O2'	1:A:1208:C:H2'	2.10	0.52
20:S:132:ARG:NH2	40:S:8582:HOH:O	2.43	0.52
25:X:38:THR:O	25:X:42:ARG:HB2	2.10	0.52
1:A:2361:A:H2'	1:A:2362:A:C8	2.44	0.52
1:A:256:C:H2'	1:A:257:G:O4'	2.10	0.52
7:F:140:ARG:O	7:F:144:ARG:HG2	2.09	0.52
1:A:2111:G:H1'	40:A:8563:HOH:O	2.09	0.52
7:F:22:VAL:HG22	7:F:74:THR:HG22	1.91	0.52
29:2:25:LYS:HE2	40:2:7213:HOH:O	2.08	0.52
17:P:47:ARG:NH1	17:P:47:ARG:HG3	2.23	0.52
4:C:220:PRO:HD2	4:C:223:ARG:HD3	1.92	0.52
22:U:41:ARG:HG2	22:U:41:ARG:NH1	2.25	0.52
18:Q:38:GLU:HA	18:Q:41:ARG:HH11	1.75	0.52
1:A:951:A:O2'	1:A:952:G:H5'	2.09	0.52
7:F:11:HIS:C	7:F:13:MET:H	2.13	0.52
1:A:602:A:O2'	1:A:605:C:H4'	2.09	0.52
1:A:1353:C:P	40:A:4194:HOH:O	2.66	0.52
4:C:165:THR:HG22	40:C:8615:HOH:O	2.09	0.52
1:A:2502:C:H2'	1:A:2503:A:H5'	1.91	0.52
1:A:1701:A:H5''	1:A:1702:U:H3'	1.92	0.52
12:K:131:THR:HG22	12:K:134:GLU:H	1.75	0.52
1:A:1120:U:H5''	1:A:1120:U:C6	2.45	0.52
26:Y:66:THR:HG23	26:Y:67:PRO:HD2	1.91	0.52
7:F:103:ASN:ND2	7:F:134:LEU:H	2.07	0.52
26:Y:78:GLU:HG2	26:Y:79:GLU:N	2.24	0.52
5:D:168:GLY:N	5:D:174:ARG:HD3	2.24	0.52
9:H:46:GLU:O	9:H:73:PRO:HD2	2.09	0.52
1:A:447:A:OP1	22:U:2:LYS:HG2	2.10	0.52
1:A:2443:C:H3'	40:A:9983:HOH:O	2.09	0.52
14:M:61:ALA:HA	40:M:8564:HOH:O	2.09	0.52
15:N:30:GLU:O	15:N:34:GLU:HG3	2.09	0.52
1:A:283:U:H5''	1:A:284:C:P	2.50	0.52
1:A:1189:A:H1'	1:A:1209:C:H1'	1.92	0.52
1:A:1151:G:OP1	10:I:63:ARG:NH1	2.43	0.52
9:H:46:GLU:N	40:H:3461:HOH:O	2.43	0.52
25:X:38:THR:HG22	25:X:39:ASP:H	1.75	0.52
1:A:661:G:C5	1:A:686:A:C2	2.98	0.52
1:A:2251:G:H2'	1:A:2252:A:C8	2.45	0.52
1:A:1250:C:O2'	1:A:1251:C:H5'	2.09	0.52
21:T:8:PRO:HD2	24:W:32:ALA:HA	1.91	0.52
7:F:99:ASP:CB	7:F:103:ASN:HB2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:41:LEU:HA	7:F:44:ILE:CG2	2.39	0.51
1:A:21:G:H5''	20:S:1:GLY:O	2.10	0.51
5:D:212:GLN:OE1	5:D:216:LYS:HD3	2.10	0.51
1:A:1874:U:H2'	4:C:120:ARG:HG3	1.92	0.51
7:F:94:ALA:HB3	7:F:174:VAL:HA	1.92	0.51
1:A:1787:C:H4'	1:A:2883:A:O4'	2.10	0.51
1:A:407:A:H2'	1:A:408:A:C8	2.45	0.51
1:A:2894:C:O2'	1:A:2895:C:H5'	2.09	0.51
1:A:328:U:O4'	6:E:202:THR:HG22	2.10	0.51
2:B:3042:C:H2'	40:B:6700:HOH:O	2.10	0.51
7:F:67:ASP:O	7:F:69:ILE:HG13	2.10	0.51
1:A:290:C:O2'	1:A:291:C:H5'	2.10	0.51
12:K:45:VAL:HG22	12:K:46:ILE:N	2.24	0.51
4:C:105:VAL:HG11	4:C:154:ALA:CB	2.40	0.51
5:D:139:ASP:HB2	5:D:165:ARG:HE	1.75	0.51
11:J:35:ASN:ND2	11:J:79:ALA:O	2.43	0.51
1:A:380:A:OP2	15:N:9:ARG:HD2	2.09	0.51
25:X:108:ARG:NH2	40:X:2359:HOH:O	2.44	0.51
7:F:10:PHE:CD1	7:F:11:HIS:N	2.78	0.51
1:A:417:G:P	40:A:6928:HOH:O	2.67	0.51
22:U:63:ILE:HD11	22:U:75:GLU:HB2	1.92	0.51
1:A:1484:G:H2'	40:A:8618:HOH:O	2.10	0.51
11:J:45:GLN:HB3	11:J:163:PRO:CD	2.21	0.51
7:F:99:ASP:O	7:F:159:PRO:HG3	2.09	0.51
25:X:84:VAL:HG12	40:X:6679:HOH:O	2.09	0.51
4:C:211:LYS:HD3	40:C:8608:HOH:O	2.10	0.51
25:X:21:LEU:HD22	25:X:26:ILE:HD13	1.93	0.51
1:A:558:C:C2'	1:A:559:U:C5'	2.88	0.51
23:V:47:ARG:CG	40:V:4381:HOH:O	2.58	0.51
1:A:136:C:H2'	1:A:137:U:O4'	2.10	0.51
22:U:111:ARG:HB3	22:U:119:ALA:HB2	1.92	0.51
27:Z:144:ARG:CZ	40:Z:8608:HOH:O	2.58	0.51
16:O:170:GLU:O	16:O:174:GLU:HG3	2.10	0.51
5:D:16:ARG:NE	40:D:8550:HOH:O	2.30	0.51
11:J:59:ASN:N	11:J:59:ASN:ND2	2.54	0.51
14:M:143:THR:CG2	14:M:144:ASP:H	2.22	0.51
16:O:48:VAL:HG11	16:O:55:ASP:HB3	1.90	0.51
1:A:1515:A:H2'	1:A:1516:C:C6	2.45	0.51
1:A:1304:U:H2'	1:A:1305:C:C6	2.46	0.51
1:A:2832:C:H5	40:A:6721:HOH:O	1.92	0.51
40:A:6934:HOH:O	22:U:9:LYS:HD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:3:41:HIS:H	30:3:45:ASN:ND2	2.06	0.51
1:A:1641:A:C2'	1:A:1642:A:H5'	2.40	0.51
5:D:280:VAL:HG13	5:D:333:GLU:O	2.10	0.51
14:M:73:VAL:HG11	14:M:118:LEU:HD21	1.91	0.51
40:A:6536:HOH:O	4:C:211:LYS:HG2	2.10	0.51
1:A:2717:C:H2'	1:A:2718:C:C5'	2.35	0.51
17:P:26:TRP:HB2	40:P:3062:HOH:O	2.11	0.51
15:N:182:LYS:HD2	15:N:193:LYS:HB2	1.91	0.51
1:A:714:U:H3'	40:A:6455:HOH:O	2.11	0.51
2:B:3035:C:H5''	40:B:4078:HOH:O	2.11	0.51
4:C:125:ASN:HB3	4:C:158:VAL:HG12	1.91	0.51
12:K:90:LYS:HB2	35:K:8502:CL:CL	2.48	0.51
13:L:125:ALA:C	13:L:127:ALA:H	2.14	0.51
1:A:101:C:H2'	1:A:102:A:H8	1.75	0.51
26:Y:74:ALA:CB	26:Y:85:VAL:HG22	2.40	0.51
2:B:3049:G:H2'	2:B:3050:G:O4'	2.11	0.51
16:O:182:GLY:O	16:O:183:ASP:O	2.28	0.51
1:A:588:G:O6	25:X:154:ARG:NH1	2.44	0.51
9:H:99:THR:O	9:H:100:ASP:HB2	2.10	0.51
16:O:143:ARG:HA	16:O:172:PHE:CD2	2.45	0.51
2:B:3027:C:H1'	40:B:2772:HOH:O	2.10	0.51
25:X:38:THR:HG22	25:X:39:ASP:N	2.25	0.51
1:A:1342:C:C2'	1:A:1343:C:H5'	2.41	0.51
15:N:80:GLY:O	15:N:81:ARG:HD3	2.11	0.51
1:A:155:C:OP2	15:N:188:ARG:HD3	2.11	0.51
14:M:30:ARG:NH2	40:M:8521:HOH:O	2.31	0.51
15:N:5:TYR:HE2	15:N:46:LEU:HD13	1.76	0.51
21:T:73:ASP:OD1	21:T:76:GLU:HG3	2.11	0.51
2:B:3006:C:C5'	16:O:37:ARG:HH12	2.18	0.51
20:S:96:VAL:HG13	20:S:106:GLY:HA3	1.92	0.51
25:X:21:LEU:HB3	25:X:26:ILE:CG1	2.41	0.51
29:2:8:GLN:HE22	29:2:11:LYS:HZ1	1.59	0.51
12:K:39:VAL:HG12	12:K:40:ASN:ND2	2.26	0.51
22:U:41:ARG:NH1	22:U:42:VAL:O	2.43	0.51
40:A:9207:HOH:O	5:D:254:GLN:HG3	2.09	0.51
16:O:141:ARG:HB3	40:O:8571:HOH:O	2.10	0.51
1:A:380:A:H5''	15:N:48:ARG:NH2	2.25	0.51
15:N:107:ARG:NH1	40:N:8578:HOH:O	2.42	0.51
6:E:16:VAL:HG12	6:E:17:ASP:N	2.25	0.51
16:O:47:LEU:CD1	16:O:97:VAL:HG11	2.40	0.51
15:N:157:LEU:HD23	40:N:8629:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:14:LEU:HD23	17:P:102:ILE:HD11	1.92	0.51
7:F:167:GLU:OE2	7:F:173:GLU:HG2	2.10	0.51
1:A:1525:G:H5'	1:A:1526:A:OP2	2.11	0.51
1:A:2866:U:H4'	1:A:2867:G:H5'	1.92	0.51
2:B:3049:G:O2'	2:B:3050:G:H5'	2.11	0.51
1:A:1733:A:H4'	5:D:212:GLN:HA	1.91	0.51
7:F:57:THR:HG23	7:F:63:ILE:CB	2.41	0.51
1:A:1500:U:OP2	18:Q:41:ARG:NH2	2.43	0.51
5:D:85:ARG:NH1	40:D:8629:HOH:O	2.44	0.51
1:A:1130:U:H5'	40:A:7191:HOH:O	2.10	0.51
1:A:2898:G:H4'	5:D:288:GLY:HA2	1.93	0.51
5:D:16:ARG:NH2	40:D:8550:HOH:O	2.36	0.51
29:2:10:LYS:HG3	40:2:2979:HOH:O	2.10	0.51
1:A:818:A:O2'	28:1:13:ARG:HD3	2.11	0.51
23:V:11:THR:HG22	23:V:53:ASP:OD2	2.11	0.51
8:G:118:ILE:HG23	8:G:144:THR:HG21	1.93	0.51
15:N:63:VAL:HG21	15:N:109:PHE:CZ	2.46	0.50
28:1:46:LYS:NZ	40:1:8439:HOH:O	2.43	0.50
5:D:156:LYS:HE3	40:D:8625:HOH:O	2.11	0.50
27:Z:216:ARG:HD3	40:Z:8564:HOH:O	2.11	0.50
16:O:180:LEU:O	16:O:181:ASP:HB3	2.11	0.50
16:O:23:ARG:NH1	40:O:8548:HOH:O	2.44	0.50
12:K:131:THR:HG22	12:K:133:GLY:H	1.75	0.50
16:O:159:TYR:HE2	16:O:163:PHE:HE2	1.60	0.50
16:O:73:ALA:HB2	16:O:163:PHE:CZ	2.47	0.50
9:H:111:ILE:O	9:H:115:VAL:HG23	2.10	0.50
14:M:104:ASP:HB3	40:M:8564:HOH:O	2.12	0.50
8:G:24:GLY:HA3	8:G:76:VAL:HB	1.93	0.50
31:4:3:MET:O	31:4:90:PHE:HA	2.11	0.50
1:A:2314:G:C2'	1:A:2315:C:H5'	2.41	0.50
11:J:47:GLU:HG2	11:J:133:ILE:HD12	1.92	0.50
13:L:87:ARG:NE	40:L:4854:HOH:O	2.44	0.50
1:A:1592:G:O2'	1:A:1593:C:O4'	2.28	0.50
18:Q:103:THR:O	18:Q:107:GLU:HG3	2.10	0.50
1:A:475:G:OP1	6:E:73:LEU:HD22	2.11	0.50
40:A:3574:HOH:O	5:D:27:ASN:HB2	2.10	0.50
5:D:198:GLU:HB3	40:D:8590:HOH:O	2.11	0.50
15:N:113:ARG:NH2	15:N:156:ARG:HG2	2.27	0.50
12:K:75:PRO:HG2	12:K:105:LEU:HD21	1.93	0.50
1:A:1471:A:H2'	1:A:1472:C:C6	2.46	0.50
1:A:1007:A:H2'	11:J:19:TYR:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:47:GLU:CB	11:J:133:ILE:HD13	2.41	0.50
11:J:150:LYS:HG2	40:J:8383:HOH:O	2.12	0.50
5:D:140:LEU:HD23	40:D:8574:HOH:O	2.12	0.50
1:A:777:U:O2'	29:2:11:LYS:HG2	2.12	0.50
1:A:1450:C:C4'	1:A:1451:C:OP2	2.59	0.50
2:B:3030:C:OP1	7:F:137:PRO:O	2.29	0.50
9:H:80:GLN:HB3	40:H:2563:HOH:O	2.12	0.50
10:I:20:VAL:O	10:I:24:VAL:HG23	2.12	0.50
1:A:2428:G:N7	31:4:60:LYS:NZ	2.57	0.50
20:S:33:ARG:NH1	40:S:8541:HOH:O	2.45	0.50
1:A:371:U:H2'	1:A:372:A:C8	2.45	0.50
25:X:125:HIS:HE1	40:X:3071:HOH:O	1.94	0.50
4:C:125:ASN:CB	4:C:158:VAL:HG12	2.42	0.50
6:E:153:VAL:O	6:E:157:LEU:HG	2.11	0.50
11:J:144:GLU:HA	11:J:144:GLU:OE1	2.11	0.50
1:A:2670:G:O2'	1:A:2671:U:H5'	2.11	0.50
4:C:164:ARG:NE	40:C:8586:HOH:O	2.44	0.50
5:D:14:GLY:HA2	5:D:15:PRO:C	2.31	0.50
15:N:185:PRO:HG2	15:N:189:VAL:HG11	1.93	0.50
11:J:39:GLY:O	11:J:41:THR:N	2.45	0.50
40:A:7074:HOH:O	31:4:60:LYS:HG3	2.10	0.50
17:P:25:VAL:HG23	17:P:26:TRP:N	2.26	0.50
30:3:48:ASP:O	30:3:49:GLU:HB2	2.12	0.50
5:D:279:THR:OG1	5:D:290:VAL:HB	2.12	0.50
22:U:49:GLU:OE2	22:U:97:ARG:HD2	2.12	0.50
25:X:130:HIS:O	25:X:136:GLY:HA3	2.12	0.50
40:A:6218:HOH:O	27:Z:165:GLU:HB3	2.11	0.50
1:A:1180:U:H2'	1:A:1181:A:O4'	2.11	0.50
5:D:24:PRO:CG	5:D:204:GLY:HA2	2.42	0.50
27:Z:186:ARG:NH1	27:Z:186:ARG:HG2	2.26	0.50
15:N:55:LYS:HB2	15:N:60:ILE:CD1	2.41	0.50
1:A:710:G:P	17:P:24:ALA:HB3	2.52	0.50
25:X:31:HIS:HB3	40:X:5420:HOH:O	2.11	0.50
19:R:40:HIS:HD2	19:R:60:THR:OG1	1.94	0.50
1:A:949:U:O2'	19:R:40:HIS:HE1	1.94	0.50
6:E:140:VAL:HG12	6:E:141:SER:N	2.26	0.50
15:N:169:ARG:NH1	40:N:8572:HOH:O	2.44	0.50
15:N:74:ARG:HG3	15:N:74:ARG:NH1	2.27	0.50
1:A:2269:C:C2'	1:A:2270:G:H5'	2.41	0.50
23:V:52:THR:HG22	23:V:54:THR:HB	1.94	0.50
15:N:134:ILE:CG2	15:N:141:ILE:HD13	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:11:HIS:O	7:F:12:GLU:HB3	2.11	0.50
1:A:1527:A:H1'	1:A:1528:A:C8	2.46	0.50
1:A:2387:U:H2'	1:A:2388:C:C6	2.46	0.50
1:A:814:G:H4'	40:A:9641:HOH:O	2.11	0.50
4:C:186:TRP:CG	4:C:187:PRO:HA	2.47	0.50
1:A:1205:U:C2'	1:A:1206:U:H5''	2.41	0.50
13:L:82:ARG:HH21	13:L:115:ARG:HG2	1.77	0.50
4:C:153:ARG:HD3	40:C:8532:HOH:O	2.10	0.50
8:G:132:THR:HG23	8:G:132:THR:O	2.11	0.50
1:A:776:A:OP1	29:2:28:HIS:HE1	1.95	0.50
16:O:11:ARG:HG3	16:O:14:ARG:NH1	2.26	0.50
27:Z:144:ARG:NE	40:Z:8608:HOH:O	2.44	0.50
1:A:101:C:H2'	1:A:102:A:C8	2.47	0.50
7:F:49:PRO:HG3	40:F:5828:HOH:O	2.12	0.50
1:A:2004:U:O2	1:A:2004:U:H2'	2.11	0.50
28:1:30:GLU:O	28:1:33:HIS:HB3	2.12	0.50
5:D:144:THR:HG22	5:D:145:HIS:N	2.27	0.50
6:E:129:HIS:CE1	6:E:231:ARG:HA	2.47	0.50
8:G:152:THR:HG21	8:G:165:GLY:HA2	1.93	0.50
11:J:95:GLU:HB3	11:J:119:VAL:HG11	1.94	0.50
40:A:5707:HOH:O	30:3:44:ARG:HG2	2.11	0.50
21:T:11:THR:H	21:T:14:ALA:HB3	1.77	0.50
7:F:149:ARG:NH1	40:F:3066:HOH:O	2.24	0.50
16:O:184:ILE:HG22	16:O:185:GLU:N	2.26	0.50
1:A:1173:A:H2'	40:A:3860:HOH:O	2.12	0.49
7:F:23:VAL:HG21	7:F:45:THR:HG21	1.94	0.49
1:A:2768:A:O2'	1:A:2769:C:H5'	2.11	0.49
4:C:53:ALA:HB3	40:C:8603:HOH:O	2.12	0.49
12:K:42:GLU:O	12:K:131:THR:HG23	2.11	0.49
5:D:43:GLY:O	5:D:308:LEU:HD12	2.12	0.49
5:D:51:VAL:HG23	5:D:329:TYR:O	2.12	0.49
5:D:336:GLN:NE2	40:D:8523:HOH:O	2.45	0.49
1:A:1819:G:H5'	40:A:4224:HOH:O	2.12	0.49
25:X:22:GLU:HG2	25:X:27:HIS:CD2	2.47	0.49
15:N:155:HIS:CE1	15:N:158:ARG:HE	2.30	0.49
1:A:812:A:H1'	40:A:3466:HOH:O	2.11	0.49
5:D:132:HIS:HB2	5:D:137:LEU:HD22	1.94	0.49
1:A:383:A:H4'	40:A:4846:HOH:O	2.12	0.49
7:F:99:ASP:HB2	7:F:103:ASN:H	1.77	0.49
25:X:139:GLY:O	25:X:141:HIS:HD2	1.95	0.49
4:C:192:VAL:O	4:C:192:VAL:HG12	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2896:A:N3	1:A:2896:A:H2'	2.27	0.49
1:A:1730:G:C5'	1:A:1731:C:C6	2.95	0.49
10:I:64:ASN:N	10:I:64:ASN:ND2	2.60	0.49
1:A:2589:U:H2'	1:A:2590:U:C6	2.47	0.49
5:D:27:ASN:HB3	40:D:8622:HOH:O	2.13	0.49
1:A:1236:A:H2'	1:A:1237:U:O4'	2.13	0.49
9:H:79:GLN:HB2	9:H:82:ASP:OD2	2.13	0.49
1:A:1003:U:O2'	11:J:90:PHE:HE1	1.95	0.49
25:X:6:GLN:CB	25:X:26:ILE:HD12	2.34	0.49
15:N:87:MET:HB2	15:N:91:ILE:HD11	1.94	0.49
16:O:77:ASN:OD1	16:O:80:SER:HB2	2.12	0.49
1:A:2420:G:H4'	40:A:3605:HOH:O	2.12	0.49
17:P:26:TRP:N	40:P:3062:HOH:O	2.44	0.49
1:A:2613:G:O2'	1:A:2614:C:H5'	2.12	0.49
1:A:74:A:H2'	1:A:75:U:C6	2.47	0.49
1:A:1717:A:H5''	18:Q:54:LYS:HB2	1.95	0.49
1:A:1268:C:O2'	1:A:1269:G:H5'	2.11	0.49
1:A:2010:A:H2'	40:A:5474:HOH:O	2.13	0.49
1:A:1098:A:H2'	1:A:1099:G:O4'	2.12	0.49
1:A:542:A:H2'	1:A:543:G:O4'	2.12	0.49
1:A:1942:A:O2'	1:A:1943:C:H5'	2.13	0.49
15:N:172:GLY:C	15:N:183:VAL:HG11	2.33	0.49
8:G:11:VAL:CG1	8:G:12:ASP:N	2.75	0.49
7:F:93:LEU:HG	40:F:3862:HOH:O	2.11	0.49
14:M:57:VAL:HG12	14:M:57:VAL:O	2.13	0.49
1:A:2619:U:H2'	1:A:2620:U:C6	2.47	0.49
1:A:432:G:O2'	1:A:433:C:H5'	2.12	0.49
1:A:1535:G:H2'	1:A:1536:C:C6	2.47	0.49
1:A:349:U:O2'	1:A:350:C:H5'	2.12	0.49
4:C:173:GLY:O	4:C:176:HIS:HB3	2.12	0.49
5:D:7:ARG:CG	5:D:7:ARG:HH11	2.20	0.49
8:G:7:ILE:HD11	8:G:11:VAL:O	2.12	0.49
4:C:94:LEU:HG	4:C:99:ILE:CD1	2.42	0.49
25:X:13:MET:CE	25:X:17:ILE:HG22	2.42	0.49
1:A:926:A:O2'	14:M:41:HIS:CD2	2.65	0.49
4:C:164:ARG:HB2	28:1:68:CYS:SG	2.52	0.49
11:J:129:ASN:HD22	11:J:129:ASN:N	2.10	0.49
14:M:97:VAL:HG12	14:M:98:GLU:O	2.13	0.49
11:J:45:GLN:HE21	11:J:135:TRP:HE1	1.60	0.49
7:F:27:ILE:HD11	7:F:37:ALA:CB	2.42	0.49
7:F:23:VAL:HG23	7:F:41:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:113:HIS:O	20:S:145:LEU:HD12	2.12	0.49
13:L:34:VAL:HB	40:L:7169:HOH:O	2.13	0.49
4:C:153:ARG:CB	4:C:153:ARG:HH11	2.25	0.49
31:4:48:ASN:ND2	31:4:50:GLY:H	2.10	0.49
16:O:15:GLU:HB2	16:O:17:ARG:HG3	1.94	0.49
1:A:821:U:H2'	1:A:822:C:H6	1.76	0.49
1:A:559:U:H2'	1:A:560:C:O4'	2.13	0.49
28:1:22:ILE:O	28:1:26:VAL:HG23	2.11	0.49
8:G:116:THR:HG22	8:G:151:LEU:HD22	1.94	0.49
1:A:1168:C:H5	40:A:7011:HOH:O	1.96	0.49
27:Z:144:ARG:NH1	40:Z:8571:HOH:O	2.37	0.49
7:F:158:ASN:HB2	7:F:161:ASP:OD2	2.12	0.49
1:A:2353:A:H4'	1:A:2354:A:O5'	2.12	0.49
1:A:2365:G:H4'	19:R:45:PRO:O	2.12	0.49
22:U:78:THR:HB	22:U:87:VAL:O	2.13	0.49
1:A:703:G:O2'	1:A:704:C:H5'	2.13	0.49
20:S:44:VAL:O	20:S:48:GLU:HG3	2.12	0.49
4:C:36:ASP:HA	4:C:83:GLY:HA3	1.95	0.49
7:F:59:GLY:C	7:F:61:PHE:H	2.16	0.49
5:D:84:LEU:HD13	5:D:84:LEU:O	2.12	0.49
1:A:1056:U:H2'	1:A:1057:A:O4'	2.13	0.49
11:J:65:ARG:HB3	40:J:8385:HOH:O	2.12	0.49
25:X:3:ALA:O	25:X:54:PHE:HA	2.13	0.49
30:3:40:ARG:HG3	30:3:45:ASN:CB	2.43	0.49
1:A:875:A:C2	4:C:194:MET:SD	3.06	0.49
1:A:1730:G:H5'	1:A:1731:C:C6	2.48	0.49
21:T:81:ILE:HG12	40:T:8336:HOH:O	2.11	0.49
8:G:126:ILE:HB	8:G:131:LEU:HD23	1.94	0.49
22:U:49:GLU:HB3	22:U:59:GLU:CG	2.43	0.49
16:O:43:VAL:HG11	16:O:81:ALA:HA	1.94	0.49
25:X:1:MET:HB2	25:X:103:GLU:HG2	1.95	0.49
1:A:1735:C:O2'	1:A:1736:A:H5'	2.12	0.49
1:A:1926:G:H2'	1:A:1927:A:C8	2.48	0.49
1:A:1656:A:H2'	1:A:1657:A:O4'	2.13	0.49
6:E:127:ARG:NH1	6:E:127:ARG:HG2	2.28	0.49
15:N:154:ARG:HG3	40:N:8614:HOH:O	2.12	0.49
11:J:75:SER:HB3	11:J:79:ALA:CB	2.43	0.49
1:A:2274:A:H1'	15:N:86:MET:HE1	1.95	0.49
16:O:58:LEU:HD12	16:O:58:LEU:N	2.28	0.49
1:A:514:G:OP1	1:A:514:G:H2'	2.12	0.49
8:G:92:PRO:HB2	40:G:4917:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:4:15:ASN:ND2	40:4:8547:HOH:O	2.46	0.49
20:S:82:GLU:O	20:S:86:LYS:HG3	2.12	0.49
15:N:65:VAL:HG21	15:N:105:ALA:HB2	1.94	0.49
1:A:2073:G:OP2	1:A:2490:A:H5'	2.13	0.49
1:A:377:C:H5	40:A:9819:HOH:O	1.95	0.49
5:D:223:ARG:HG3	5:D:232:TRP:O	2.13	0.49
1:A:920:C:H5''	1:A:921:G:O5'	2.13	0.49
8:G:5:LEU:HD21	8:G:66:GLN:HG3	1.93	0.49
2:B:3064:C:H2'	2:B:3065:A:H5'	1.95	0.49
1:A:1119:G:C8	12:K:52:GLN:NE2	2.81	0.48
25:X:122:ARG:HG2	25:X:152:ALA:O	2.11	0.48
27:Z:106:THR:CG2	27:Z:107:PRO:HD2	2.43	0.48
17:P:38:ARG:NH1	40:P:7674:HOH:O	2.46	0.48
1:A:1003:U:O2	11:J:90:PHE:CZ	2.65	0.48
4:C:39:ALA:O	4:C:61:GLU:HG3	2.13	0.48
2:B:3076:G:C3'	2:B:3077:A:H5''	2.32	0.48
5:D:217:ARG:HG3	5:D:257:THR:CG2	2.42	0.48
16:O:163:PHE:HE1	16:O:171:HIS:HD1	1.61	0.48
20:S:132:ARG:NH1	40:S:8582:HOH:O	2.45	0.48
19:R:11:ARG:HD3	40:R:5620:HOH:O	2.12	0.48
1:A:816:G:C6	1:A:817:G:N1	2.81	0.48
4:C:97:ALA:HB2	4:C:150:PRO:HB2	1.95	0.48
26:Y:43:VAL:CG1	26:Y:44:ASP:N	2.75	0.48
5:D:305:ASP:O	5:D:306:LYS:CB	2.61	0.48
1:A:2361:A:H5''	40:A:8523:HOH:O	2.13	0.48
5:D:268:ARG:NH2	5:D:325:PRO:HG3	2.28	0.48
29:2:25:LYS:HG3	30:3:49:GLU:H	1.76	0.48
14:M:73:VAL:HG23	14:M:74:THR:N	2.28	0.48
1:A:1137:G:H1'	40:A:3388:HOH:O	2.12	0.48
1:A:1699:C:H4'	40:A:5952:HOH:O	2.13	0.48
1:A:1211:G:O2'	1:A:1212:C:H5'	2.13	0.48
25:X:119:HIS:HD2	25:X:120:PRO:O	1.96	0.48
15:N:104:ARG:O	15:N:108:LYS:HG2	2.13	0.48
40:B:7568:HOH:O	16:O:107:ASN:HB3	2.13	0.48
1:A:538:C:H5''	1:A:539:G:C8	2.48	0.48
28:1:56:MET:HA	28:1:62:TYR:O	2.13	0.48
1:A:625:U:H5''	1:A:1044:C:N4	2.28	0.48
20:S:34:GLU:HG2	20:S:46:TYR:OH	2.12	0.48
6:E:133:ARG:HD2	40:E:8409:HOH:O	2.13	0.48
11:J:157:ILE:CG2	11:J:158:ASN:N	2.76	0.48
20:S:104:PHE:HB2	20:S:109:MET:HE1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:A:4595:HOH:O	5:D:216:LYS:HA	2.13	0.48
5:D:168:GLY:H	5:D:174:ARG:HD3	1.79	0.48
1:A:1505:U:C6	1:A:1505:U:H5'	2.44	0.48
1:A:553:G:H5'	40:A:3009:HOH:O	2.13	0.48
5:D:74:ILE:HG13	40:D:8600:HOH:O	2.12	0.48
26:Y:30:MET:HE1	26:Y:55:ASN:HA	1.95	0.48
1:A:2385:G:H2'	1:A:2386:U:C6	2.48	0.48
31:4:87:ARG:HG3	40:4:8573:HOH:O	2.13	0.48
1:A:482:G:H4'	1:A:508:A:N1	2.29	0.48
7:F:81:GLU:O	7:F:85:GLN:HG3	2.13	0.48
4:C:211:LYS:NZ	40:C:8573:HOH:O	2.47	0.48
11:J:13:ALA:HA	11:J:91:HIS:HE1	1.78	0.48
15:N:67:ILE:CD1	15:N:104:ARG:HD2	2.43	0.48
21:T:57:THR:CG2	21:T:58:MET:N	2.77	0.48
7:F:146:LYS:HZ1	16:O:107:ASN:ND2	2.08	0.48
13:L:65:ARG:HD3	40:L:5358:HOH:O	2.14	0.48
15:N:149:TRP:O	15:N:152:ARG:HG2	2.14	0.48
10:I:27:ILE:HD12	10:I:70:ALA:HB1	1.96	0.48
11:J:81:TYR:C	11:J:81:TYR:CD1	2.86	0.48
27:Z:115:ARG:NE	40:Z:8553:HOH:O	2.47	0.48
2:B:3001:U:O3'	2:B:3003:A:H5''	2.14	0.48
30:3:19:SER:HB3	40:3:4479:HOH:O	2.13	0.48
1:A:1139:U:H2'	1:A:1140:C:C6	2.49	0.48
1:A:790:A:H2'	1:A:791:A:O4'	2.14	0.48
7:F:170:TYR:O	7:F:171:ASP:HB3	2.12	0.48
17:P:112:ARG:HA	40:P:1484:HOH:O	2.11	0.48
8:G:32:ARG:O	8:G:33:LEU:HD23	2.12	0.48
9:H:36:THR:HG23	9:H:97:ALA:HB2	1.95	0.48
1:A:1666:C:H2'	1:A:1667:A:C5'	2.43	0.48
4:C:48:ASP:HB3	40:C:8603:HOH:O	2.12	0.48
8:G:31:ARG:NH1	40:G:5919:HOH:O	2.45	0.48
9:H:46:GLU:OE1	9:H:100:ASP:HA	2.14	0.48
7:F:65:GLU:HG3	40:F:6752:HOH:O	2.12	0.48
40:A:6916:HOH:O	22:U:2:LYS:HE2	2.13	0.48
1:A:1384:C:H5'	26:Y:30:MET:HG2	1.96	0.48
1:A:1497:G:H4'	1:A:1627:G:O2'	2.13	0.48
1:A:2090:G:H2'	1:A:2091:G:C8	2.48	0.48
1:A:954:U:O2'	1:A:955:A:H5'	2.13	0.48
40:A:8832:HOH:O	28:1:16:PRO:HG3	2.14	0.48
22:U:1:SER:N	40:U:5837:HOH:O	2.46	0.48
16:O:21:HIS:HB2	40:O:8533:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:147:ARG:HA	11:J:150:LYS:NZ	2.29	0.48
13:L:10:GLN:NE2	13:L:10:GLN:N	2.43	0.48
6:E:16:VAL:HG12	6:E:17:ASP:H	1.79	0.48
5:D:320:GLN:HG3	5:D:321:PRO:HD2	1.95	0.48
1:A:1603:A:H5''	1:A:1605:G:H5'	1.95	0.48
10:I:63:ARG:N	40:I:2569:HOH:O	2.47	0.48
18:Q:10:ALA:HA	18:Q:13:VAL:CG1	2.43	0.48
14:M:53:ARG:NH2	14:M:57:VAL:CG1	2.77	0.48
18:Q:134:VAL:O	18:Q:137:LEU:HB3	2.13	0.48
9:H:47:LEU:HD22	9:H:108:LEU:CD1	2.44	0.48
1:A:1268:C:H2'	1:A:1269:G:H8	1.79	0.48
1:A:2435:U:H1'	40:A:4946:HOH:O	2.14	0.48
19:R:25:PRO:HB2	40:R:4350:HOH:O	2.13	0.48
13:L:58:THR:HG22	13:L:59:LYS:HG3	1.95	0.48
1:A:2821:C:H4'	5:D:116:PRO:HB3	1.95	0.48
7:F:23:VAL:CG2	7:F:23:VAL:O	2.61	0.48
2:B:3042:C:O2	7:F:76:ARG:NH1	2.47	0.48
1:A:2712:G:O2'	1:A:2713:G:H5'	2.14	0.48
6:E:107:ARG:HB3	6:E:107:ARG:NH1	2.29	0.48
31:4:65:THR:HB	31:4:83:TRP:H	1.78	0.48
7:F:57:THR:HG23	7:F:63:ILE:CG2	2.42	0.48
1:A:2064:U:H5'	1:A:2652:U:H4'	1.95	0.48
1:A:120:A:H2'	1:A:120:A:N3	2.29	0.48
1:A:1878:G:O2'	1:A:1879:U:P	2.71	0.48
6:E:150:THR:HA	6:E:203:ALA:O	2.12	0.48
1:A:1423:C:O2'	1:A:1424:A:H5'	2.14	0.48
1:A:1614:G:H2'	40:A:4142:HOH:O	2.12	0.48
2:B:3107:C:H5	40:B:3167:HOH:O	1.97	0.48
1:A:2326:U:H4'	1:A:2412:G:H4'	1.96	0.48
2:B:3056:A:H1'	7:F:14:ARG:HG2	1.96	0.48
16:O:47:LEU:HD12	16:O:92:ALA:CB	2.44	0.48
1:A:1666:C:C2'	1:A:1667:A:C5'	2.92	0.48
1:A:2054:A:H2	20:S:128:ARG:HH22	1.58	0.48
16:O:163:PHE:HA	40:O:8519:HOH:O	2.13	0.48
1:A:2269:C:H2'	1:A:2270:G:H5'	1.94	0.48
16:O:154:LEU:O	16:O:155:GLU:CB	2.62	0.48
1:A:1654:U:H2'	4:C:47:HIS:CD2	2.47	0.48
5:D:248:ARG:O	5:D:251:VAL:HG12	2.13	0.48
29:2:25:LYS:HG2	29:2:25:LYS:O	2.14	0.48
5:D:16:ARG:NH1	40:D:8611:HOH:O	2.46	0.48
1:A:1909:A:N1	1:A:2128:G:H1'	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:G:H5'	1:A:644:G:N3	2.27	0.48
1:A:1015:C:H2'	1:A:1016:U:H6	1.79	0.48
1:A:1023:C:O2'	1:A:1024:G:H5'	2.14	0.48
40:A:6056:HOH:O	28:1:22:ILE:HG13	2.14	0.47
23:V:17:THR:HG22	23:V:18:GLY:N	2.29	0.47
1:A:2896:A:OP1	26:Y:15:ARG:NH1	2.47	0.47
9:H:22:VAL:HG21	9:H:104:ALA:HB2	1.96	0.47
1:A:2274:A:O2'	1:A:2275:G:H5'	2.13	0.47
11:J:130:HIS:CG	11:J:133:ILE:HD11	2.48	0.47
7:F:18:ILE:HG12	7:F:134:LEU:CD2	2.44	0.47
16:O:89:GLY:O	16:O:92:ALA:HB3	2.14	0.47
2:B:3023:U:C5'	2:B:3024:U:OP2	2.57	0.47
6:E:246:ARG:NH1	6:E:246:ARG:HB3	2.28	0.47
7:F:58:VAL:CG1	7:F:59:GLY:N	2.76	0.47
1:A:177:A:H2'	1:A:178:U:O4'	2.14	0.47
1:A:1762:C:H2'	1:A:1763:C:H6	1.79	0.47
11:J:163:PRO:HG2	40:J:8340:HOH:O	2.13	0.47
7:F:159:PRO:O	7:F:163:VAL:HG23	2.14	0.47
15:N:31:TRP:HA	15:N:34:GLU:HG3	1.95	0.47
1:A:2004:U:H2'	1:A:2005:G:OP1	2.14	0.47
1:A:1151:G:OP1	10:I:16:LYS:NZ	2.45	0.47
23:V:33:SER:O	23:V:37:GLU:HG3	2.15	0.47
5:D:132:HIS:CE1	5:D:171:VAL:HG21	2.50	0.47
22:U:101:LEU:HD13	22:U:112:LEU:HD11	1.96	0.47
1:A:1406:A:H4'	1:A:1407:A:H5''	1.96	0.47
19:R:93:ARG:HG3	19:R:93:ARG:HH11	1.79	0.47
1:A:1462:C:H2'	1:A:1463:A:C8	2.50	0.47
8:G:86:VAL:CG1	8:G:129:GLU:HA	2.44	0.47
1:A:1669:A:H2'	1:A:1670:G:C8	2.49	0.47
15:N:114:VAL:HB	15:N:159:THR:HG23	1.96	0.47
20:S:39:THR:CG2	20:S:42:GLU:HG3	2.44	0.47
16:O:73:ALA:N	40:O:8568:HOH:O	2.47	0.47
1:A:1187:U:H2'	40:A:6408:HOH:O	2.13	0.47
8:G:126:ILE:HB	8:G:131:LEU:CD2	2.44	0.47
1:A:1060:C:H6	1:A:1060:C:H5'	1.80	0.47
1:A:2266:A:OP2	15:N:90:ARG:NH2	2.47	0.47
1:A:2281:C:H2'	1:A:2282:U:H5'	1.96	0.47
1:A:154:C:P	15:N:188:ARG:HH12	2.37	0.47
1:A:2649:A:H5'	1:A:2649:A:H8	1.78	0.47
15:N:122:GLU:OE2	15:N:127:LYS:HE2	2.13	0.47
14:M:149:ARG:O	14:M:150:GLN:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:A:H3'	1:A:128:A:C8	2.49	0.47
21:T:6:LYS:HB2	21:T:27:ALA:O	2.14	0.47
1:A:2403:C:H3'	40:A:4729:HOH:O	2.15	0.47
16:O:71:TRP:N	40:O:8539:HOH:O	2.46	0.47
15:N:99:ARG:CD	15:N:167:GLY:HA2	2.45	0.47
1:A:1010:C:H4'	16:O:4:PRO:HB2	1.97	0.47
5:D:41:PHE:HA	5:D:79:MET:HE2	1.95	0.47
1:A:182:G:O3'	15:N:157:LEU:CD1	2.62	0.47
6:E:214:THR:HG23	40:E:8437:HOH:O	2.14	0.47
5:D:207:LYS:HG2	5:D:304:PRO:HB3	1.96	0.47
1:A:656:G:H5'	17:P:3:THR:HG22	1.96	0.47
11:J:35:ASN:HD21	11:J:80:ASN:HA	1.79	0.47
1:A:2730:G:O2'	1:A:2731:G:H5'	2.14	0.47
27:Z:107:PRO:HB3	27:Z:182:PHE:CE2	2.49	0.47
1:A:2443:C:O3'	14:M:56:LYS:HE3	2.15	0.47
5:D:56:ASP:OD1	5:D:322:ARG:HB3	2.13	0.47
12:K:77:GLY:O	12:K:78:ILE:C	2.53	0.47
7:F:41:LEU:CA	7:F:44:ILE:HG22	2.44	0.47
11:J:139:ASP:HB2	40:J:8348:HOH:O	2.15	0.47
4:C:51:ARG:HB2	40:C:8603:HOH:O	2.14	0.47
1:A:2094:G:C4'	5:D:245:SER:HB3	2.41	0.47
4:C:194:MET:CE	4:C:199:HIS:HB2	2.45	0.47
12:K:19:MET:HE2	12:K:79:PHE:HA	1.97	0.47
7:F:65:GLU:HA	40:F:6752:HOH:O	2.13	0.47
1:A:1123:A:C2	1:A:1129:C:H4'	2.49	0.47
19:R:32:GLU:HA	19:R:71:TYR:OH	2.15	0.47
19:R:93:ARG:HG3	19:R:93:ARG:NH1	2.30	0.47
1:A:794:U:H3	1:A:819:A:H61	1.63	0.47
26:Y:21:PRO:HG2	26:Y:24:LYS:HD3	1.95	0.47
1:A:797:A:O4'	28:1:10:ARG:N	2.48	0.47
11:J:14:TYR:N	11:J:91:HIS:HE1	2.12	0.47
7:F:154:LYS:H	7:F:154:LYS:CD	2.15	0.47
20:S:39:THR:CB	20:S:42:GLU:HG3	2.45	0.47
4:C:51:ARG:NH2	4:C:69:LEU:HD13	2.29	0.47
16:O:73:ALA:HB1	16:O:74:PRO:CD	2.45	0.47
11:J:127:GLY:O	11:J:128:ALA:CB	2.63	0.47
14:M:72:ASN:O	14:M:76:LEU:HG	2.14	0.47
27:Z:154:ARG:NH1	27:Z:155:ARG:HG3	2.30	0.47
16:O:139:TRP:HA	16:O:139:TRP:HE3	1.80	0.47
13:L:28:GLU:OE2	13:L:58:THR:HG21	2.14	0.47
1:A:1015:C:H2'	1:A:1016:U:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3051:A:H5'	16:O:160:SER:HB3	1.97	0.47
31:4:69:TYR:HB2	31:4:78:HIS:CE1	2.50	0.47
1:A:669:G:O2'	1:A:670:G:H5'	2.15	0.47
4:C:217:ARG:HH11	4:C:217:ARG:CG	2.28	0.47
2:B:3031:C:H2'	2:B:3032:G:O4'	2.15	0.47
8:G:107:PHE:CE2	8:G:108:LEU:HD13	2.50	0.47
11:J:85:ILE:HB	11:J:132:PHE:HE2	1.80	0.47
11:J:150:LYS:HA	11:J:153:VAL:HG22	1.96	0.47
11:J:26:LYS:HA	11:J:58:HIS:CD2	2.49	0.47
27:Z:187:VAL:HB	40:Z:8565:HOH:O	2.14	0.47
18:Q:13:VAL:HG13	18:Q:14:LEU:N	2.30	0.47
1:A:424:C:H2'	1:A:425:U:C6	2.50	0.47
4:C:70:ALA:HA	4:C:71:PRO:HD3	1.76	0.47
6:E:61:PHE:HB3	40:E:8446:HOH:O	2.14	0.47
1:A:2842:G:H2'	1:A:2843:A:H5'	1.96	0.47
17:P:77:ALA:HB1	17:P:98:LEU:HD12	1.97	0.47
14:M:101:ASP:C	14:M:103:ALA:H	2.18	0.47
11:J:31:PHE:HD2	11:J:85:ILE:O	1.97	0.47
1:A:797:A:H4'	28:1:10:ARG:N	2.28	0.47
40:A:6970:HOH:O	6:E:188:ARG:HD3	2.15	0.47
6:E:234:VAL:O	6:E:234:VAL:HG22	2.15	0.47
22:U:75:GLU:O	22:U:76:ASP:HB2	2.13	0.47
1:A:2563:U:H2'	1:A:2565:C:O5'	2.14	0.47
9:H:26:THR:HB	9:H:102:GLY:HA3	1.97	0.47
17:P:96:VAL:HG13	17:P:100:GLN:HB2	1.97	0.47
22:U:38:ARG:HG3	22:U:38:ARG:HH11	1.79	0.47
4:C:95:PRO:HA	4:C:153:ARG:HA	1.97	0.47
26:Y:41:PHE:O	26:Y:43:VAL:HG23	2.14	0.47
1:A:2472:C:O2'	1:A:2634:G:H4'	2.14	0.47
1:A:1331:A:OP2	27:Z:142:SER:OG	2.31	0.47
1:A:1192:A:H3'	1:A:1193:A:H5'	1.96	0.46
18:Q:59:ARG:HH22	18:Q:66:GLN:HE22	1.59	0.46
6:E:246:ARG:CZ	40:E:8423:HOH:O	2.63	0.46
1:A:816:G:H5'	1:A:1598:A:H4'	1.96	0.46
1:A:1864:C:OP1	15:N:75:THR:HG23	2.16	0.46
11:J:147:ARG:HA	11:J:150:LYS:HZ2	1.79	0.46
1:A:2812:A:C2	1:A:2814:A:N6	2.72	0.46
1:A:2768:A:H3'	40:A:3940:HOH:O	2.15	0.46
9:H:110:GLU:O	9:H:114:LYS:HG3	2.14	0.46
1:A:1730:G:C5'	1:A:1731:C:H6	2.27	0.46
21:T:51:GLN:HE21	21:T:53:ASN:ND2	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2724:U:H2'	1:A:2725:G:O4'	2.15	0.46
1:A:1418:U:OP1	30:3:42:TRP:HB3	2.15	0.46
1:A:629:A:H2'	1:A:630:A:O4'	2.15	0.46
27:Z:178:HIS:CG	27:Z:179:PRO:HD2	2.51	0.46
26:Y:37:LEU:HD21	26:Y:72:VAL:HG11	1.98	0.46
15:N:115:LEU:HD13	15:N:116:ASN:HB2	1.98	0.46
5:D:7:ARG:NH1	5:D:7:ARG:HG2	2.26	0.46
26:Y:30:MET:CE	26:Y:58:ALA:HB3	2.46	0.46
22:U:49:GLU:OE2	22:U:97:ARG:NH1	2.40	0.46
2:B:3088:G:OP1	25:X:130:HIS:NE2	2.45	0.46
1:A:1789:G:O6	18:Q:73:HIS:HE1	1.98	0.46
1:A:1503:U:H2'	1:A:1504:A:O4'	2.16	0.46
11:J:109:ASP:HB2	40:J:8347:HOH:O	2.15	0.46
1:A:2464:C:H5''	1:A:2465:A:OP1	2.15	0.46
1:A:2720:C:O2	13:L:87:ARG:NH2	2.49	0.46
7:F:19:GLU:O	7:F:133:ASN:HB3	2.15	0.46
1:A:2769:C:H2'	1:A:2770:G:C5'	2.45	0.46
2:B:3092:G:C6	2:B:3093:A:C6	3.04	0.46
11:J:71:TYR:C	11:J:73:GLN:N	2.67	0.46
1:A:1235:G:C1'	12:K:63:ILE:HG23	2.45	0.46
1:A:544:G:H2'	1:A:545:G:C5'	2.40	0.46
8:G:11:VAL:HG13	8:G:23:GLU:O	2.14	0.46
24:W:57:LYS:HA	24:W:60:GLN:HE21	1.80	0.46
23:V:49:LEU:HD11	40:V:3805:HOH:O	2.16	0.46
16:O:93:GLN:HG2	40:O:8559:HOH:O	2.15	0.46
1:A:1862:C:H1'	40:A:6727:HOH:O	2.15	0.46
1:A:1555:G:H4'	1:A:1630:A:H2	1.81	0.46
28:1:58:GLY:CA	40:1:8437:HOH:O	2.45	0.46
1:A:2072:G:C6	1:A:2533:C:H1'	2.51	0.46
7:F:86:THR:C	7:F:89:PRO:HD2	2.35	0.46
30:3:18:ASN:ND2	30:3:40:ARG:H	2.14	0.46
15:N:78:ASN:C	15:N:79:LYS:HG2	2.36	0.46
28:1:42:CYS:SG	28:1:43:GLY:N	2.89	0.46
14:M:54:PRO:HG2	14:M:57:VAL:CG2	2.46	0.46
1:A:581:G:H5'	40:A:7202:HOH:O	2.16	0.46
13:L:98:VAL:HG13	13:L:99:ASP:N	2.30	0.46
5:D:75:GLU:C	5:D:77:PRO:HD3	2.36	0.46
24:W:11:MET:HB3	24:W:15:GLU:HB2	1.97	0.46
1:A:1666:C:C2'	1:A:1667:A:H5''	2.45	0.46
2:B:3078:G:N2	2:B:3103:A:OP2	2.45	0.46
15:N:87:MET:HE2	40:N:8593:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:119:VAL:CG1	20:S:119:VAL:O	2.63	0.46
16:O:184:ILE:HG22	16:O:185:GLU:HG3	1.96	0.46
9:H:48:VAL:HG23	9:H:74:PHE:CB	2.46	0.46
18:Q:14:LEU:HD13	18:Q:51:ALA:HB2	1.97	0.46
8:G:95:VAL:O	8:G:126:ILE:HD13	2.15	0.46
20:S:114:VAL:O	20:S:114:VAL:HG13	2.15	0.46
40:C:8610:HOH:O	28:1:75:ALA:HB3	2.16	0.46
26:Y:26:ALA:HB1	26:Y:59:TRP:CE2	2.50	0.46
1:A:2338:G:H2'	7:F:129:ASP:OD1	2.15	0.46
1:A:1667:A:H2'	1:A:1668:U:H6	1.80	0.46
14:M:130:ARG:HA	40:M:8558:HOH:O	2.15	0.46
1:A:283:U:H5	1:A:284:C:N4	2.14	0.46
9:H:91:VAL:CG1	9:H:92:GLY:N	2.76	0.46
12:K:93:ARG:HB3	12:K:93:ARG:NH1	2.30	0.46
1:A:130:C:H5'	40:A:4731:HOH:O	2.14	0.46
8:G:101:GLU:OE2	8:G:115:ARG:NH1	2.48	0.46
19:R:32:GLU:O	19:R:93:ARG:NH2	2.49	0.46
9:H:48:VAL:CG2	9:H:74:PHE:HB3	2.45	0.46
6:E:20:ASP:O	6:E:23:GLU:HB2	2.15	0.46
21:T:10:VAL:HG11	24:W:36:ALA:HA	1.98	0.46
5:D:119:HIS:O	5:D:121:PRO:HD3	2.16	0.46
1:A:1919:A:H4'	40:A:4363:HOH:O	2.16	0.46
1:A:2597:U:H2'	1:A:2598:U:H5'	1.98	0.46
20:S:68:HIS:CG	20:S:76:ASP:HB2	2.51	0.46
28:1:57:CYS:SG	28:1:59:HIS:HB3	2.55	0.46
28:1:29:VAL:O	28:1:33:HIS:HB2	2.15	0.46
27:Z:144:ARG:NH2	40:Z:8608:HOH:O	2.48	0.46
1:A:1506:U:H6	1:A:1506:U:H5'	1.80	0.46
23:V:39:ASN:ND2	23:V:44:ARG:HH11	2.14	0.46
1:A:764:C:H2'	1:A:765:G:O4'	2.16	0.46
22:U:80:GLU:OE2	22:U:84:GLY:HA2	2.16	0.46
1:A:1687:C:O2	29:2:9:GLY:HA2	2.16	0.46
1:A:1682:A:H5''	40:A:8964:HOH:O	2.15	0.46
1:A:37:A:H2'	1:A:38:G:C8	2.51	0.46
1:A:2506:A:H1'	40:A:5568:HOH:O	2.16	0.45
5:D:41:PHE:CE1	5:D:79:MET:HG3	2.50	0.45
4:C:199:HIS:HD2	4:C:201:PHE:HB2	1.80	0.45
18:Q:131:PHE:CE1	18:Q:137:LEU:HD13	2.51	0.45
1:A:170:U:H2'	1:A:171:C:H5'	1.98	0.45
5:D:301:VAL:HG13	5:D:302:PRO:HD2	1.97	0.45
40:A:9048:HOH:O	18:Q:81:LYS:HG2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:A:C2	1:A:378:A:H4'	2.51	0.45
1:A:834:G:H3'	1:A:835:U:H4'	1.98	0.45
5:D:241:PRO:HD2	40:D:8650:HOH:O	2.15	0.45
1:A:2780:C:H2'	1:A:2781:U:C6	2.51	0.45
7:F:86:THR:HG23	40:F:7477:HOH:O	2.16	0.45
9:H:28:ALA:HB3	9:H:99:THR:O	2.15	0.45
17:P:32:ARG:HE	17:P:35:LYS:HD2	1.81	0.45
1:A:736:A:H2'	1:A:737:A:O4'	2.16	0.45
20:S:25:PHE:CE2	20:S:29:LYS:CE	3.00	0.45
26:Y:70:ILE:O	26:Y:70:ILE:HG23	2.16	0.45
1:A:2078:U:O2'	1:A:2079:G:H5'	2.16	0.45
11:J:112:ARG:O	11:J:113:ALA:C	2.54	0.45
5:D:152:PRO:HD2	40:D:8626:HOH:O	2.16	0.45
1:A:2507:G:H2'	1:A:2510:C:H42	1.81	0.45
25:X:122:ARG:HH22	25:X:154:ARG:C	2.20	0.45
30:3:40:ARG:HA	30:3:45:ASN:HD22	1.79	0.45
5:D:304:PRO:HD2	5:D:307:ARG:HD2	1.98	0.45
16:O:61:ALA:CB	16:O:88:ALA:HB2	2.47	0.45
36:5:9080:SPS:O1	36:5:9080:SPS:H91	2.16	0.45
4:C:8:ARG:NH1	40:C:8552:HOH:O	2.48	0.45
1:A:184:G:H5''	15:N:153:THR:HG22	1.98	0.45
15:N:153:THR:O	15:N:156:ARG:HG3	2.16	0.45
1:A:1783:A:O2'	1:A:1784:U:H5'	2.16	0.45
5:D:129:ARG:NH2	5:D:176:ASP:OD1	2.47	0.45
31:4:6:ARG:NE	40:4:8524:HOH:O	2.48	0.45
1:A:51:G:O2'	1:A:52:A:H5'	2.16	0.45
1:A:1119:G:N2	1:A:1246:A:H2	2.09	0.45
4:C:34:ASP:OD1	4:C:35:GLY:N	2.46	0.45
5:D:7:ARG:HD3	5:D:9:GLY:O	2.16	0.45
1:A:566:A:H2'	1:A:567:U:O4'	2.16	0.45
26:Y:9:VAL:HG13	26:Y:88:GLU:OE1	2.16	0.45
4:C:55:VAL:HG13	4:C:67:LEU:HD22	1.98	0.45
4:C:194:MET:HE1	4:C:199:HIS:HB2	1.98	0.45
1:A:1819:G:H2'	1:A:1820:G:C4'	2.47	0.45
6:E:39:GLN:O	6:E:43:LYS:HD3	2.17	0.45
18:Q:16:VAL:CG1	18:Q:17:GLY:N	2.79	0.45
1:A:2831:C:H2'	1:A:2832:C:H5'	1.99	0.45
1:A:2649:A:C8	1:A:2649:A:H5'	2.52	0.45
1:A:249:G:O2'	1:A:250:C:H5'	2.16	0.45
1:A:2243:C:H5''	40:A:3263:HOH:O	2.16	0.45
1:A:1352:A:N1	6:E:48:SER:HB3	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:51:GLU:O	12:K:55:GLU:HG3	2.16	0.45
1:A:558:C:H5'	40:A:4774:HOH:O	2.16	0.45
25:X:122:ARG:CG	25:X:152:ALA:O	2.64	0.45
25:X:13:MET:HE3	25:X:17:ILE:CG2	2.44	0.45
7:F:94:ALA:HB3	7:F:174:VAL:CA	2.47	0.45
5:D:24:PRO:HG2	5:D:204:GLY:HA2	1.97	0.45
28:1:56:MET:HE2	28:1:63:LYS:HG3	1.99	0.45
14:M:73:VAL:HG23	14:M:74:THR:H	1.81	0.45
28:1:13:ARG:NH1	28:1:14:PHE:CE2	2.85	0.45
1:A:1028:U:H1'	40:A:3159:HOH:O	2.17	0.45
5:D:81:ALA:O	5:D:186:GLY:HA3	2.17	0.45
14:M:90:ARG:NH2	14:M:121:ILE:HD11	2.31	0.45
6:E:34:ALA:HB3	6:E:220:THR:HG21	1.99	0.45
1:A:1562:C:H42	1:A:2738:G:H1	1.64	0.45
1:A:56:G:H5''	24:W:50:ARG:NH1	2.32	0.45
1:A:2791:U:H1'	1:A:2792:A:H5''	1.99	0.45
11:J:132:PHE:O	11:J:133:ILE:HD13	2.17	0.45
40:A:3203:HOH:O	8:G:143:GLN:HG2	2.17	0.45
5:D:7:ARG:NH1	5:D:11:LEU:HD22	2.31	0.45
16:O:163:PHE:O	16:O:164:ASP:O	2.34	0.45
10:I:67:LEU:O	10:I:71:LEU:HG	2.16	0.45
40:L:7438:HOH:O	23:V:20:MET:HE1	2.17	0.45
2:B:3092:G:H22	11:J:52:LYS:NZ	2.15	0.45
1:A:2265:U:H2'	1:A:2266:A:H8	1.81	0.45
18:Q:16:VAL:CG1	18:Q:20:ARG:HB2	2.47	0.45
25:X:125:HIS:HD2	25:X:127:GLY:H	1.64	0.45
4:C:179:MET:HG2	4:C:186:TRP:CB	2.47	0.45
27:Z:122:ARG:NH2	40:Z:8535:HOH:O	2.48	0.45
1:A:321:A:H1'	40:A:6543:HOH:O	2.17	0.45
9:H:41:GLU:OE2	15:N:2:ARG:HB2	2.16	0.45
11:J:157:ILE:HG22	11:J:158:ASN:N	2.31	0.45
15:N:52:LEU:HD13	15:N:116:ASN:CB	2.46	0.45
4:C:99:ILE:O	4:C:131:HIS:CE1	2.70	0.45
1:A:951:A:H2'	1:A:952:G:H5'	1.97	0.45
1:A:20:G:H1'	20:S:5:SER:HB3	1.98	0.45
1:A:795:G:N3	1:A:817:G:C2	2.85	0.45
29:2:25:LYS:HD2	30:3:48:ASP:HA	1.97	0.45
5:D:202:VAL:HG11	5:D:301:VAL:HG13	1.99	0.45
1:A:2372:A:H2'	1:A:2373:U:C6	2.52	0.45
1:A:2478:U:O2'	1:A:2479:A:H5'	2.17	0.45
1:A:2904:U:H4'	26:Y:8:ARG:NH1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:8:ARG:NH1	40:Y:2479:HOH:O	2.50	0.45
7:F:99:ASP:HB2	7:F:103:ASN:CB	2.46	0.45
1:A:1205:U:H2'	1:A:1206:U:C5'	2.47	0.45
1:A:2005:G:OP2	1:A:2005:G:H3'	2.17	0.45
6:E:107:ARG:O	6:E:111:VAL:HG23	2.17	0.45
4:C:81:GLN:HB2	4:C:92:ASN:HD22	1.80	0.45
1:A:2421:G:H3'	1:A:2422:U:H5''	1.98	0.45
5:D:55:ASN:HB3	5:D:64:GLY:H	1.82	0.45
15:N:87:MET:HG3	15:N:87:MET:H	1.26	0.45
14:M:53:ARG:HH22	14:M:57:VAL:HG12	1.78	0.45
25:X:38:THR:HB	40:X:5390:HOH:O	2.16	0.45
1:A:2274:A:H1'	15:N:86:MET:SD	2.57	0.45
4:C:179:MET:HG2	4:C:186:TRP:CG	2.51	0.45
6:E:123:LEU:HA	6:E:123:LEU:HD23	1.85	0.45
1:A:168:C:O2'	1:A:169:A:H5'	2.17	0.45
21:T:37:VAL:O	21:T:41:VAL:HG23	2.16	0.45
26:Y:37:LEU:CD1	26:Y:85:VAL:HG21	2.24	0.45
16:O:34:LEU:HA	16:O:47:LEU:HD23	1.99	0.45
1:A:1191:A:C3'	1:A:1192:A:H5''	2.43	0.45
15:N:138:HIS:C	15:N:139:PRO:O	2.48	0.45
1:A:338:C:H4'	6:E:174:ILE:HD11	1.98	0.45
7:F:91:ALA:HB1	40:F:5198:HOH:O	2.17	0.45
29:2:21:ARG:HD2	29:2:39:PHE:HB2	1.98	0.45
9:H:117:GLU:C	9:H:119:ARG:H	2.20	0.45
8:G:145:ALA:HB1	8:G:168:ILE:HD11	1.99	0.45
2:B:3064:C:C2'	2:B:3065:A:H5'	2.47	0.45
31:4:87:ARG:NH1	40:4:8525:HOH:O	2.49	0.45
1:A:1565:C:O4'	1:A:2738:G:H1'	2.17	0.45
10:I:69:ARG:NH1	40:I:3513:HOH:O	2.50	0.45
1:A:613:C:H2'	1:A:614:U:H6	1.82	0.45
9:H:56:PRO:CG	15:N:44:THR:HA	2.46	0.45
6:E:19:PRO:HG2	6:E:22:PHE:CD1	2.52	0.45
31:4:73:GLU:HB2	40:4:8527:HOH:O	2.16	0.44
28:1:30:GLU:HB3	28:1:34:LYS:HE3	1.99	0.44
28:1:31:ILE:HG23	28:1:32:LYS:N	2.32	0.44
1:A:2456:A:H2'	1:A:2457:U:C6	2.52	0.44
20:S:29:LYS:HD3	40:S:8530:HOH:O	2.18	0.44
27:Z:154:ARG:HH12	27:Z:155:ARG:HG3	1.82	0.44
15:N:81:ARG:HG3	15:N:85:ARG:HB2	1.99	0.44
14:M:92:ASP:OD1	14:M:94:ARG:HB2	2.17	0.44
1:A:440:C:H2'	1:A:441:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:66:LYS:HB2	19:R:70:ALA:O	2.17	0.44
6:E:236:THR:HG22	6:E:239:ALA:CB	2.47	0.44
6:E:5:ILE:CD1	6:E:16:VAL:HG23	2.35	0.44
1:A:797:A:H5'	28:1:10:ARG:HG2	1.99	0.44
1:A:1634:G:H2'	1:A:1635:U:C6	2.52	0.44
12:K:39:VAL:CG1	12:K:107:ASN:HB2	2.47	0.44
22:U:38:ARG:NH1	22:U:38:ARG:HG3	2.31	0.44
30:3:40:ARG:HD2	30:3:47:THR:HG22	1.99	0.44
1:A:1641:A:H2'	1:A:1642:A:C5'	2.46	0.44
1:A:88:G:N7	30:3:28:LYS:HD2	2.31	0.44
7:F:10:PHE:CE1	7:F:11:HIS:HB3	2.52	0.44
11:J:112:ARG:HB3	40:J:8395:HOH:O	2.17	0.44
14:M:77:ALA:HB3	40:M:8530:HOH:O	2.16	0.44
1:A:517:U:H1'	40:A:7095:HOH:O	2.17	0.44
1:A:716:G:C2'	1:A:717:C:O5'	2.65	0.44
25:X:34:LEU:CD1	25:X:100:LEU:HD13	2.47	0.44
4:C:192:VAL:CG1	4:C:192:VAL:O	2.65	0.44
29:2:8:GLN:NE2	29:2:11:LYS:NZ	2.60	0.44
4:C:69:LEU:CD2	4:C:120:ARG:HB3	2.43	0.44
9:H:28:ALA:CB	9:H:99:THR:HG23	2.47	0.44
1:A:1269:G:H2'	1:A:1270:U:C6	2.53	0.44
1:A:2326:U:H4'	1:A:2412:G:C4'	2.47	0.44
1:A:1681:G:H5''	1:A:1682:A:H5'	1.99	0.44
5:D:127:GLN:HG3	40:D:8636:HOH:O	2.16	0.44
13:L:78:LYS:HA	13:L:79:PRO:HD3	1.87	0.44
1:A:960:G:N3	1:A:960:G:C2'	2.80	0.44
1:A:1592:G:HO2'	1:A:1593:C:C5'	2.30	0.44
15:N:108:LYS:HE3	40:N:8615:HOH:O	2.17	0.44
31:4:70:ARG:NH1	40:4:8539:HOH:O	2.46	0.44
27:Z:189:ASN:CA	27:Z:217:ILE:HD11	2.46	0.44
14:M:67:ARG:HB2	14:M:112:GLY:HA3	1.99	0.44
1:A:2415:A:N3	16:O:26:LEU:HD13	2.32	0.44
1:A:2748:G:H5'	40:A:7058:HOH:O	2.18	0.44
26:Y:76:ARG:HG3	26:Y:76:ARG:NH1	2.31	0.44
2:B:3003:A:H2	2:B:3021:G:N3	2.15	0.44
14:M:125:PHE:CE1	14:M:140:VAL:HG13	2.53	0.44
12:K:75:PRO:HG2	12:K:105:LEU:CD2	2.47	0.44
40:A:5137:HOH:O	18:Q:55:LYS:HA	2.17	0.44
1:A:2104:C:O2	1:A:2485:A:N1	2.51	0.44
20:S:47:LEU:O	20:S:51:ILE:HG13	2.18	0.44
6:E:27:ARG:HG2	6:E:30:LEU:HG	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:189:ASN:ND2	27:Z:189:ASN:C	2.70	0.44
1:A:1450:C:O2'	1:A:1494:A:H5'	2.17	0.44
22:U:45:GLY:C	40:U:3851:HOH:O	2.55	0.44
15:N:78:ASN:O	15:N:79:LYS:HG2	2.18	0.44
23:V:20:MET:CG	23:V:28:THR:HG23	2.48	0.44
16:O:42:HIS:CG	16:O:62:HIS:HE1	2.35	0.44
7:F:56:ARG:N	40:F:6752:HOH:O	2.51	0.44
5:D:175:LEU:HD23	5:D:175:LEU:O	2.17	0.44
7:F:59:GLY:O	7:F:61:PHE:N	2.39	0.44
22:U:73:HIS:CD2	22:U:88:PRO:CG	3.00	0.44
14:M:121:ILE:HG12	14:M:141:GLU:HB2	1.99	0.44
1:A:716:G:H2'	1:A:717:C:O5'	2.18	0.44
27:Z:126:PRO:HG2	27:Z:128:PHE:CE1	2.53	0.44
1:A:1921:A:C6	1:A:1922:A:C2	3.05	0.44
13:L:72:VAL:HG11	13:L:121:PHE:CD1	2.52	0.44
11:J:56:ILE:HG21	11:J:61:LEU:HD13	2.00	0.44
12:K:74:ARG:NH1	12:K:76:ASP:HB2	2.33	0.44
15:N:37:VAL:HG21	15:N:108:LYS:CG	2.48	0.44
4:C:33:GLU:CD	4:C:33:GLU:H	2.21	0.44
6:E:214:THR:HB	40:E:8326:HOH:O	2.18	0.44
17:P:35:LYS:HD3	40:P:3360:HOH:O	2.17	0.44
8:G:84:MET:HE3	8:G:148:ILE:HG21	1.99	0.44
9:H:21:GLU:O	9:H:24:ARG:CG	2.66	0.44
1:A:2252:A:C5	1:A:2253:G:H1'	2.52	0.44
1:A:441:A:H1'	1:A:442:A:N7	2.32	0.44
1:A:333:G:O2'	1:A:334:G:H5'	2.18	0.44
14:M:12:THR:HG21	14:M:16:GLY:O	2.17	0.44
1:A:278:A:H2'	1:A:279:C:O4'	2.18	0.44
25:X:122:ARG:NH2	40:X:4276:HOH:O	2.44	0.44
4:C:170:VAL:HG13	28:1:22:ILE:CG2	2.46	0.44
5:D:168:GLY:O	5:D:169:GLY:O	2.36	0.44
4:C:81:GLN:CB	4:C:92:ASN:ND2	2.80	0.44
23:V:44:ARG:HB3	40:V:3805:HOH:O	2.18	0.44
1:A:587:A:H5''	40:A:6797:HOH:O	2.17	0.44
1:A:1966:U:H2'	1:A:1967:U:C6	2.52	0.44
14:M:89:PHE:N	40:M:8572:HOH:O	2.50	0.44
25:X:107:LEU:O	25:X:112:LEU:HB2	2.17	0.44
27:Z:109:LEU:HA	40:Z:8566:HOH:O	2.18	0.44
1:A:1021:G:O2'	1:A:1022:A:H5'	2.18	0.44
11:J:163:PRO:O	11:J:164:ALA:HB2	2.18	0.44
16:O:37:ARG:NH2	40:O:8534:HOH:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:67:ALA:HA	16:O:71:TRP:H	1.82	0.44
11:J:55:GLN:HE21	11:J:124:ARG:NE	2.01	0.44
40:A:3265:HOH:O	15:N:108:LYS:HD2	2.18	0.44
28:1:34:LYS:HE2	40:1:8425:HOH:O	2.17	0.44
9:H:22:VAL:CG2	9:H:104:ALA:HB2	2.47	0.44
12:K:75:PRO:HD3	12:K:136:SER:OG	2.17	0.44
1:A:2385:G:H2'	1:A:2386:U:H6	1.83	0.44
1:A:581:G:O2'	1:A:582:C:H5'	2.17	0.44
17:P:81:PHE:N	17:P:81:PHE:CD1	2.85	0.44
1:A:303:C:H2'	1:A:304:G:O4'	2.18	0.44
1:A:2767:C:OP1	5:D:318:ASN:ND2	2.51	0.44
22:U:3:GLN:HA	22:U:4:PRO:HD3	1.85	0.44
13:L:132:VAL:C	40:L:3160:HOH:O	2.55	0.44
2:B:3022:G:N7	2:B:3055:U:O2'	2.35	0.44
1:A:2506:A:C1'	40:A:5568:HOH:O	2.66	0.44
13:L:109:LEU:HD13	13:L:113:ILE:HD11	2.00	0.44
5:D:63:GLU:HG3	5:D:63:GLU:O	2.17	0.44
2:B:3008:G:O6	16:O:11:ARG:NH1	2.51	0.44
1:A:475:G:H5'	6:E:73:LEU:HD23	2.00	0.44
5:D:232:TRP:CD1	5:D:235:ARG:HD2	2.52	0.44
19:R:25:PRO:HA	19:R:26:PRO:HD3	1.86	0.44
1:A:1902:G:H2'	1:A:1903:U:O4'	2.18	0.44
1:A:638:C:H2'	1:A:639:A:C8	2.53	0.44
20:S:4:TYR:N	40:S:8546:HOH:O	2.51	0.44
22:U:50:VAL:HG12	22:U:56:ALA:HA	2.00	0.44
1:A:1592:G:O2'	1:A:1593:C:O5'	2.31	0.43
5:D:312:ARG:HD3	5:D:315:VAL:HG13	1.99	0.43
1:A:262:A:OP2	9:H:91:VAL:HG11	2.18	0.43
1:A:2415:A:C2	16:O:25:ARG:HB3	2.53	0.43
1:A:603:A:H4'	1:A:604:G:O5'	2.18	0.43
8:G:84:MET:HB2	8:G:131:LEU:HB2	2.00	0.43
24:W:23:LEU:HD12	24:W:56:ILE:HD12	2.00	0.43
1:A:1249:U:H2'	1:A:1250:C:C6	2.53	0.43
5:D:279:THR:CG2	5:D:280:VAL:N	2.80	0.43
12:K:63:ILE:HG22	12:K:64:GLY:N	2.31	0.43
5:D:177:HIS:O	5:D:181:ILE:HG13	2.17	0.43
1:A:2015:A:H2'	1:A:2016:U:O4'	2.18	0.43
8:G:34:TRP:O	12:K:127:ILE:HD11	2.18	0.43
12:K:17:CYS:HA	12:K:119:THR:O	2.18	0.43
9:H:34:ASN:HA	15:N:4:ALA:HB2	2.00	0.43
1:A:941:G:O2'	1:A:942:U:H5'	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:83:PHE:HE1	11:J:146:TRP:CZ2	2.36	0.43
1:A:1752:G:H2'	40:A:7066:HOH:O	2.19	0.43
15:N:95:LYS:HG2	15:N:99:ARG:HB3	2.00	0.43
6:E:77:ALA:O	6:E:78:ARG:HG3	2.18	0.43
28:1:25:ARG:O	28:1:29:VAL:HG23	2.19	0.43
5:D:51:VAL:HG21	5:D:327:VAL:HG13	1.99	0.43
13:L:22:ASP:OD1	13:L:22:ASP:C	2.57	0.43
1:A:1730:G:H5'	1:A:1731:C:H5	1.81	0.43
12:K:80:LYS:HE2	12:K:98:PHE:CZ	2.53	0.43
40:A:8971:HOH:O	20:S:83:LYS:HD3	2.18	0.43
18:Q:7:LYS:HD2	18:Q:21:VAL:CG2	2.46	0.43
11:J:1:LYS:N	40:J:8371:HOH:O	2.51	0.43
24:W:5:VAL:CG1	24:W:9:ARG:NH1	2.81	0.43
1:A:2324:G:N2	1:A:2377:U:H1'	2.33	0.43
1:A:270:U:H1'	40:A:3234:HOH:O	2.17	0.43
22:U:37:GLN:OE1	22:U:118:SER:HA	2.17	0.43
1:A:156:C:H5''	15:N:171:ARG:CD	2.26	0.43
1:A:1182:C:H1'	1:A:1192:A:C8	2.50	0.43
7:F:23:VAL:HG12	7:F:130:VAL:HG22	2.00	0.43
5:D:60:SER:C	5:D:62:ARG:H	2.20	0.43
15:N:38:VAL:O	15:N:38:VAL:HG12	2.17	0.43
8:G:133:VAL:HG12	8:G:141:VAL:HG13	2.00	0.43
31:4:74:CYS:N	40:4:8561:HOH:O	2.51	0.43
16:O:161:GLY:O	16:O:162:ASP:C	2.56	0.43
5:D:87:TYR:OH	5:D:163:GLU:OE2	2.25	0.43
14:M:54:PRO:HG2	14:M:57:VAL:HG21	1.99	0.43
1:A:695:C:H2'	1:A:696:C:C6	2.53	0.43
14:M:80:ASP:HB2	14:M:90:ARG:O	2.18	0.43
6:E:154:VAL:O	6:E:158:GLU:HG3	2.18	0.43
1:A:1523:G:H2'	1:A:1524:U:C6	2.53	0.43
5:D:80:ARG:HD3	40:D:8601:HOH:O	2.18	0.43
8:G:83:GLY:O	8:G:169:THR:N	2.39	0.43
2:B:3060:C:O2'	2:B:3061:C:H5'	2.17	0.43
1:A:1857:A:N6	1:A:2247:C:H1'	2.33	0.43
6:E:140:VAL:CG1	6:E:141:SER:N	2.82	0.43
11:J:86:ARG:HD3	11:J:130:HIS:HD2	1.83	0.43
25:X:21:LEU:CD2	25:X:48:VAL:HG11	2.47	0.43
25:X:4:LEU:HD23	25:X:4:LEU:HA	1.84	0.43
1:A:289:G:O2'	1:A:290:C:H5'	2.18	0.43
5:D:7:ARG:CD	5:D:9:GLY:O	2.66	0.43
1:A:1158:G:O2'	1:A:1159:G:H5'	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:154:VAL:HA	5:D:155:PRO:HD3	1.84	0.43
1:A:795:G:H1'	1:A:817:G:N2	2.33	0.43
7:F:144:ARG:NH2	40:F:3839:HOH:O	2.45	0.43
23:V:6:CYS:C	23:V:8:TYR:H	2.20	0.43
6:E:7:ASP:OD1	6:E:11:ASN:O	2.36	0.43
1:A:1375:A:C2'	1:A:1376:G:H5'	2.48	0.43
24:W:12:THR:HG23	24:W:14:ALA:H	1.83	0.43
16:O:37:ARG:CZ	40:O:8534:HOH:O	2.66	0.43
7:F:67:ASP:OD2	7:F:69:ILE:HD11	2.19	0.43
6:E:1:MET:HG2	6:E:2:GLN:NE2	2.33	0.43
4:C:35:GLY:O	4:C:36:ASP:CB	2.60	0.43
4:C:130:THR:HG22	4:C:131:HIS:O	2.17	0.43
1:A:67:A:H5''	1:A:69:A:C8	2.53	0.43
1:A:1470:A:OP1	15:N:93:ARG:HD2	2.18	0.43
16:O:24:LEU:HD13	19:R:26:PRO:HB3	2.00	0.43
13:L:28:GLU:HB3	13:L:59:LYS:HB2	2.00	0.43
1:A:128:A:O2'	1:A:129:A:H5'	2.18	0.43
12:K:22:VAL:O	12:K:26:VAL:HG23	2.18	0.43
1:A:324:G:O2'	1:A:325:U:H5'	2.19	0.43
5:D:274:GLU:HA	5:D:292:GLY:O	2.18	0.43
1:A:2061:C:C2'	1:A:2062:A:H5'	2.49	0.43
26:Y:34:ARG:NH1	26:Y:48:VAL:O	2.50	0.43
20:S:59:PHE:CZ	20:S:79:ARG:HB2	2.54	0.43
11:J:47:GLU:CB	11:J:133:ILE:CD1	2.95	0.43
28:1:10:ARG:HG3	28:1:11:THR:N	2.34	0.43
24:W:38:GLY:C	24:W:40:PRO:HD2	2.38	0.43
10:I:63:ARG:O	10:I:67:LEU:HG	2.18	0.43
7:F:95:THR:C	7:F:97:GLN:N	2.71	0.43
13:L:4:LEU:HD22	13:L:116:GLU:HB3	2.01	0.43
18:Q:10:ALA:CA	18:Q:13:VAL:HG12	2.46	0.43
21:T:51:GLN:NE2	21:T:53:ASN:HD21	2.12	0.43
5:D:125:GLU:O	5:D:129:ARG:HG3	2.18	0.43
1:A:612:U:H2'	1:A:613:C:C6	2.54	0.43
1:A:671:A:O2'	1:A:672:G:H2'	2.19	0.43
22:U:77:VAL:HG11	22:U:91:LEU:HD11	1.99	0.43
1:A:2776:A:H2'	1:A:2777:G:O4'	2.18	0.43
1:A:796:A:HO2'	28:1:10:ARG:N	2.16	0.43
7:F:64:ARG:HG2	7:F:66:GLY:O	2.19	0.43
27:Z:187:VAL:HB	27:Z:203:VAL:HG22	2.01	0.43
26:Y:43:VAL:HG12	26:Y:47:ALA:HB3	2.00	0.43
1:A:2044:G:OP1	26:Y:23:HIS:HE1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2274:A:N3	15:N:86:MET:CE	2.82	0.43
40:A:4896:HOH:O	28:I:13:ARG:NH1	2.51	0.43
13:L:101:ASN:O	13:L:102:GLU:HB2	2.19	0.43
26:Y:27:ASP:N	26:Y:27:ASP:OD2	2.52	0.43
1:A:2413:A:N7	16:O:109:PRO:HB3	2.34	0.43
1:A:1413:A:H2'	1:A:1414:A:O4'	2.19	0.43
1:A:2115:U:H2'	1:A:2116:U:C6	2.54	0.43
1:A:1287:A:O4'	25:X:117:ARG:HD3	2.17	0.43
11:J:46:VAL:O	11:J:146:TRP:CH2	2.68	0.43
1:A:1191:A:N1	1:A:1206:U:O4	2.52	0.43
10:I:16:LYS:O	10:I:20:VAL:HG23	2.19	0.43
1:A:737:A:H2'	1:A:738:G:O4'	2.18	0.43
11:J:72:VAL:HG11	11:J:81:TYR:CZ	2.54	0.43
9:H:101:ALA:HB2	9:H:108:LEU:HD22	1.99	0.43
27:Z:117:LEU:HA	27:Z:174:VAL:HG11	2.00	0.43
17:P:26:TRP:HA	17:P:26:TRP:CE3	2.54	0.43
1:A:1109:U:O4	12:K:21:ARG:HA	2.19	0.43
14:M:21:ARG:N	40:M:8531:HOH:O	2.51	0.43
5:D:142:LEU:HG	5:D:166:VAL:CG2	2.49	0.43
7:F:62:ASP:HA	40:F:4233:HOH:O	2.19	0.43
8:G:112:ALA:HA	8:G:113:PRO:HD3	1.90	0.43
1:A:189:A:OP1	15:N:171:ARG:NH2	2.52	0.43
11:J:26:LYS:HG2	11:J:28:ILE:N	2.29	0.43
8:G:11:VAL:HG11	8:G:22:VAL:HG13	2.00	0.43
1:A:1603:A:C5'	1:A:1605:G:H5'	2.49	0.43
4:C:199:HIS:CD2	4:C:201:PHE:HB2	2.53	0.43
15:N:55:LYS:O	15:N:60:ILE:HD12	2.19	0.43
1:A:903:U:O4	14:M:18:HIS:HB2	2.18	0.43
1:A:1926:G:H2'	1:A:1927:A:H8	1.84	0.43
40:A:4243:HOH:O	16:O:21:HIS:HD2	2.01	0.43
24:W:5:VAL:HG11	24:W:9:ARG:NH1	2.34	0.43
4:C:30:ARG:HB3	4:C:30:ARG:HE	1.69	0.43
1:A:2356:A:H2'	1:A:2357:G:O4'	2.18	0.43
1:A:970:U:H2'	40:A:5838:HOH:O	2.19	0.43
17:P:107:GLU:O	17:P:108:GLY:C	2.57	0.43
22:U:48:VAL:CG1	22:U:96:VAL:HG13	2.49	0.43
20:S:72:VAL:CG1	20:S:75:TRP:HB3	2.48	0.43
25:X:88:THR:CG2	25:X:110:GLN:NE2	2.75	0.43
1:A:1175:G:H1'	1:A:1193:A:H2'	2.01	0.43
25:X:54:PHE:CZ	25:X:140:LYS:HB2	2.53	0.43
1:A:291:C:H2'	1:A:292:G:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:U:H5''	1:A:284:C:OP2	2.19	0.43
9:H:63:ILE:HB	9:H:64:PRO:CD	2.44	0.43
1:A:187:A:H3'	1:A:188:C:H6	1.83	0.43
22:U:49:GLU:HB3	22:U:59:GLU:HG3	2.01	0.43
25:X:142:ASP:HB3	25:X:145:GLY:H	1.82	0.43
1:A:245:C:H2'	1:A:246:G:H5'	2.01	0.43
1:A:344:C:H2'	1:A:345:G:O4'	2.18	0.43
1:A:958:G:H2'	1:A:959:C:C6	2.53	0.43
11:J:48:LEU:HD13	11:J:146:TRP:HB3	2.02	0.42
1:A:1166:A:H61	1:A:1180:U:H3	1.67	0.42
7:F:23:VAL:HG21	7:F:45:THR:CG2	2.48	0.42
15:N:37:VAL:HG21	15:N:108:LYS:HG3	2.01	0.42
1:A:289:G:N1	1:A:363:A:C2	2.85	0.42
14:M:143:THR:HG21	40:M:8537:HOH:O	2.19	0.42
1:A:559:U:C6	1:A:559:U:H5'	2.45	0.42
1:A:35:U:H5'	6:E:47:GLY:O	2.19	0.42
1:A:1684:A:O2'	1:A:1685:A:H5''	2.19	0.42
20:S:119:VAL:HG21	20:S:142:ASP:CG	2.39	0.42
1:A:1314:U:H5''	1:A:1316:G:O4'	2.19	0.42
1:A:664:U:O4	1:A:681:G:H5''	2.18	0.42
1:A:920:C:H4'	1:A:921:G:C2	2.54	0.42
1:A:1588:G:C6	1:A:1589:G:N1	2.87	0.42
1:A:1135:G:H5'	40:A:5445:HOH:O	2.19	0.42
1:A:1231:A:N3	1:A:2553:A:H5''	2.34	0.42
1:A:2755:G:H1'	40:A:4197:HOH:O	2.19	0.42
1:A:912:A:C4	1:A:1294:A:C2	3.07	0.42
1:A:2401:A:H2'	1:A:2402:A:C8	2.55	0.42
14:M:128:GLY:O	14:M:132:LYS:HG3	2.18	0.42
1:A:240:C:H4'	15:N:146:GLN:NE2	2.34	0.42
18:Q:115:SER:O	18:Q:117:SER:N	2.52	0.42
15:N:67:ILE:HD13	15:N:104:ARG:HH11	1.84	0.42
1:A:2781:U:C2'	1:A:2782:G:H5'	2.49	0.42
1:A:2712:G:H5'	40:L:4183:HOH:O	2.18	0.42
24:W:1:THR:HG23	24:W:2:VAL:N	2.23	0.42
17:P:96:VAL:CG1	17:P:100:GLN:HB2	2.49	0.42
1:A:2269:C:H2'	1:A:2270:G:C5'	2.49	0.42
1:A:710:G:N2	1:A:719:C:C2	2.88	0.42
20:S:119:VAL:HG11	40:S:8583:HOH:O	2.18	0.42
1:A:694:A:H2'	1:A:695:C:H5'	2.01	0.42
1:A:2362:A:H2'	1:A:2363:G:C8	2.54	0.42
1:A:485:A:O2'	1:A:487:G:H5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:186:TRP:CD1	4:C:187:PRO:HA	2.54	0.42
8:G:108:LEU:HD11	8:G:164:ASP:HB2	2.01	0.42
1:A:1309:U:O2'	1:A:1310:U:H5'	2.17	0.42
1:A:2088:C:H1'	1:A:2841:A:N1	2.35	0.42
1:A:1114:A:H2'	1:A:1115:U:H6	1.84	0.42
7:F:84:LEU:C	7:F:86:THR:H	2.22	0.42
1:A:585:C:H6	40:A:5609:HOH:O	2.01	0.42
11:J:114:PRO:O	11:J:115:PHE:C	2.58	0.42
2:B:3020:G:O2'	2:B:3021:G:H5'	2.19	0.42
1:A:1335:C:H2'	1:A:1336:U:C6	2.54	0.42
1:A:2787:C:H5	40:A:4147:HOH:O	2.01	0.42
4:C:211:LYS:CB	4:C:212:PRO:CD	2.98	0.42
1:A:1206:U:H5'	1:A:1206:U:C6	2.45	0.42
16:O:38:LYS:HE2	16:O:107:ASN:ND2	2.34	0.42
1:A:2004:U:H5''	1:A:2005:G:C8	2.55	0.42
26:Y:71:ARG:HD3	40:Y:2171:HOH:O	2.19	0.42
5:D:254:GLN:HG2	5:D:255:GLY:H	1.82	0.42
2:B:3014:G:O2'	16:O:1:ALA:HB2	2.20	0.42
9:H:28:ALA:HB3	9:H:99:THR:HG23	2.01	0.42
24:W:20:LEU:HD22	24:W:60:GLN:HE22	1.84	0.42
9:H:101:ALA:HA	40:H:5413:HOH:O	2.19	0.42
2:B:3091:C:H2'	2:B:3092:G:O4'	2.18	0.42
29:2:28:HIS:CD2	29:2:31:LYS:HG3	2.55	0.42
2:B:3114:G:O6	16:O:11:ARG:HD3	2.19	0.42
1:A:2911:C:H3'	40:A:5070:HOH:O	2.19	0.42
6:E:79:ARG:O	6:E:87:ARG:HG2	2.20	0.42
1:A:1827:G:C6	1:A:1828:G:C6	3.08	0.42
1:A:1744:G:H2'	1:A:1745:G:H5'	2.00	0.42
1:A:1756:G:H1'	40:A:5773:HOH:O	2.19	0.42
16:O:182:GLY:N	40:O:8572:HOH:O	2.50	0.42
40:A:5758:HOH:O	23:V:56:ARG:HD3	2.19	0.42
40:A:9673:HOH:O	15:N:87:MET:HE3	2.18	0.42
12:K:131:THR:HB	12:K:134:GLU:HG3	2.00	0.42
1:A:2909:G:H2'	1:A:2910:A:H8	1.85	0.42
5:D:51:VAL:HA	5:D:329:TYR:O	2.19	0.42
1:A:1881:A:OP1	4:C:199:HIS:HE1	2.01	0.42
23:V:37:GLU:O	23:V:40:ALA:HB3	2.19	0.42
1:A:1819:G:H2'	1:A:1820:G:C5'	2.50	0.42
7:F:167:GLU:C	7:F:169:THR:H	2.23	0.42
17:P:29:VAL:O	17:P:33:LEU:HG	2.20	0.42
1:A:2816:A:H5''	1:A:2817:G:H5'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:U:O4	1:A:532:A:OP2	2.37	0.42
1:A:451:C:O2'	1:A:452:G:H5'	2.19	0.42
6:E:236:THR:O	6:E:237:GLU:C	2.57	0.42
25:X:146:ILE:HG22	25:X:147:ASP:N	2.33	0.42
16:O:90:LEU:CB	16:O:186:LEU:HD22	2.49	0.42
11:J:165:GLY:C	11:J:166:ASN:HD22	2.23	0.42
20:S:39:THR:HB	20:S:42:GLU:OE1	2.20	0.42
6:E:107:ARG:HB3	6:E:107:ARG:CZ	2.49	0.42
1:A:182:G:H4'	15:N:157:LEU:HD13	2.01	0.42
8:G:31:ARG:NH1	8:G:68:HIS:ND1	2.67	0.42
4:C:128:LEU:HD21	4:C:131:HIS:HE1	1.84	0.42
7:F:174:VAL:CG1	40:F:6555:HOH:O	2.59	0.42
5:D:243:ASN:HA	5:D:244:PRO:C	2.39	0.42
1:A:1595:G:O2'	1:A:1596:U:H5'	2.20	0.42
1:A:2897:C:H2'	1:A:2898:G:C8	2.53	0.42
5:D:82:VAL:HG12	5:D:101:TRP:CE3	2.55	0.42
1:A:1236:A:C8	12:K:63:ILE:HD11	2.55	0.42
1:A:2821:C:H4'	5:D:116:PRO:CB	2.50	0.42
11:J:1:LYS:N	40:J:8353:HOH:O	2.52	0.42
16:O:108:SER:HA	16:O:109:PRO:HD3	1.78	0.42
17:P:59:VAL:HG23	17:P:111:VAL:HG23	2.01	0.42
1:A:2900:G:H2'	1:A:2901:C:O4'	2.20	0.42
40:A:7227:HOH:O	6:E:94:THR:HG21	2.19	0.42
11:J:149:ALA:C	11:J:151:MET:H	2.23	0.42
15:N:159:THR:HA	40:N:8520:HOH:O	2.20	0.42
1:A:1116:U:O2'	1:A:1118:A:C2	2.49	0.42
9:H:57:GLU:O	9:H:61:MET:HG3	2.20	0.42
24:W:42:ASN:O	24:W:44:GLY:N	2.52	0.42
26:Y:15:ARG:HH11	26:Y:15:ARG:CB	2.30	0.42
1:A:771:G:OP2	15:N:79:LYS:HE3	2.19	0.42
16:O:143:ARG:HH12	16:O:173:ASP:CG	2.19	0.42
1:A:907:A:H4'	1:A:1328:A:C2	2.55	0.42
1:A:709:G:O2'	17:P:25:VAL:CG1	2.67	0.42
4:C:66:ARG:HB2	4:C:66:ARG:NH1	2.34	0.42
4:C:175:LYS:HE2	40:C:8576:HOH:O	2.19	0.42
21:T:76:GLU:HB3	40:T:8345:HOH:O	2.19	0.42
1:A:1504:A:H4'	1:A:1506:U:C5	2.55	0.42
20:S:68:HIS:CD2	20:S:76:ASP:HB2	2.54	0.42
1:A:37:A:H2'	1:A:38:G:H8	1.84	0.42
14:M:10:SER:O	14:M:12:THR:N	2.51	0.42
1:A:2271:G:N3	1:A:2271:G:H2'	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2515:C:H2'	1:A:2516:G:O4'	2.20	0.42
1:A:1218:U:H2'	1:A:1219:U:C6	2.54	0.42
1:A:23:G:H1'	1:A:520:A:N6	2.35	0.42
1:A:1675:C:H5''	30:3:5:LYS:HD2	2.02	0.42
27:Z:172:THR:HG22	27:Z:173:ALA:N	2.35	0.42
15:N:32:ARG:NH2	40:N:8597:HOH:O	2.52	0.42
1:A:932:U:H2'	1:A:933:C:C6	2.55	0.42
6:E:236:THR:C	40:E:8450:HOH:O	2.57	0.42
2:B:3056:A:C3'	2:B:3057:A:H5''	2.50	0.42
15:N:164:THR:HB	40:N:8520:HOH:O	2.19	0.42
1:A:2494:G:H4'	11:J:5:MET:SD	2.60	0.42
25:X:122:ARG:CG	25:X:122:ARG:HH11	2.26	0.42
1:A:338:C:H4'	6:E:174:ILE:HD12	2.00	0.42
1:A:553:G:P	27:Z:204:ARG:NH2	2.91	0.42
16:O:154:LEU:CG	16:O:155:GLU:H	2.27	0.42
17:P:26:TRP:HA	17:P:26:TRP:HE3	1.84	0.42
20:S:82:GLU:HG3	20:S:83:LYS:N	2.34	0.42
1:A:2820:A:H2'	1:A:2821:C:C6	2.55	0.42
1:A:2911:C:H2'	1:A:2912:C:C6	2.55	0.42
1:A:2912:C:H2'	1:A:2913:A:O4'	2.20	0.42
1:A:1311:G:C2	1:A:1312:G:C8	3.08	0.42
16:O:175:LEU:HA	16:O:175:LEU:HD12	1.87	0.42
6:E:223:LEU:HD12	6:E:223:LEU:HA	1.86	0.42
7:F:51:ARG:HA	40:F:7636:HOH:O	2.20	0.42
25:X:139:GLY:O	25:X:141:HIS:CD2	2.72	0.42
1:A:2769:C:H2'	1:A:2770:G:H5'	2.02	0.42
12:K:39:VAL:HG11	12:K:107:ASN:HB2	2.02	0.42
16:O:73:ALA:HB1	16:O:74:PRO:HD2	2.01	0.42
5:D:25:ARG:HA	5:D:310:ARG:HH21	1.85	0.42
1:A:1972:U:C2'	1:A:1973:A:C5'	2.98	0.42
16:O:63:SER:O	16:O:66:LEU:HB2	2.19	0.42
15:N:122:GLU:HB2	15:N:126:HIS:O	2.20	0.42
1:A:1976:G:O2'	1:A:1977:U:H5'	2.20	0.42
6:E:51:TYR:CE2	29:2:53:LYS:HB3	2.55	0.42
1:A:1805:G:O2'	1:A:1806:G:H5'	2.20	0.42
1:A:2383:G:N3	40:A:6217:HOH:O	2.36	0.42
1:A:1289:C:O2'	1:A:1290:G:H5'	2.19	0.42
31:4:91:GLN:O	31:4:92:GLU:HB2	2.19	0.42
26:Y:74:ALA:HB1	26:Y:85:VAL:HG22	2.01	0.42
6:E:115:LEU:CD2	6:E:243:VAL:HG13	2.37	0.42
1:A:1943:C:H4'	4:C:211:LYS:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:21:LEU:HD21	25:X:48:VAL:HG13	2.01	0.42
15:N:67:ILE:HD13	15:N:104:ARG:NH1	2.35	0.42
5:D:170:SER:O	5:D:174:ARG:HG2	2.20	0.42
25:X:14:HIS:HB2	25:X:17:ILE:HG13	2.01	0.42
18:Q:10:ALA:O	18:Q:13:VAL:HG12	2.20	0.42
1:A:2421:G:H3'	1:A:2422:U:C5'	2.50	0.42
40:A:4038:HOH:O	15:N:94:LYS:CE	2.61	0.42
1:A:138:U:OP2	1:A:139:C:H5	2.01	0.42
1:A:1477:C:O2'	1:A:1478:U:H5'	2.20	0.42
17:P:14:LEU:HG	17:P:102:ILE:HD11	2.02	0.42
22:U:40:VAL:HG23	22:U:119:ALA:C	2.41	0.42
27:Z:205:ILE:O	27:Z:206:ALA:C	2.59	0.42
23:V:50:GLU:CD	40:V:7349:HOH:O	2.58	0.42
1:A:40:C:H4'	40:A:6511:HOH:O	2.18	0.42
1:A:57:C:H5''	40:A:6270:HOH:O	2.19	0.42
1:A:1943:C:O4'	4:C:212:PRO:HA	2.19	0.41
9:H:91:VAL:CG1	9:H:92:GLY:H	2.29	0.41
5:D:162:MET:HG3	5:D:310:ARG:CZ	2.50	0.41
26:Y:15:ARG:NH1	26:Y:15:ARG:HB3	2.31	0.41
7:F:93:LEU:HB2	40:F:5198:HOH:O	2.19	0.41
11:J:71:TYR:O	11:J:73:GLN:N	2.53	0.41
14:M:104:ASP:O	14:M:105:TYR:HB3	2.20	0.41
5:D:49:THR:CG2	5:D:280:VAL:CG2	2.98	0.41
8:G:73:PHE:O	8:G:76:VAL:HG22	2.20	0.41
15:N:113:ARG:NH1	15:N:150:ILE:O	2.48	0.41
4:C:39:ALA:HB3	4:C:61:GLU:OE2	2.20	0.41
1:A:1114:A:H2'	1:A:1115:U:C6	2.55	0.41
1:A:1339:G:C6	1:A:1340:G:N1	2.87	0.41
40:A:9494:HOH:O	14:M:22:ARG:HG2	2.20	0.41
40:A:5539:HOH:O	19:R:50:GLY:HA2	2.19	0.41
1:A:772:G:H2'	1:A:773:A:O4'	2.19	0.41
1:A:1275:C:C2'	1:A:1276:U:H5'	2.50	0.41
1:A:2329:C:O2'	1:A:2330:U:H5'	2.20	0.41
1:A:204:A:C2'	1:A:205:U:H5'	2.50	0.41
7:F:99:ASP:HB2	7:F:103:ASN:CA	2.50	0.41
1:A:240:C:O2	1:A:240:C:H2'	2.21	0.41
28:1:33:HIS:HE1	28:1:49:ARG:NE	2.18	0.41
1:A:2756:U:N3	1:A:2896:A:H2	2.15	0.41
2:B:3048:C:H4'	16:O:141:ARG:NH2	2.35	0.41
2:B:3026:C:O2'	2:B:3027:C:H5'	2.20	0.41
1:A:2467:A:O2'	1:A:2468:A:H2'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2314:G:H2'	1:A:2315:C:H5'	2.02	0.41
1:A:941:G:C5	1:A:942:U:C4	3.08	0.41
1:A:1433:G:O2'	1:A:1434:A:H5'	2.20	0.41
19:R:46:SER:O	19:R:48:PRO:HD3	2.19	0.41
16:O:122:ALA:O	16:O:127:LEU:HB2	2.20	0.41
15:N:39:ARG:HA	15:N:63:VAL:HG22	2.03	0.41
25:X:52:VAL:HG13	25:X:53:ALA:N	2.34	0.41
27:Z:112:GLU:OE1	27:Z:112:GLU:HA	2.21	0.41
5:D:17:LYS:O	5:D:260:HIS:HD2	2.03	0.41
6:E:57:PRO:HG2	6:E:73:LEU:HD13	2.01	0.41
6:E:21:VAL:C	6:E:23:GLU:H	2.23	0.41
1:A:2377:U:H6	1:A:2377:U:O5'	2.03	0.41
1:A:1434:A:H2'	1:A:1436:C:C5	2.55	0.41
27:Z:116:LEU:HD23	27:Z:116:LEU:HA	1.80	0.41
19:R:23:THR:HA	40:R:4792:HOH:O	2.20	0.41
1:A:1252:A:H2'	1:A:1253:C:O4'	2.20	0.41
1:A:2424:U:H1'	19:R:7:LEU:HD12	2.02	0.41
17:P:73:ASP:HA	17:P:92:VAL:O	2.21	0.41
1:A:100:C:H4'	22:U:16:LEU:HB2	2.02	0.41
1:A:2055:A:H5'	20:S:134:SER:HB2	2.02	0.41
11:J:86:ARG:HG2	11:J:86:ARG:H	1.54	0.41
11:J:26:LYS:CD	11:J:28:ILE:HB	2.51	0.41
1:A:870:G:C3'	1:A:871:G:H5''	2.50	0.41
15:N:165:SER:HB2	40:N:8549:HOH:O	2.20	0.41
16:O:127:LEU:HA	16:O:127:LEU:HD12	1.83	0.41
1:A:1205:U:H2'	1:A:1206:U:H5''	2.01	0.41
5:D:62:ARG:CB	5:D:65:MET:HE3	2.50	0.41
15:N:108:LYS:N	15:N:108:LYS:HD3	2.35	0.41
1:A:1845:A:OP2	4:C:190:ARG:NH1	2.52	0.41
22:U:9:LYS:NZ	22:U:13:ARG:NH1	2.69	0.41
1:A:1298:U:H2'	1:A:1299:G:C8	2.55	0.41
12:K:39:VAL:HG13	12:K:106:GLY:O	2.19	0.41
10:I:71:LEU:C	10:I:73:ASP:H	2.23	0.41
13:L:6:ALA:HB3	13:L:116:GLU:HG2	2.03	0.41
16:O:149:GLU:O	16:O:152:GLU:HB2	2.21	0.41
40:B:3472:HOH:O	16:O:41:LYS:HD3	2.19	0.41
1:A:708:A:H2'	1:A:709:G:O4'	2.20	0.41
25:X:35:VAL:CG2	25:X:41:TYR:CD2	3.04	0.41
1:A:2308:U:C5	1:A:2310:G:C8	3.08	0.41
6:E:129:HIS:HE1	6:E:231:ARG:HA	1.85	0.41
1:A:920:C:H5'	1:A:921:G:C4	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:99:ASP:OD1	13:L:101:ASN:N	2.52	0.41
1:A:2667:G:H1'	1:A:2914:A:N3	2.35	0.41
1:A:2825:C:H4'	1:A:2826:G:O5'	2.20	0.41
1:A:2642:G:H2'	1:A:2643:G:O4'	2.20	0.41
25:X:63:GLU:HG2	25:X:93:ILE:HG22	2.01	0.41
5:D:215:VAL:HB	5:D:234:ARG:HH12	1.85	0.41
40:A:6141:HOH:O	11:J:150:LYS:NZ	2.50	0.41
11:J:68:ALA:HB2	11:J:149:ALA:HB2	2.01	0.41
1:A:870:G:OP2	4:C:3:ARG:HD3	2.19	0.41
14:M:144:ASP:HA	14:M:147:GLU:HG3	2.02	0.41
23:V:9:CYS:HA	23:V:52:THR:CG2	2.46	0.41
2:B:3013:A:H3'	2:B:3014:G:H5'	2.01	0.41
7:F:92:GLU:O	7:F:93:LEU:O	2.38	0.41
31:4:38:ARG:O	31:4:42:ARG:HB2	2.21	0.41
9:H:21:GLU:HA	9:H:24:ARG:HE	1.85	0.41
25:X:35:VAL:HA	25:X:36:PRO:HD3	1.80	0.41
2:B:3003:A:OP2	2:B:3025:G:N2	2.53	0.41
1:A:1878:G:O2'	1:A:1879:U:OP2	2.38	0.41
26:Y:66:THR:HG22	26:Y:67:PRO:O	2.21	0.41
4:C:135:VAL:N	40:C:8593:HOH:O	2.52	0.41
1:A:1772:C:H5'	1:A:1773:G:C5	2.55	0.41
13:L:90:PHE:CD1	13:L:90:PHE:N	2.89	0.41
1:A:2070:G:H5''	40:A:3293:HOH:O	2.20	0.41
1:A:503:G:H2'	1:A:504:G:H8	1.85	0.41
1:A:513:A:N3	40:A:3173:HOH:O	2.36	0.41
1:A:622:G:O2'	1:A:623:U:H5'	2.20	0.41
5:D:221:GLN:HE22	13:L:42:ASN:HD22	1.68	0.41
1:A:2786:G:H2'	40:A:6694:HOH:O	2.20	0.41
1:A:1482:A:O2'	1:A:1483:C:H5'	2.21	0.41
6:E:115:LEU:HD12	6:E:115:LEU:HA	1.87	0.41
25:X:26:ILE:O	25:X:26:ILE:HG13	2.21	0.41
1:A:2780:C:H2'	1:A:2781:U:H6	1.86	0.41
4:C:36:ASP:O	4:C:37:VAL:C	2.59	0.41
5:D:139:ASP:HB3	40:D:8546:HOH:O	2.20	0.41
1:A:1878:G:O2'	1:A:1879:U:C6	2.71	0.41
1:A:1406:A:H4'	1:A:1407:A:C5'	2.50	0.41
5:D:277:GLU:N	5:D:278:PRO:HD2	2.35	0.41
1:A:90:A:H2'	1:A:91:G:O4'	2.21	0.41
1:A:2575:C:H2'	1:A:2576:A:O4'	2.20	0.41
40:A:8599:HOH:O	15:N:174:ARG:HG3	2.21	0.41
1:A:42:C:H1'	40:A:4191:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:48:LEU:CG	11:J:157:ILE:HG21	2.50	0.41
2:B:3040:C:N4	7:F:51:ARG:HB2	2.35	0.41
5:D:60:SER:C	5:D:62:ARG:N	2.73	0.41
1:A:2591:C:H2'	1:A:2592:G:O4'	2.21	0.41
5:D:320:GLN:HG3	5:D:321:PRO:CD	2.50	0.41
36:5:9080:SPS:H71	36:5:9080:SPS:H81	1.82	0.41
1:A:1003:U:O2	11:J:90:PHE:HZ	2.03	0.41
2:B:3107:C:H2'	2:B:3108:C:C6	2.55	0.41
1:A:10:U:H1'	1:A:532:A:H62	1.86	0.41
5:D:189:ALA:HB1	40:D:8561:HOH:O	2.19	0.41
1:A:2364:A:H5''	19:R:15:LYS:HD3	2.01	0.41
1:A:2559:C:H4'	40:A:6765:HOH:O	2.20	0.41
1:A:162:C:H2'	1:A:163:U:H5'	2.03	0.41
2:B:3104:A:O2'	2:B:3105:A:H5'	2.20	0.41
1:A:2846:C:H4'	40:A:4593:HOH:O	2.19	0.41
1:A:731:U:H2'	1:A:732:C:C6	2.55	0.41
5:D:148:PRO:HD2	40:D:8575:HOH:O	2.21	0.41
1:A:1829:A:H2'	1:A:1830:C:H5'	2.03	0.41
1:A:690:G:H4'	1:A:741:C:O2	2.20	0.41
1:A:542:A:C8	1:A:542:A:C5'	2.99	0.41
1:A:1164:U:O4'	1:A:1165:G:OP1	2.38	0.41
1:A:1166:A:H1'	1:A:1192:A:N1	2.32	0.41
1:A:2781:U:H2'	1:A:2782:G:H5'	2.03	0.41
1:A:2768:A:H5''	40:A:3940:HOH:O	2.21	0.41
4:C:48:ASP:HA	4:C:49:PRO:HD3	1.92	0.41
7:F:95:THR:HG21	7:F:174:VAL:HG22	2.03	0.41
5:D:145:HIS:CD2	5:D:146:THR:O	2.65	0.41
1:A:396:U:OP2	31:4:38:ARG:NH1	2.47	0.41
7:F:57:THR:HG23	7:F:63:ILE:HA	2.03	0.41
11:J:97:LYS:HD3	11:J:117:LYS:HE2	2.03	0.41
1:A:876:A:N3	1:A:876:A:H2'	2.36	0.41
1:A:221:G:H2'	1:A:222:A:C8	2.55	0.41
30:3:24:TRP:CD1	40:3:6863:HOH:O	2.73	0.41
1:A:1609:C:H2'	1:A:1610:G:H8	1.86	0.41
31:4:23:GLU:HG2	31:4:24:LYS:N	2.36	0.41
12:K:88:PRO:O	12:K:94:GLY:HA3	2.20	0.41
1:A:1754:A:H2'	1:A:1755:A:O4'	2.20	0.41
1:A:1174:A:C5	1:A:1201:C:H4'	2.55	0.41
5:D:238:ASN:ND2	5:D:240:GLY:N	2.66	0.41
16:O:38:LYS:HB2	16:O:38:LYS:HE3	1.70	0.41
25:X:5:VAL:O	25:X:52:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:58:GLU:HG3	9:H:61:MET:CE	2.50	0.41
5:D:7:ARG:NH1	5:D:7:ARG:CG	2.80	0.41
28:1:39:CYS:HA	28:1:40:PRO:HD3	1.98	0.41
13:L:49:LEU:HD21	13:L:74:VAL:O	2.20	0.41
24:W:39:ALA:C	24:W:41:GLU:N	2.74	0.41
12:K:130:VAL:CG1	12:K:131:THR:N	2.83	0.41
1:A:1299:G:H5'	40:A:3582:HOH:O	2.21	0.41
12:K:6:PHE:HB3	12:K:109:TYR:OH	2.21	0.41
4:C:105:VAL:CG1	4:C:106:CYS:N	2.83	0.41
5:D:36:PRO:CA	5:D:168:GLY:HA3	2.48	0.41
4:C:29:HIS:HB2	4:C:153:ARG:HH12	1.86	0.41
18:Q:41:ARG:O	18:Q:44:VAL:HB	2.20	0.41
16:O:154:LEU:CG	16:O:155:GLU:N	2.83	0.41
1:A:2419:U:H5''	1:A:2420:G:C5'	2.50	0.41
20:S:29:LYS:HB3	40:S:8530:HOH:O	2.21	0.41
1:A:2256:G:O2'	1:A:2257:G:H5'	2.20	0.41
27:Z:117:LEU:HD12	27:Z:174:VAL:HG13	2.02	0.41
4:C:66:ARG:CB	4:C:66:ARG:NH1	2.84	0.41
4:C:164:ARG:CZ	40:C:8586:HOH:O	2.69	0.41
1:A:1095:U:O2	25:X:120:PRO:HG2	2.21	0.41
1:A:1014:A:H2'	1:A:1015:C:H5'	2.03	0.41
20:S:79:ARG:C	20:S:81:PRO:HD3	2.41	0.41
1:A:1804:A:H2'	1:A:1805:G:C8	2.55	0.41
40:A:4388:HOH:O	15:N:174:ARG:HG2	2.20	0.41
20:S:149:GLU:HA	20:S:150:PRO:HD3	1.93	0.41
1:A:2425:A:H2'	40:A:8743:HOH:O	2.20	0.41
1:A:2621:U:H5	40:A:9490:HOH:O	2.04	0.41
1:A:1421:C:O2'	1:A:1422:U:H5'	2.21	0.41
13:L:27:ARG:HD2	40:L:4747:HOH:O	2.21	0.41
1:A:1079:A:N1	1:A:2068:G:O2'	2.50	0.41
28:1:81:LYS:O	28:1:82:ALA:C	2.59	0.41
1:A:2107:U:O2'	1:A:2108:A:H5'	2.21	0.41
12:K:92:GLN:HB3	40:K:1405:HOH:O	2.20	0.41
6:E:118:THR:CG2	6:E:137:PRO:HB3	2.50	0.41
24:W:1:THR:O	24:W:4:HIS:CE1	2.74	0.41
1:A:1543:G:N1	1:A:1641:A:OP2	2.43	0.41
18:Q:141:ILE:C	18:Q:143:ALA:H	2.24	0.41
18:Q:37:ARG:O	18:Q:41:ARG:HG3	2.20	0.41
5:D:5:ARG:HD2	5:D:8:LYS:NZ	2.36	0.41
22:U:52:ARG:HB2	22:U:95:ASN:HB3	2.03	0.41
18:Q:94:TRP:CZ2	18:Q:98:ILE:HG13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:46:LEU:HG	40:N:8623:HOH:O	2.21	0.41
4:C:150:PRO:HD3	40:C:8593:HOH:O	2.21	0.41
1:A:1453:G:N2	1:A:1675:C:C2	2.89	0.41
1:A:228:C:H2'	1:A:229:G:H5'	2.03	0.41
9:H:78:GLU:HG3	40:H:5966:HOH:O	2.20	0.41
1:A:2761:A:C4	1:A:2763:G:C8	3.09	0.41
1:A:962:C:C1'	16:O:5:ARG:NH1	2.76	0.40
16:O:22:GLN:HG2	16:O:26:LEU:HD22	2.03	0.40
1:A:445:U:H1'	40:A:6846:HOH:O	2.21	0.40
24:W:20:LEU:HD22	24:W:60:GLN:NE2	2.36	0.40
1:A:86:A:C2	30:3:25:VAL:HG13	2.57	0.40
1:A:2251:G:H2'	1:A:2252:A:H8	1.87	0.40
1:A:1762:C:H2'	1:A:1763:C:C6	2.56	0.40
1:A:2061:C:H2'	1:A:2062:A:H5'	2.03	0.40
8:G:162:PHE:CD1	8:G:162:PHE:N	2.88	0.40
1:A:1946:C:H2'	1:A:1971:G:C8	2.56	0.40
1:A:1456:C:H2'	1:A:1457:U:C6	2.56	0.40
7:F:128:LEU:N	40:F:6007:HOH:O	2.53	0.40
11:J:33:MET:SD	11:J:65:ARG:HD2	2.62	0.40
15:N:169:ARG:NH2	40:N:8549:HOH:O	2.46	0.40
1:A:1173:A:H4'	1:A:1174:A:C8	2.56	0.40
7:F:49:PRO:HA	7:F:73:VAL:HG22	2.03	0.40
25:X:48:VAL:O	25:X:48:VAL:HG12	2.21	0.40
11:J:43:PRO:HD2	11:J:137:ASN:HA	2.03	0.40
8:G:137:ASP:O	8:G:141:VAL:HG23	2.21	0.40
1:A:545:G:H2'	1:A:546:C:O4'	2.21	0.40
27:Z:187:VAL:HB	27:Z:203:VAL:CG2	2.51	0.40
15:N:74:ARG:HD3	15:N:91:ILE:HD12	2.02	0.40
16:O:164:ASP:OD1	16:O:164:ASP:C	2.59	0.40
17:P:25:VAL:HG23	17:P:26:TRP:H	1.86	0.40
18:Q:98:ILE:O	18:Q:98:ILE:HD13	2.21	0.40
5:D:279:THR:HG22	5:D:280:VAL:N	2.35	0.40
2:B:3106:C:O2'	2:B:3107:C:H5'	2.22	0.40
1:A:644:G:H1'	40:A:5916:HOH:O	2.21	0.40
27:Z:126:PRO:HG2	27:Z:128:PHE:CZ	2.55	0.40
1:A:1805:G:H2'	1:A:1806:G:H8	1.86	0.40
18:Q:2:ASP:OD1	18:Q:2:ASP:C	2.58	0.40
40:A:4136:HOH:O	4:C:6:GLY:HA3	2.21	0.40
1:A:326:G:O2'	1:A:327:A:H5'	2.20	0.40
1:A:1883:U:O2'	1:A:1884:G:H5'	2.21	0.40
5:D:294:TYR:HE2	40:D:8645:HOH:O	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:A:6509:HOH:O	19:R:9:GLY:HA2	2.20	0.40
40:A:8731:HOH:O	4:C:11:ARG:HD3	2.22	0.40
16:O:67:ALA:HA	16:O:71:TRP:HB3	2.03	0.40
15:N:98:GLN:HB2	15:N:129:HIS:NE2	2.36	0.40
1:A:2812:A:H1'	40:A:5306:HOH:O	2.21	0.40
15:N:67:ILE:HD11	15:N:104:ARG:HD2	2.02	0.40
13:L:75:ARG:NH2	40:L:4172:HOH:O	2.54	0.40
5:D:41:PHE:CZ	5:D:79:MET:HG3	2.56	0.40
5:D:24:PRO:HG3	5:D:204:GLY:HA2	2.04	0.40
1:A:450:C:H4'	6:E:46:TYR:CE1	2.56	0.40
20:S:33:ARG:NH2	40:S:8530:HOH:O	2.40	0.40
5:D:258:GLY:N	5:D:260:HIS:CE1	2.88	0.40
1:A:2266:A:H2'	1:A:2267:G:C8	2.57	0.40
1:A:1343:C:C2'	27:Z:208:LYS:HZ1	2.32	0.40
1:A:704:C:H2'	1:A:705:C:H6	1.85	0.40
1:A:1773:G:C8	28:1:16:PRO:HA	2.56	0.40
1:A:1761:U:H5'	18:Q:81:LYS:O	2.22	0.40
22:U:48:VAL:HG13	22:U:96:VAL:HG13	2.04	0.40
1:A:222:A:H2'	1:A:223:G:O4'	2.20	0.40
30:3:11:LEU:HD23	30:3:11:LEU:HA	1.86	0.40
27:Z:99:ALA:HB2	27:Z:233:TYR:CZ	2.56	0.40
1:A:264:G:H1'	1:A:265:U:H5	1.86	0.40
12:K:71:TYR:CD1	12:K:72:PRO:HD2	2.56	0.40
1:A:295:C:H2'	1:A:296:G:O4'	2.20	0.40
6:E:98:ARG:NH1	40:E:8357:HOH:O	2.50	0.40
1:A:1398:G:H2'	1:A:1399:A:C8	2.56	0.40
11:J:65:ARG:CZ	40:J:8385:HOH:O	2.70	0.40
6:E:76:ARG:HG2	6:E:78:ARG:NH1	2.36	0.40
1:A:2890:A:C1'	23:V:56:ARG:NH2	2.77	0.40
24:W:42:ASN:N	24:W:43:PRO:HD3	2.36	0.40
9:H:32:GLY:N	40:H:3111:HOH:O	2.53	0.40
12:K:107:ASN:HD22	12:K:108:PRO:N	2.20	0.40
1:A:2416:G:O2'	16:O:25:ARG:HG2	2.21	0.40
1:A:445:U:H2'	1:A:446:G:H8	1.86	0.40
40:A:3702:HOH:O	27:Z:186:ARG:HD2	2.21	0.40
2:B:3026:C:P	40:B:3472:HOH:O	2.80	0.40
1:A:1613:C:H2'	1:A:1614:G:O4'	2.21	0.40
9:H:26:THR:HG21	9:H:103:ALA:CB	2.50	0.40
1:A:1052:G:N3	1:A:1052:G:H2'	2.37	0.40
13:L:66:ARG:HG2	13:L:66:ARG:HH11	1.87	0.40
1:A:1224:G:H2'	1:A:1225:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2093:G:H5''	40:A:8989:HOH:O	2.21	0.40
20:S:15:LYS:HE3	40:S:8577:HOH:O	2.22	0.40
2:B:3116:C:O2'	2:B:3117:G:H5'	2.21	0.40
1:A:1815:A:H4'	1:A:2751:C:O4'	2.22	0.40
2:B:3052:A:H2'	2:B:3053:G:O4'	2.22	0.40
1:A:2379:G:N7	1:A:2408:A:N1	2.69	0.40
1:A:47:G:N3	1:A:114:A:C2	2.90	0.40
1:A:2718:C:C6	1:A:2718:C:H5'	2.54	0.40
1:A:2779:G:H21	8:G:143:GLN:NE2	2.19	0.40
14:M:146:GLY:C	14:M:148:GLU:H	2.25	0.40
12:K:45:VAL:CG2	12:K:46:ILE:N	2.85	0.40
29:2:21:ARG:CD	29:2:37:CYS:SG	3.09	0.40
1:A:1891:G:H1'	1:A:1972:U:C2	2.56	0.40
1:A:907:A:H2'	1:A:908:A:H8	1.86	0.40
1:A:2657:G:OP1	5:D:17:LYS:HB2	2.22	0.40
1:A:1044:C:H5''	40:A:8542:HOH:O	2.21	0.40
1:A:332:G:O2'	1:A:333:G:H5'	2.22	0.40
1:A:512:G:O3'	1:A:513:A:H8	2.05	0.40
4:C:17:ARG:HD2	40:C:8542:HOH:O	2.22	0.40
20:S:61:GLN:NE2	40:S:8537:HOH:O	2.55	0.40
1:A:2325:C:H1'	40:A:3658:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	C	235/239 (98%)	209 (89%)	21 (9%)	5 (2%)	9	29
5	D	335/337 (99%)	303 (90%)	25 (8%)	7 (2%)	9	29
6	E	244/246 (99%)	218 (89%)	25 (10%)	1 (0%)	39	74
7	F	134/176 (76%)	98 (73%)	28 (21%)	8 (6%)	2	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	G	170/177 (96%)	159 (94%)	10 (6%)	1 (1%)	30	65
9	H	117/119 (98%)	102 (87%)	12 (10%)	3 (3%)	7	22
10	I	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
11	J	152/167 (91%)	133 (88%)	13 (9%)	6 (4%)	4	12
12	K	140/145 (97%)	126 (90%)	11 (8%)	3 (2%)	9	29
13	L	130/132 (98%)	118 (91%)	10 (8%)	2 (2%)	13	40
14	M	141/164 (86%)	120 (85%)	19 (14%)	2 (1%)	14	42
15	N	192/194 (99%)	174 (91%)	16 (8%)	2 (1%)	19	52
16	O	184/186 (99%)	167 (91%)	11 (6%)	6 (3%)	5	16
17	P	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
18	Q	141/148 (95%)	137 (97%)	3 (2%)	1 (1%)	26	62
19	R	93/95 (98%)	85 (91%)	8 (9%)	0	100	100
20	S	148/154 (96%)	140 (95%)	7 (5%)	1 (1%)	26	62
21	T	79/84 (94%)	75 (95%)	4 (5%)	0	100	100
22	U	117/119 (98%)	111 (95%)	5 (4%)	1 (1%)	21	55
23	V	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
24	W	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	5	17
25	X	152/154 (99%)	147 (97%)	3 (2%)	2 (1%)	15	44
26	Y	80/91 (88%)	70 (88%)	8 (10%)	2 (2%)	7	24
27	Z	140/240 (58%)	139 (99%)	1 (1%)	0	100	100
28	1	71/73 (97%)	63 (89%)	7 (10%)	1 (1%)	14	42
29	2	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
30	3	42/48 (88%)	42 (100%)	0	0	100	100
31	4	90/92 (98%)	85 (94%)	3 (3%)	2 (2%)	8	28
All	All	3633/4235 (86%)	3313 (91%)	262 (7%)	58 (2%)	12	38

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	139	ASP
7	F	20	LYS
7	F	93	LEU
7	F	95	THR
7	F	173	GLU

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Mol	Chain	Res	Type
9	H	101	ALA
11	J	162	SER
14	M	80	ASP
16	O	154	LEU
16	O	164	ASP
16	O	183	ASP
24	W	43	PRO
4	C	34	ASP
4	C	37	VAL
4	C	132	ASP
5	D	34	GLY
5	D	169	GLY
7	F	11	HIS
7	F	171	ASP
11	J	164	ALA
12	K	5	GLU
16	O	162	ASP
28	1	81	LYS
31	4	56	PRO
31	4	57	GLY
5	D	184	ASP
7	F	137	PRO
9	H	64	PRO
11	J	40	PRO
11	J	138	PRO
12	K	143	LYS
13	L	126	SER
15	N	140	ALA
16	O	65	ASP
16	O	181	ASP
25	X	49	ASN
25	X	77	ALA
26	Y	77	PHE
4	C	119	ALA
5	D	185	GLY
18	Q	116	SER
22	U	53	GLY
4	C	211	LYS
5	D	2	GLN
5	D	107	SER
9	H	61	MET
12	K	7	ASP

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Mol	Chain	Res	Type
14	M	21	ARG
20	S	81	PRO
6	E	8	LEU
13	L	119	GLN
24	W	40	PRO
11	J	72	VAL
7	F	16	PRO
8	G	44	GLY
26	Y	70	ILE
15	N	110	PRO
11	J	110	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	C	179/181 (99%)	166 (93%)	13 (7%)	17	44
5	D	282/282 (100%)	264 (94%)	18 (6%)	22	52
6	E	193/193 (100%)	177 (92%)	16 (8%)	14	38
7	F	117/147 (80%)	109 (93%)	8 (7%)	20	49
8	G	152/155 (98%)	148 (97%)	4 (3%)	54	86
9	H	92/92 (100%)	91 (99%)	1 (1%)	80	95
10	I	27/283 (10%)	27 (100%)	0	100	100
11	J	122/122 (100%)	110 (90%)	12 (10%)	10	28
12	K	118/121 (98%)	109 (92%)	9 (8%)	16	42
13	L	106/106 (100%)	103 (97%)	3 (3%)	51	84
14	M	112/126 (89%)	109 (97%)	3 (3%)	52	85
15	N	166/166 (100%)	157 (95%)	9 (5%)	27	60
16	O	149/149 (100%)	144 (97%)	5 (3%)	44	78
17	P	93/93 (100%)	91 (98%)	2 (2%)	60	89
18	Q	113/116 (97%)	110 (97%)	3 (3%)	52	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	R	79/79 (100%)	75 (95%)	4 (5%)	29	63
20	S	117/121 (97%)	113 (97%)	4 (3%)	44	78
21	T	71/73 (97%)	71 (100%)	0	100	100
22	U	105/105 (100%)	104 (99%)	1 (1%)	82	96
23	V	44/52 (85%)	44 (100%)	0	100	100
24	W	51/56 (91%)	50 (98%)	1 (2%)	63	90
25	X	130/130 (100%)	123 (95%)	7 (5%)	27	60
26	Y	66/73 (90%)	62 (94%)	4 (6%)	23	55
27	Z	120/195 (62%)	113 (94%)	7 (6%)	25	57
28	1	56/56 (100%)	51 (91%)	5 (9%)	12	34
29	2	46/46 (100%)	46 (100%)	0	100	100
30	3	42/44 (96%)	41 (98%)	1 (2%)	57	87
31	4	79/79 (100%)	76 (96%)	3 (4%)	40	74
All	All	3027/3441 (88%)	2884 (95%)	143 (5%)	32	67

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	3	ARG
4	C	33	GLU
4	C	36	ASP
4	C	55	VAL
4	C	68	ILE
4	C	69	LEU
4	C	78	ASP
4	C	94	LEU
4	C	120	ARG
4	C	131	HIS
4	C	153	ARG
4	C	179	MET
4	C	217	ARG
5	D	7	ARG
5	D	11	LEU
5	D	27	ASN
5	D	33	ASP
5	D	63	GLU
5	D	97	LEU

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Mol	Chain	Res	Type
5	D	98	THR
5	D	103	ASP
5	D	162	MET
5	D	190	MET
5	D	234	ARG
5	D	245	SER
5	D	251	VAL
5	D	254	GLN
5	D	264	GLU
5	D	304	PRO
5	D	307	ARG
5	D	312	ARG
6	E	2	GLN
6	E	27	ARG
6	E	67	GLN
6	E	76	ARG
6	E	78	ARG
6	E	91	PRO
6	E	94	THR
6	E	101	ASP
6	E	136	VAL
6	E	187	ARG
6	E	214	THR
6	E	222	ASP
6	E	223	LEU
6	E	234	VAL
6	E	236	THR
6	E	240	LEU
7	F	24	HIS
7	F	61	PHE
7	F	99	ASP
7	F	131	THR
7	F	133	ASN
7	F	136	ARG
7	F	137	PRO
7	F	149	ARG
8	G	7	ILE
8	G	54	ASP
8	G	102	VAL
8	G	164	ASP
9	H	1	PRO
11	J	1	LYS

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Mol	Chain	Res	Type
11	J	30	GLN
11	J	59	ASN
11	J	61	LEU
11	J	72	VAL
11	J	73	GLN
11	J	82	LYS
11	J	86	ARG
11	J	129	ASN
11	J	142	VAL
11	J	150	LYS
11	J	166	ASN
12	K	46	ILE
12	K	52	GLN
12	K	74	ARG
12	K	79	PHE
12	K	107	ASN
12	K	112	ASP
12	K	120	SER
12	K	125	SER
12	K	127	ILE
13	L	7	ASP
13	L	10	GLN
13	L	98	VAL
14	M	35	ARG
14	M	80	ASP
14	M	117	GLU
15	N	38	VAL
15	N	46	LEU
15	N	68	ARG
15	N	81	ARG
15	N	87	MET
15	N	93	ARG
15	N	99	ARG
15	N	116	ASN
15	N	164	THR
16	O	26	LEU
16	O	127	LEU
16	O	128	ASP
16	O	152	GLU
16	O	163	PHE
17	P	3	THR
17	P	98	LEU

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Mol	Chain	Res	Type
18	Q	52	LYS
18	Q	91	LYS
18	Q	98	ILE
19	R	11	ARG
19	R	16	ASN
19	R	57	ASP
19	R	95	GLU
20	S	13	THR
20	S	39	THR
20	S	82	GLU
20	S	132	ARG
22	U	39	ASN
24	W	43	PRO
25	X	35	VAL
25	X	52	VAL
25	X	73	LEU
25	X	122	ARG
25	X	142	ASP
25	X	146	ILE
25	X	154	ARG
26	Y	15	ARG
26	Y	27	ASP
26	Y	49	ARG
26	Y	72	VAL
27	Z	141	THR
27	Z	163	THR
27	Z	172	THR
27	Z	186	ARG
27	Z	189	ASN
27	Z	200	THR
27	Z	203	VAL
28	1	11	THR
28	1	42	CYS
28	1	44	PHE
28	1	49	ARG
28	1	64	ILE
30	3	18	ASN
31	4	42	ARG
31	4	56	PRO
31	4	65	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	47	HIS
4	C	92	ASN
4	C	127	GLN
4	C	199	HIS
5	D	27	ASN
5	D	145	HIS
5	D	238	ASN
5	D	256	GLN
5	D	260	HIS
5	D	332	ASN
6	E	2	GLN
6	E	39	GLN
6	E	129	HIS
6	E	163	HIS
7	F	103	ASN
7	F	133	ASN
8	G	106	ASN
8	G	143	GLN
10	I	17	GLN
10	I	64	ASN
11	J	8	ASN
11	J	35	ASN
11	J	55	GLN
11	J	58	HIS
11	J	59	ASN
11	J	69	ASN
11	J	74	ASN
11	J	80	ASN
11	J	91	HIS
11	J	129	ASN
11	J	130	HIS
11	J	137	ASN
11	J	166	ASN
12	K	52	GLN
12	K	107	ASN
12	K	126	ASN
13	L	10	GLN
13	L	42	ASN
14	M	18	HIS
14	M	41	HIS
14	M	42	ASN
14	M	116	HIS
15	N	26	HIS

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Mol	Chain	Res	Type
15	N	58	GLN
15	N	89	ASN
15	N	176	GLN
16	O	107	ASN
16	O	153	GLN
17	P	53	GLN
18	Q	50	GLN
18	Q	66	GLN
18	Q	73	HIS
18	Q	118	GLN
19	R	16	ASN
19	R	40	HIS
20	S	61	GLN
20	S	94	ASN
20	S	98	ASN
20	S	113	HIS
20	S	117	HIS
20	S	122	GLN
21	T	53	ASN
22	U	39	ASN
22	U	43	ASN
22	U	73	HIS
23	V	39	ASN
23	V	48	ASN
24	W	60	GLN
25	X	27	HIS
25	X	87	HIS
25	X	110	GLN
25	X	119	HIS
25	X	125	HIS
25	X	141	HIS
26	Y	23	HIS
27	Z	133	HIS
27	Z	134	HIS
27	Z	149	GLN
27	Z	189	ASN
28	1	33	HIS
28	1	70	GLN
29	2	8	GLN
29	2	16	HIS
29	2	28	HIS
30	3	16	ASN

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Mol	Chain	Res	Type
30	3	18	ASN
30	3	41	HIS
30	3	45	ASN
31	4	30	GLN
31	4	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	237 (8%)	38 (1%)
2	B	121/122 (99%)	15 (12%)	3 (2%)
3	5	2/3 (66%)	1 (50%)	0
All	All	2870/3047 (94%)	253 (8%)	41 (1%)

All (253) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	A
1	A	31	C
1	A	60	A
1	A	67	A
1	A	69	A
1	A	70	A
1	A	71	G
1	A	87	C
1	A	88	G
1	A	114	A
1	A	115	U
1	A	120	A
1	A	130	C
1	A	139	C
1	A	141	C
1	A	151	A
1	A	166	A
1	A	169	A
1	A	185	G
1	A	186	A
1	A	191	A
1	A	192	A
1	A	219	G
1	A	237	G

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Mol	Chain	Res	Type
1	A	271	C
1	A	272	A
1	A	273	G
1	A	283	U
1	A	284	C
1	A	285	A
1	A	308	U
1	A	309	C
1	A	318	C
1	A	336	G
1	A	337	A
1	A	345	G
1	A	358	G
1	A	381	G
1	A	397	A
1	A	417	G
1	A	461	C
1	A	487	G
1	A	498	A
1	A	510	U
1	A	511	A
1	A	514	G
1	A	537	G
1	A	538	C
1	A	539	G
1	A	542	A
1	A	545	G
1	A	553	G
1	A	559	U
1	A	588	G
1	A	604	G
1	A	620	A
1	A	632	A
1	A	644	G
1	A	660	A
1	A	688	A
1	A	701	U
1	A	705	C
1	A	717	C
1	A	759	C
1	A	777	U
1	A	809	G

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Mol	Chain	Res	Type
1	A	821	U
1	A	835	U
1	A	840	U
1	A	857	A
1	A	868	G
1	A	869	G
1	A	871	G
1	A	872	U
1	A	875	A
1	A	877	G
1	A	878	G
1	A	882	A
1	A	885	G
1	A	898	G
1	A	905	C
1	A	920	C
1	A	921	G
1	A	923	A
1	A	953	G
1	A	960	G
1	A	961	A
1	A	1006	A
1	A	1008	C
1	A	1029	U
1	A	1045	G
1	A	1059	G
1	A	1060	C
1	A	1072	G
1	A	1081	A
1	A	1087	G
1	A	1088	A
1	A	1109	U
1	A	1110	G
1	A	1119	G
1	A	1130	U
1	A	1161	A
1	A	1162	G
1	A	1164	U
1	A	1165	G
1	A	1166	A
1	A	1171	A
1	A	1174	A

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Mol	Chain	Res	Type
1	A	1175	G
1	A	1177	A
1	A	1185	U
1	A	1192	A
1	A	1193	A
1	A	1206	U
1	A	1208	C
1	A	1216	G
1	A	1237	U
1	A	1238	C
1	A	1239	G
1	A	1279	U
1	A	1289	C
1	A	1342	C
1	A	1353	C
1	A	1360	C
1	A	1377	C
1	A	1407	A
1	A	1451	C
1	A	1474	C
1	A	1485	A
1	A	1488	U
1	A	1505	U
1	A	1506	U
1	A	1524	U
1	A	1525	G
1	A	1526	A
1	A	1564	C
1	A	1580	A
1	A	1592	G
1	A	1625	U
1	A	1626	A
1	A	1633	C
1	A	1634	G
1	A	1656	A
1	A	1667	A
1	A	1682	A
1	A	1684	A
1	A	1685	A
1	A	1692	C
1	A	1701	A
1	A	1722	U

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Mol	Chain	Res	Type
1	A	1723	G
1	A	1725	C
1	A	1731	C
1	A	1752	G
1	A	1778	A
1	A	1798	C
1	A	1820	G
1	A	1829	A
1	A	1856	C
1	A	1879	U
1	A	1904	A
1	A	1919	A
1	A	1942	A
1	A	1971	G
1	A	1973	A
1	A	1974	G
1	A	1978	A
1	A	1979	G
1	A	1980	U
1	A	1982	C
1	A	1996	U
1	A	2008	U
1	A	2011	A
1	A	2012	U
1	A	2013	G
1	A	2033	G
1	A	2034	U
1	A	2064	U
1	A	2072	G
1	A	2073	G
1	A	2074	A
1	A	2096	A
1	A	2101	A
1	A	2102	G
1	A	2103	A
1	A	2110	G
1	A	2238	A
1	A	2258	A
1	A	2271	G
1	A	2272	G
1	A	2317	C
1	A	2321	A

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Mol	Chain	Res	Type
1	A	2354	A
1	A	2361	A
1	A	2369	A
1	A	2422	U
1	A	2462	G
1	A	2469	A
1	A	2476	C
1	A	2480	G
1	A	2483	A
1	A	2507	G
1	A	2511	A
1	A	2533	C
1	A	2537	G
1	A	2541	U
1	A	2553	A
1	A	2564	G
1	A	2589	U
1	A	2601	A
1	A	2602	G
1	A	2608	C
1	A	2613	G
1	A	2637	A
1	A	2649	A
1	A	2664	A
1	A	2681	A
1	A	2682	C
1	A	2719	A
1	A	2726	U
1	A	2747	C
1	A	2748	G
1	A	2749	U
1	A	2750	G
1	A	2762	C
1	A	2768	A
1	A	2786	G
1	A	2792	A
1	A	2800	A
1	A	2811	A
1	A	2825	C
1	A	2850	C
1	A	2876	G
1	A	2890	A

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Mol	Chain	Res	Type
1	A	2896	A
1	A	2903	C
1	A	2914	A
2	B	3002	U
2	B	3011	A
2	B	3014	G
2	B	3022	G
2	B	3024	U
2	B	3041	C
2	B	3043	G
2	B	3044	A
2	B	3052	A
2	B	3056	A
2	B	3057	A
2	B	3066	G
2	B	3077	A
2	B	3114	G
2	B	3122	C
3	5	9076	A

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	10	U
1	A	69	A
1	A	129	A
1	A	284	C
1	A	338	C
1	A	603	A
1	A	644	G
1	A	699	C
1	A	716	G
1	A	834	G
1	A	857	A
1	A	871	G
1	A	877	G
1	A	1080	C
1	A	1164	U
1	A	1232	A
1	A	1237	U
1	A	1352	A
1	A	1377	C

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Mol	Chain	Res	Type
1	A	1450	C
1	A	1563	G
1	A	1667	A
1	A	1684	A
1	A	1692	C
1	A	1730	G
1	A	1856	C
1	A	1942	A
1	A	1979	G
1	A	2011	A
1	A	2313	C
1	A	2467	A
1	A	2526	C
1	A	2536	C
1	A	2649	A
1	A	2718	C
1	A	2726	U
1	A	2761	A
1	A	2791	U
2	B	3023	U
2	B	3065	A
2	B	3103	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 237 ligands modelled in this entry, 234 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
37	PHA	5	9077	3,38	10,11,11	0.78	0	10,13,13	0.40	0
38	ACA	5	9078	37	7,7,8	1.80	2 (28%)	5,6,8	0.79	0
36	SPS	5	9080	32	17,23,23	1.97	5 (29%)	15,30,30	2.12	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	PHA	5	9077	3,38	-	0/4/6/6	0/1/1/1
38	ACA	5	9078	37	-	0/4/5/6	0/0/0/0
36	SPS	5	9080	32	-	0/15/18/18	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	9080	SPS	C9-C10	-3.26	1.41	1.48
36	5	9080	SPS	O15-S15	-2.63	1.41	1.50
38	5	9078	ACA	C3-C2	-2.47	1.42	1.52
36	5	9080	SPS	C1-N2	2.71	1.38	1.33
36	5	9080	SPS	C5-N4	2.93	1.38	1.34
38	5	9078	ACA	C2-C1	3.65	1.60	1.49
36	5	9080	SPS	C1-C6	4.89	1.54	1.44

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	9080	SPS	C7-C5-C6	-2.43	120.75	123.69
36	5	9080	SPS	C9-C10-N11	2.15	118.85	114.12
36	5	9080	SPS	C1-N2-C3	6.58	120.94	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	5	9080	SPS	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	2754/2922 (94%)	0.01	69 (2%) 61 48	18, 43, 87, 135	0
2	B	122/122 (100%)	0.30	4 (3%) 50 38	35, 60, 87, 145	0
3	5	3/3 (100%)	-0.07	0 100 100	33, 33, 35, 36	0
4	C	237/239 (99%)	0.13	11 (4%) 36 25	24, 47, 79, 101	0
5	D	337/337 (100%)	-0.00	5 (1%) 76 68	25, 53, 79, 88	0
6	E	246/246 (100%)	-0.28	0 100 100	21, 42, 64, 75	0
7	F	140/176 (79%)	2.06	73 (52%) 0 0	51, 94, 112, 118	0
8	G	172/177 (97%)	0.95	17 (9%) 9 4	44, 67, 85, 92	0
9	H	119/119 (100%)	0.58	12 (10%) 9 4	45, 66, 91, 97	0
10	I	29/348 (8%)	2.43	19 (65%) 0 0	66, 85, 93, 96	0
11	J	156/167 (93%)	0.33	10 (6%) 23 14	34, 52, 77, 80	0
12	K	142/145 (97%)	0.00	0 100 100	33, 49, 68, 86	0
13	L	132/132 (100%)	-0.10	2 (1%) 76 68	31, 50, 70, 80	0
14	M	145/164 (88%)	0.41	11 (7%) 17 9	20, 60, 98, 111	0
15	N	194/194 (100%)	-0.14	3 (1%) 76 68	28, 39, 58, 68	0
16	O	186/186 (100%)	0.54	20 (10%) 8 3	36, 59, 99, 111	0
17	P	115/115 (100%)	-0.05	1 (0%) 85 79	35, 49, 67, 77	0
18	Q	143/148 (96%)	0.13	1 (0%) 89 84	36, 52, 64, 74	0
19	R	95/95 (100%)	-0.11	1 (1%) 82 74	29, 40, 54, 70	0
20	S	150/154 (97%)	-0.22	0 100 100	29, 41, 61, 70	0
21	T	81/84 (96%)	0.10	2 (2%) 61 48	40, 54, 73, 80	0
22	U	119/119 (100%)	0.34	10 (8%) 14 6	36, 52, 76, 90	0
23	V	53/66 (80%)	0.22	1 (1%) 70 59	39, 53, 69, 77	0
24	W	65/70 (92%)	1.29	14 (21%) 1 1	49, 68, 105, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	154/154 (100%)	-0.25	0 100 100	32, 45, 63, 72	0
26	Y	82/91 (90%)	0.15	4 (4%) 33 22	40, 57, 79, 99	0
27	Z	142/240 (59%)	-0.09	2 (1%) 78 69	24, 41, 65, 82	0
28	1	73/73 (100%)	0.24	4 (5%) 29 18	46, 60, 71, 79	0
29	2	56/56 (100%)	-0.60	0 100 100	24, 29, 35, 43	0
30	3	46/48 (95%)	0.41	4 (8%) 13 6	31, 57, 84, 98	0
31	4	92/92 (100%)	0.10	1 (1%) 82 74	31, 51, 64, 78	0
All	All	6580/7282 (90%)	0.13	301 (4%) 36 25	18, 48, 88, 145	0

All (301) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	W	1	THR	10.9
1	A	1172	G	6.8
2	B	3001	U	6.5
7	F	88	LEU	6.2
7	F	57	THR	6.1
7	F	69	ILE	5.9
16	O	166	ALA	5.8
1	A	1173	A	5.8
7	F	62	ASP	5.6
21	T	81	ILE	5.5
16	O	186	LEU	5.5
1	A	1177	A	5.4
5	D	1	PRO	5.4
7	F	63	ILE	5.4
7	F	18	ILE	5.3
24	W	40	PRO	5.1
10	I	24	VAL	5.0
9	H	106	THR	5.0
7	F	90	LEU	4.8
8	G	45	ASP	4.8
1	A	2237	G	4.7
7	F	10	PHE	4.7
16	O	162	ASP	4.6
7	F	27	ILE	4.5
24	W	39	ALA	4.5
10	I	23	ILE	4.5
24	W	43	PRO	4.4
1	A	735	C	4.3

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Mol	Chain	Res	Type	RSRZ
7	F	66	GLY	4.3
10	I	27	ILE	4.3
1	A	1175	G	4.3
7	F	56	ARG	4.2
10	I	26	MET	4.1
1	A	1525	G	4.1
1	A	1951	G	4.1
7	F	26	GLY	4.1
4	C	85	ASP	3.9
24	W	38	GLY	3.9
1	A	960	G	3.9
28	1	22	ILE	3.9
7	F	170	TYR	3.9
4	C	36	ASP	3.8
1	A	1950	G	3.8
1	A	1171	A	3.8
26	Y	80	GLU	3.8
7	F	67	ASP	3.8
11	J	32	ASP	3.8
14	M	104	ASP	3.7
2	B	3023	U	3.7
7	F	92	GLU	3.7
1	A	1199	A	3.7
1	A	1192	A	3.7
7	F	44	ILE	3.7
16	O	152	GLU	3.6
1	A	1181	A	3.6
1	A	282	C	3.6
7	F	58	VAL	3.6
7	F	84	LEU	3.6
7	F	102	GLY	3.6
10	I	65	THR	3.6
8	G	100	ASP	3.6
7	F	104	PHE	3.6
26	Y	88	GLU	3.5
28	1	11	THR	3.5
16	O	165	ALA	3.5
1	A	1198	U	3.5
16	O	139	TRP	3.5
1	A	1168	C	3.5
7	F	25	MET	3.5
7	F	165	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
16	O	148	ALA	3.4
14	M	102	ASP	3.4
7	F	72	LYS	3.4
7	F	24	HIS	3.4
1	A	1200	A	3.4
9	H	17	LEU	3.4
16	O	143	ARG	3.4
7	F	166	ILE	3.4
24	W	41	GLU	3.3
14	M	100	ALA	3.3
1	A	1182	C	3.3
14	M	60	GLU	3.3
1	A	1201	C	3.3
2	B	3122	C	3.3
7	F	17	ARG	3.3
19	R	95	GLU	3.3
4	C	35	GLY	3.3
7	F	85	GLN	3.3
7	F	53	LYS	3.2
11	J	83	PHE	3.2
7	F	129	ASP	3.2
1	A	1169	U	3.2
4	C	31	LYS	3.2
1	A	1203	G	3.2
16	O	138	ASP	3.2
1	A	285	A	3.2
7	F	128	LEU	3.2
8	G	10	ASP	3.2
1	A	1167	G	3.2
1	A	2238	A	3.2
7	F	51	ARG	3.2
7	F	65	GLU	3.2
7	F	89	PRO	3.1
7	F	75	LEU	3.1
7	F	157	LEU	3.1
4	C	37	VAL	3.1
23	V	47	ARG	3.1
7	F	64	ARG	3.1
1	A	1190	G	3.1
22	U	116	ASP	3.1
8	G	28	SER	3.1
22	U	119	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
22	U	115	GLU	3.1
10	I	12	ILE	3.0
10	I	20	VAL	3.0
8	G	122	THR	3.0
1	A	1162	G	3.0
1	A	1178	G	3.0
1	A	284	C	3.0
14	M	105	TYR	3.0
14	M	97	VAL	3.0
7	F	45	THR	3.0
10	I	15	TRP	3.0
4	C	32	VAL	3.0
7	F	73	VAL	3.0
1	A	1174	A	3.0
1	A	1186	C	3.0
27	Z	235	GLU	3.0
1	A	1163	G	3.0
16	O	145	ALA	2.9
14	M	80	ASP	2.9
16	O	178	THR	2.9
7	F	70	GLY	2.9
1	A	370	G	2.9
9	H	26	THR	2.9
26	Y	74	ALA	2.9
7	F	81	GLU	2.9
2	B	3002	U	2.9
7	F	130	VAL	2.9
10	I	13	PRO	2.8
1	A	372	A	2.8
10	I	71	LEU	2.8
22	U	117	ASP	2.8
1	A	1204	C	2.8
16	O	159	TYR	2.8
7	F	55	LYS	2.8
10	I	66	LEU	2.7
1	A	1184	C	2.7
14	M	106	VAL	2.7
11	J	36	ASN	2.7
7	F	86	THR	2.7
7	F	41	LEU	2.7
7	F	29	HIS	2.7
13	L	119	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	999	C	2.7
5	D	117	GLU	2.7
11	J	72	VAL	2.7
7	F	61	PHE	2.6
8	G	42	VAL	2.6
7	F	106	PHE	2.6
1	A	1166	A	2.6
1	A	2345	A	2.6
24	W	2	VAL	2.6
10	I	72	ASP	2.6
1	A	1202	A	2.6
7	F	87	ALA	2.6
17	P	23	GLY	2.6
28	1	44	PHE	2.6
9	H	108	LEU	2.6
22	U	118	SER	2.6
7	F	68	PRO	2.6
8	G	72	MET	2.6
16	O	150	TYR	2.6
1	A	1161	A	2.6
4	C	133	ARG	2.6
9	H	103	ALA	2.6
8	G	82	TYR	2.6
30	3	49	GLU	2.5
8	G	154	ILE	2.5
16	O	140	GLN	2.5
1	A	2344	G	2.5
7	F	47	GLN	2.5
1	A	2239	C	2.5
8	G	128	GLY	2.5
24	W	37	GLY	2.5
9	H	44	SER	2.5
4	C	237	GLY	2.5
10	I	21	ASP	2.5
1	A	970	U	2.5
5	D	133	GLU	2.5
16	O	158	LEU	2.5
18	Q	77	ALA	2.5
9	H	119	ARG	2.5
1	A	805	G	2.5
1	A	128	A	2.5
7	F	49	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
7	F	172	VAL	2.5
1	A	969	G	2.4
7	F	43	GLU	2.4
7	F	98	PHE	2.4
11	J	81	TYR	2.4
1	A	1193	A	2.4
1	A	1948	G	2.4
7	F	135	VAL	2.4
10	I	16	LYS	2.4
24	W	6	GLN	2.4
7	F	23	VAL	2.4
1	A	280	C	2.4
22	U	112	LEU	2.4
7	F	71	ALA	2.4
1	A	1208	C	2.4
7	F	40	ILE	2.3
24	W	59	ILE	2.3
11	J	146	TRP	2.3
7	F	134	LEU	2.3
14	M	145	LEU	2.3
7	F	154	LYS	2.3
16	O	147	ILE	2.3
7	F	50	VAL	2.3
24	W	3	LEU	2.3
30	3	36	ASN	2.3
16	O	163	PHE	2.3
28	1	38	LYS	2.3
1	A	2850	C	2.3
4	C	64	ASP	2.3
10	I	73	ASP	2.3
27	Z	108	ASP	2.3
11	J	158	ASN	2.3
24	W	44	GLY	2.3
1	A	736	A	2.3
1	A	1176	C	2.3
1	A	1165	G	2.3
22	U	1	SER	2.3
1	A	1170	U	2.3
1	A	1527	A	2.3
9	H	99	THR	2.3
22	U	107	LYS	2.3
1	A	1197	G	2.2

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Mol	Chain	Res	Type	RSRZ
21	T	70	GLU	2.2
7	F	52	THR	2.2
16	O	179	LEU	2.2
10	I	69	ARG	2.2
22	U	33	GLU	2.2
15	N	87	MET	2.2
16	O	137	ALA	2.2
7	F	11	HIS	2.2
7	F	91	ALA	2.2
8	G	126	ILE	2.2
7	F	171	ASP	2.2
4	C	38	ILE	2.2
24	W	8	ILE	2.2
1	A	2508	C	2.2
13	L	132	VAL	2.2
14	M	91	VAL	2.2
7	F	16	PRO	2.2
1	A	1179	C	2.2
10	I	17	GLN	2.2
8	G	121	ASP	2.2
16	O	177	GLU	2.2
7	F	93	LEU	2.2
9	H	19	ALA	2.2
15	N	152	ARG	2.2
9	H	107	VAL	2.2
22	U	35	TYR	2.2
1	A	1183	C	2.1
4	C	34	ASP	2.1
7	F	48	MET	2.1
11	J	139	ASP	2.1
7	F	137	PRO	2.1
7	F	101	THR	2.1
10	I	28	GLU	2.1
1	A	272	A	2.1
7	F	59	GLY	2.1
7	F	173	GLU	2.1
11	J	79	ALA	2.1
26	Y	7	GLU	2.1
1	A	288	A	2.1
8	G	88	TYR	2.1
1	A	2852	A	2.1
8	G	22	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
14	M	150	GLN	2.1
7	F	74	THR	2.1
30	3	35	ARG	2.1
1	A	1185	U	2.1
11	J	80	ASN	2.1
8	G	95	VAL	2.1
1	A	1949	G	2.1
31	4	92	GLU	2.1
30	3	37	HIS	2.0
5	D	181	ILE	2.0
1	A	1526	A	2.0
8	G	27	GLY	2.0
1	A	1000	C	2.0
24	W	45	ARG	2.0
9	H	22	VAL	2.0
9	H	102	GLY	2.0
15	N	194	ALA	2.0
10	I	25	GLU	2.0
1	A	1913	C	2.0
5	D	134	ALA	2.0
8	G	129	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
33	NA	A	8340	1/1	0.95	0.47	68.63	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	NA	S	8386	1/1	0.37	0.92	41.74	91,91,91,91	0
33	NA	A	8374	1/1	0.98	0.68	34.60	53,53,53,53	0
33	NA	A	8362	1/1	0.92	0.31	26.91	64,64,64,64	0
33	NA	A	8378	1/1	0.96	0.54	25.28	47,47,47,47	0
38	ACA	5	9078	8/9	0.79	0.38	24.08	45,53,55,55	0
34	K	A	8390	1/1	0.91	0.36	21.26	70,70,70,70	0
33	NA	A	8364	1/1	0.84	0.27	20.93	39,39,39,39	0
33	NA	A	8373	1/1	0.93	0.48	19.75	50,50,50,50	0
35	CL	A	8515	1/1	0.96	0.34	18.06	65,65,65,65	0
33	NA	A	8325	1/1	0.99	0.36	18.06	50,50,50,50	0
33	NA	A	8361	1/1	0.97	0.28	14.69	47,47,47,47	0
33	NA	A	8350	1/1	0.96	0.24	13.57	32,32,32,32	0
33	NA	A	8372	1/1	0.86	0.44	12.94	58,58,58,58	0
34	K	A	8391	1/1	0.99	0.24	12.67	48,48,48,48	0
33	NA	A	8371	1/1	0.85	0.32	12.36	61,61,61,61	0
33	NA	A	8356	1/1	0.95	0.28	12.09	47,47,47,47	0
33	NA	A	8359	1/1	0.84	0.38	11.56	40,40,40,40	0
33	NA	B	8383	1/1	0.80	0.61	11.53	69,69,69,69	0
33	NA	M	8380	1/1	0.89	0.41	11.49	64,64,64,64	0
37	PHA	5	9077	11/11	0.96	0.24	7.33	41,45,52,53	0
33	NA	A	8310	1/1	0.89	0.26	7.20	39,39,39,39	0
33	NA	A	8335	1/1	0.93	0.22	7.17	43,43,43,43	0
33	NA	A	8368	1/1	0.73	0.21	6.80	56,56,56,56	0
33	NA	A	8366	1/1	0.92	0.49	6.55	68,68,68,68	0
36	SPS	5	9080	23/23	0.96	0.21	5.94	30,33,47,49	0
32	MG	A	8060	1/1	0.99	0.18	3.76	42,42,42,42	0
33	NA	A	8303	1/1	0.93	0.18	3.08	43,43,43,43	0
33	NA	A	8331	1/1	0.96	0.17	2.47	31,31,31,31	0
33	NA	A	8321	1/1	0.97	0.18	2.26	54,54,54,54	0
33	NA	A	8382	1/1	0.90	0.17	1.72	72,72,72,72	0
32	MG	A	8112	1/1	0.98	0.18	1.36	28,28,28,28	0
33	NA	A	8314	1/1	0.89	0.19	1.34	38,38,38,38	0
32	MG	A	8013	1/1	0.97	0.17	1.03	32,32,32,32	0
33	NA	A	8302	1/1	0.97	0.15	0.98	46,46,46,46	0
33	NA	A	8365	1/1	0.91	0.24	0.75	43,43,43,43	0
33	NA	S	8337	1/1	0.95	0.19	0.69	28,28,28,28	0
32	MG	A	8053	1/1	0.95	0.14	0.35	50,50,50,50	0
33	NA	A	8324	1/1	0.71	0.18	0.17	55,55,55,55	0
32	MG	A	8064	1/1	0.98	0.14	0.02	31,31,31,31	0
35	CL	A	8505	1/1	0.97	0.16	-0.07	49,49,49,49	0
33	NA	A	8332	1/1	0.93	0.14	-0.10	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	8119	1/1	0.95	0.14	-0.13	41,41,41,41	0
33	NA	A	8333	1/1	0.79	0.15	-0.20	33,33,33,33	0
32	MG	A	8070	1/1	0.94	0.15	-0.24	47,47,47,47	0
33	NA	A	8353	1/1	0.94	0.15	-0.42	23,23,23,23	0
33	NA	A	8317	1/1	0.95	0.17	-0.54	45,45,45,45	0
33	NA	U	8343	1/1	0.92	0.15	-0.69	33,33,33,33	0
33	NA	R	8348	1/1	0.97	0.17	-0.86	42,42,42,42	0
33	NA	A	8339	1/1	0.97	0.14	-0.97	22,22,22,22	0
35	CL	4	8504	1/1	0.94	0.14	-1.04	67,67,67,67	0
33	NA	A	8376	1/1	0.98	0.14	-1.08	47,47,47,47	0
35	CL	A	8516	1/1	0.97	0.13	-1.13	56,56,56,56	0
33	NA	N	8347	1/1	0.93	0.12	-1.50	23,23,23,23	0
33	NA	A	8309	1/1	0.95	0.09	-1.62	32,32,32,32	0
32	MG	A	8027	1/1	0.94	0.08	-1.64	49,49,49,49	0
33	NA	A	8379	1/1	0.97	0.12	-1.67	45,45,45,45	0
32	MG	C	8065	1/1	0.99	0.11	-1.83	31,31,31,31	0
35	CL	A	8512	1/1	0.97	0.09	-1.98	47,47,47,47	0
39	CD	V	8401	1/1	1.00	0.07	-2.00	62,62,62,62	0
32	MG	A	8108	1/1	0.94	0.13	-2.00	60,60,60,60	0
35	CL	P	8508	1/1	0.96	0.10	-2.09	62,62,62,62	0
39	CD	1	8403	1/1	0.99	0.08	-2.12	62,62,62,62	0
35	CL	N	8518	1/1	0.98	0.12	-2.13	39,39,39,39	0
39	CD	4	8404	1/1	0.99	0.06	-2.20	57,57,57,57	0
33	NA	C	8345	1/1	0.94	0.13	-2.28	44,44,44,44	0
33	NA	A	8305	1/1	0.94	0.13	-2.36	35,35,35,35	0
32	MG	A	8074	1/1	0.99	0.03	-2.40	29,29,29,29	0
32	MG	A	8033	1/1	0.97	0.11	-2.62	28,28,28,28	0
39	CD	2	8402	1/1	0.99	0.07	-2.62	56,56,56,56	0
32	MG	A	8107	1/1	0.96	0.05	-2.63	43,43,43,43	0
33	NA	K	8346	1/1	0.96	0.08	-2.64	40,40,40,40	0
32	MG	A	8062	1/1	0.96	0.10	-2.68	48,48,48,48	0
35	CL	K	8521	1/1	0.93	0.10	-2.68	50,50,50,50	0
32	MG	A	8057	1/1	0.93	0.13	-2.75	40,40,40,40	0
32	MG	A	8058	1/1	0.97	0.11	-2.85	37,37,37,37	0
32	MG	U	8073	1/1	0.95	0.09	-2.88	46,46,46,46	0
35	CL	D	8519	1/1	0.98	0.11	-2.97	40,40,40,40	0
33	NA	A	8338	1/1	0.96	0.09	-3.00	41,41,41,41	0
33	NA	A	8327	1/1	0.98	0.11	-3.29	41,41,41,41	0
32	MG	A	8059	1/1	0.96	0.13	-3.36	35,35,35,35	0
32	MG	A	8003	1/1	0.99	0.12	-3.48	26,26,26,26	0
32	MG	A	8067	1/1	0.97	0.12	-3.74	43,43,43,43	0
32	MG	A	8055	1/1	0.96	0.08	-3.77	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	8001	1/1	0.98	0.07	-3.87	27,27,27,27	0
32	MG	A	8110	1/1	0.98	0.11	-4.01	35,35,35,35	0
32	MG	A	8018	1/1	0.99	0.09	-4.19	31,31,31,31	0
32	MG	A	8056	1/1	0.97	0.06	-4.21	39,39,39,39	0
33	NA	A	8320	1/1	0.98	0.11	-4.22	38,38,38,38	0
32	MG	A	8012	1/1	0.99	0.09	-4.27	28,28,28,28	0
32	MG	4	8078	1/1	0.98	0.04	-4.41	41,41,41,41	0
33	NA	A	8308	1/1	0.90	0.10	-4.47	43,43,43,43	0
32	MG	A	8039	1/1	0.99	0.08	-4.47	42,42,42,42	0
32	MG	A	8021	1/1	0.98	0.11	-4.56	33,33,33,33	0
32	MG	A	8010	1/1	0.99	0.09	-4.71	35,35,35,35	0
32	MG	5	8118	1/1	0.97	0.11	-4.73	29,29,29,29	0
32	MG	A	8015	1/1	0.98	0.09	-4.87	29,29,29,29	0
33	NA	A	8323	1/1	1.00	0.11	-5.25	42,42,42,42	0
32	MG	A	8019	1/1	0.98	0.04	-5.46	29,29,29,29	0
32	MG	Z	8109	1/1	0.97	0.07	-5.61	33,33,33,33	0
32	MG	A	8044	1/1	0.96	0.06	-5.74	36,36,36,36	0
32	MG	A	8038	1/1	0.98	0.09	-5.99	27,27,27,27	0
32	MG	A	8004	1/1	0.96	0.07	-6.01	26,26,26,26	0
32	MG	A	8007	1/1	0.96	0.06	-6.04	16,16,16,16	0
32	MG	A	8032	1/1	0.95	0.08	-6.12	28,28,28,28	0
32	MG	A	8002	1/1	0.99	0.06	-6.12	28,28,28,28	0
32	MG	A	8054	1/1	0.97	0.10	-6.39	24,24,24,24	0
32	MG	A	8096	1/1	0.96	0.07	-6.45	46,46,46,46	0
32	MG	A	8052	1/1	0.97	0.06	-7.72	40,40,40,40	0
32	MG	A	8071	1/1	0.97	0.04	-8.63	63,63,63,63	0
33	NA	A	8344	1/1	0.99	0.05	-8.67	25,25,25,25	0
32	MG	A	8017	1/1	0.99	0.03	-8.67	19,19,19,19	0
32	MG	A	8020	1/1	1.00	0.06	-8.70	28,28,28,28	0
32	MG	A	8028	1/1	0.99	0.09	-9.05	34,34,34,34	0
32	MG	A	8008	1/1	0.97	0.05	-9.79	35,35,35,35	0
32	MG	A	8006	1/1	0.98	0.04	-10.76	30,30,30,30	0
32	MG	A	8035	1/1	0.98	0.03	-10.78	52,52,52,52	0
32	MG	A	8084	1/1	0.99	0.05	-11.19	40,40,40,40	0
32	MG	A	8080	1/1	0.99	0.05	-12.48	36,36,36,36	0
32	MG	A	8077	1/1	0.99	0.06	-13.58	27,27,27,27	0
32	MG	A	8014	1/1	0.99	0.06	-24.42	25,25,25,25	0
32	MG	A	8075	1/1	0.96	0.07	-	37,37,37,37	0
32	MG	A	8115	1/1	0.98	0.06	-	42,42,42,42	0
32	MG	A	8102	1/1	0.98	0.12	-	45,45,45,45	0
33	NA	A	8358	1/1	0.95	0.79	-	82,82,82,82	0
32	MG	L	8069	1/1	0.95	0.07	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	NA	A	8377	1/1	0.93	0.22	-	66,66,66,66	0
32	MG	B	8095	1/1	0.72	0.17	-	70,70,70,70	0
33	NA	A	8363	1/1	0.85	0.25	-	49,49,49,49	0
32	MG	A	8079	1/1	0.96	0.11	-	27,27,27,27	0
32	MG	A	8034	1/1	0.99	0.07	-	33,33,33,33	0
32	MG	A	8101	1/1	0.91	0.13	-	52,52,52,52	0
33	NA	A	8367	1/1	0.95	0.10	-	44,44,44,44	0
35	CL	A	8514	1/1	0.97	0.12	-	46,46,46,46	0
33	NA	A	8375	1/1	0.92	0.60	-	47,47,47,47	0
32	MG	A	8050	1/1	0.93	0.15	-	64,64,64,64	0
32	MG	A	8088	1/1	0.95	0.09	-	30,30,30,30	0
32	MG	A	8016	1/1	0.97	0.11	-	39,39,39,39	0
32	MG	A	8086	1/1	0.99	0.17	-	45,45,45,45	0
32	MG	A	8117	1/1	0.97	0.08	-	25,25,25,25	0
33	NA	A	8328	1/1	0.96	0.32	-	34,34,34,34	0
32	MG	A	8098	1/1	0.96	0.14	-	36,36,36,36	0
32	MG	A	8037	1/1	0.97	0.05	-	34,34,34,34	0
33	NA	A	8318	1/1	0.97	0.41	-	55,55,55,55	0
33	NA	A	8354	1/1	0.96	0.27	-	34,34,34,34	0
33	NA	T	8312	1/1	0.68	0.65	-	79,79,79,79	0
33	NA	A	8334	1/1	0.96	0.06	-	32,32,32,32	0
32	MG	A	8089	1/1	0.89	0.08	-	58,58,58,58	0
35	CL	O	8507	1/1	0.84	0.27	-	59,59,59,59	0
32	MG	A	8111	1/1	0.94	0.10	-	51,51,51,51	0
32	MG	A	8048	1/1	0.98	0.16	-	58,58,58,58	0
32	MG	A	8114	1/1	0.92	0.22	-	54,54,54,54	0
32	MG	A	8093	1/1	0.98	0.07	-	49,49,49,49	0
33	NA	A	8352	1/1	0.76	0.41	-	71,71,71,71	0
32	MG	A	8066	1/1	0.93	0.23	-	84,84,84,84	0
32	MG	A	8072	1/1	0.98	0.10	-	56,56,56,56	0
32	MG	A	8082	1/1	0.91	0.11	-	53,53,53,53	0
33	NA	A	8301	1/1	0.92	0.17	-	46,46,46,46	0
32	MG	A	8030	1/1	0.99	0.10	-	32,32,32,32	0
33	NA	A	8329	1/1	0.75	0.23	-	54,54,54,54	0
33	NA	A	8306	1/1	0.95	0.52	-	32,32,32,32	0
32	MG	A	8040	1/1	0.97	0.12	-	53,53,53,53	0
35	CL	C	8509	1/1	0.94	0.18	-	56,56,56,56	0
32	MG	A	8116	1/1	0.96	0.11	-	51,51,51,51	0
35	CL	Z	8520	1/1	0.93	0.12	-	42,42,42,42	0
32	MG	A	8031	1/1	0.99	0.05	-	27,27,27,27	0
32	MG	A	8063	1/1	0.95	0.05	-	73,73,73,73	0
35	CL	A	8503	1/1	0.95	0.13	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	8042	1/1	0.97	0.12	-	31,31,31,31	0
33	NA	B	8351	1/1	0.59	0.53	-	78,78,78,78	0
33	NA	A	8355	1/1	0.92	0.55	-	56,56,56,56	0
32	MG	A	8068	1/1	0.96	0.16	-	50,50,50,50	0
33	NA	A	8330	1/1	0.98	0.21	-	34,34,34,34	0
32	MG	A	8025	1/1	0.98	0.07	-	40,40,40,40	0
33	NA	A	8315	1/1	0.99	0.10	-	32,32,32,32	0
35	CL	A	8522	1/1	0.98	0.17	-	55,55,55,55	0
32	MG	A	8049	1/1	0.92	0.62	-	77,77,77,77	0
33	NA	A	8316	1/1	0.97	0.21	-	40,40,40,40	0
35	CL	K	8501	1/1	0.96	0.12	-	55,55,55,55	0
33	NA	E	8304	1/1	0.90	0.17	-	33,33,33,33	0
32	MG	A	8041	1/1	0.95	0.16	-	53,53,53,53	0
32	MG	A	8076	1/1	0.80	0.09	-	50,50,50,50	0
32	MG	A	8022	1/1	0.97	0.12	-	40,40,40,40	0
32	MG	A	8103	1/1	0.94	0.18	-	61,61,61,61	0
35	CL	A	8513	1/1	0.98	0.11	-	50,50,50,50	0
32	MG	A	8051	1/1	0.96	0.08	-	57,57,57,57	0
33	NA	A	8349	1/1	0.97	0.14	-	41,41,41,41	0
32	MG	1	8105	1/1	0.89	0.27	-	32,32,32,32	0
32	MG	A	8104	1/1	0.95	0.26	-	52,52,52,52	0
32	MG	A	8091	1/1	0.96	0.05	-	69,69,69,69	0
32	MG	A	8061	1/1	0.96	0.08	-	34,34,34,34	0
32	MG	A	8113	1/1	0.73	0.20	-	43,43,43,43	0
32	MG	A	8094	1/1	0.94	0.04	-	63,63,63,63	0
33	NA	A	8341	1/1	0.91	0.13	-	41,41,41,41	0
33	NA	A	8370	1/1	0.97	0.41	-	57,57,57,57	0
35	CL	S	8506	1/1	0.98	0.11	-	46,46,46,46	0
32	MG	A	8043	1/1	0.97	0.08	-	39,39,39,39	0
39	CD	P	8405	1/1	0.56	0.14	-	174,174,174,174	0
33	NA	A	8384	1/1	0.38	0.82	-	75,75,75,75	0
32	MG	A	8005	1/1	0.96	0.12	-	33,33,33,33	0
33	NA	A	8369	1/1	0.91	0.14	-	49,49,49,49	0
33	NA	A	8313	1/1	0.88	0.10	-	62,62,62,62	0
32	MG	A	8009	1/1	0.99	0.04	-	26,26,26,26	0
32	MG	A	8011	1/1	0.98	0.09	-	26,26,26,26	0
32	MG	A	8036	1/1	0.98	0.05	-	32,32,32,32	0
32	MG	A	8092	1/1	0.96	0.13	-	79,79,79,79	0
32	MG	A	8090	1/1	0.91	0.29	-	70,70,70,70	0
33	NA	A	8326	1/1	0.88	0.33	-	37,37,37,37	0
33	NA	A	8385	1/1	0.68	0.41	-	50,50,50,50	0
32	MG	A	8045	1/1	0.91	0.09	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	NA	A	8336	1/1	0.96	0.06	-	53,53,53,53	0
32	MG	A	8026	1/1	0.99	0.07	-	26,26,26,26	0
32	MG	A	8085	1/1	0.92	0.11	-	45,45,45,45	0
33	NA	A	8342	1/1	0.93	0.23	-	40,40,40,40	0
32	MG	A	8106	1/1	0.92	0.08	-	52,52,52,52	0
33	NA	A	8319	1/1	0.94	0.10	-	36,36,36,36	0
33	NA	A	8357	1/1	0.89	0.08	-	53,53,53,53	0
33	NA	A	8307	1/1	0.70	0.27	-	46,46,46,46	0
35	CL	K	8502	1/1	0.87	0.14	-	66,66,66,66	0
32	MG	A	8087	1/1	0.91	0.19	-	63,63,63,63	0
35	CL	A	8517	1/1	0.93	0.14	-	59,59,59,59	0
32	MG	A	8023	1/1	0.98	0.06	-	39,39,39,39	0
32	MG	A	8083	1/1	0.94	0.09	-	41,41,41,41	0
32	MG	A	8100	1/1	0.95	0.16	-	65,65,65,65	0
33	NA	A	8360	1/1	0.95	0.56	-	39,39,39,39	0
32	MG	A	8081	1/1	0.97	0.12	-	43,43,43,43	0
32	MG	A	8099	1/1	0.95	0.12	-	48,48,48,48	0
32	MG	A	8029	1/1	0.98	0.08	-	41,41,41,41	0
35	CL	A	8511	1/1	0.94	0.11	-	48,48,48,48	0
35	CL	M	8510	1/1	0.98	0.16	-	47,47,47,47	0
33	NA	A	8381	1/1	0.98	0.23	-	44,44,44,44	0
32	MG	A	8097	1/1	0.98	0.17	-	28,28,28,28	0
32	MG	A	8024	1/1	0.48	1.23	-	89,89,89,89	0
33	NA	J	8322	1/1	0.70	0.31	-	61,61,61,61	0
33	NA	A	8311	1/1	0.76	0.30	-	55,55,55,55	0
32	MG	A	8047	1/1	0.94	0.15	-	66,66,66,66	0
32	MG	A	8046	1/1	0.94	0.08	-	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.