



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 04:09 pm GMT

PDB ID : 3CC2
Title : The Refined Crystal Structure of the Haloarcula Marismortui Large Ribosomal Subunit at 2.4 Angstrom Resolution with rrnA Sequence for the 23S rRNA and Genome-derived Sequences for r-Proteins
Authors : Gurel, G.; Blaha, G.
Deposited on : 2008-02-23
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

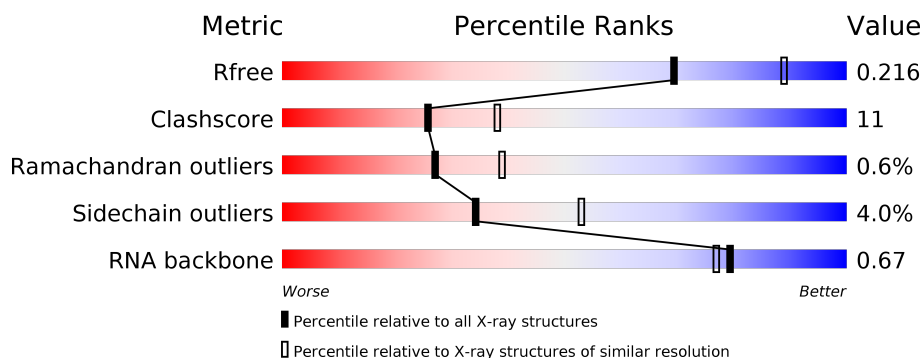
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



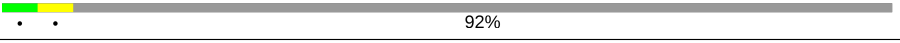















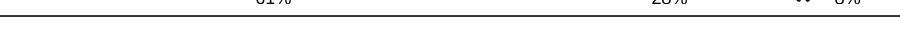
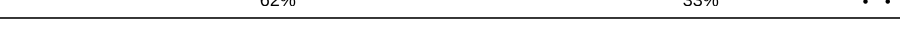
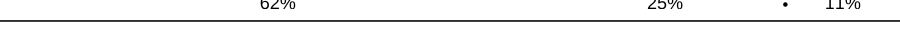
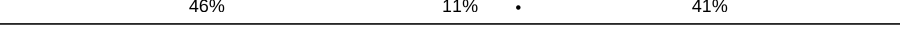
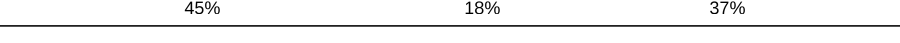
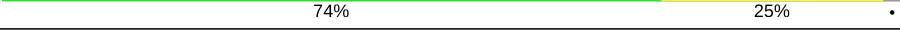



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	3481 (2.40-2.40)
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)
RNA backbone	2636	1023 (2.80-2.00)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	240	70% 26% ..
2	B	338	71% 25% .
3	C	246	75% 21% .
4	D	177	47% 29% . 21%
5	E	178	69% 28% ..
6	F	120	73% 26% ..

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Mol	Chain	Length	Quality of chain
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	
30	0	2923	
31	9	122	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 99049 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 protein called 50S ribosomal protein L2P.

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

- Molecule 2 is a protein called 50S ribosomal protein L3P.

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

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1860	1130	345	384	1			

- Molecule 4 is a protein called 50S ribosomal protein L5P.

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

- Molecule 5 is a protein called 50S ribosomal protein L6P.

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

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 7 is a protein called 50S ribosomal protein L10E.

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

- Molecule 8 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 9 is a protein called 50S ribosomal protein L11P.

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

- Molecule 10 is a protein called 50S ribosomal protein L13P.

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

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 12 is a protein called 50S ribosomal protein L15P.

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

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.

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

- Molecule 15 is a protein called 50S ribosomal protein L18e.

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

- Molecule 16 is a protein called 50S ribosomal protein L19e.

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

- Molecule 17 is a protein called 50S ribosomal protein L21e.

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

- Molecule 18 is a protein called 50S ribosomal protein L22P.

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

- Molecule 19 is a protein called 50S ribosomal protein L23P.

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

- Molecule 20 is a protein called 50S ribosomal protein L24P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24e.

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

- Molecule 22 is a protein called 50S ribosomal protein L29P.

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

- Molecule 23 is a protein called 50S ribosomal protein L30P.

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

- Molecule 24 is a protein called 50S ribosomal protein L31e.

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

- Molecule 25 is a protein called 50S ribosomal protein L32e.

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

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59021	26349	10873	19054	2745			

- Molecule 31 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	109	Total	Mg	0	0
			109	109		
32	9	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		
32	3	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	0	73	Total Na 73 73	0	0
33	J	1	Total Na 1 1	0	0
33	Q	1	Total Na 1 1	0	0
33	H	1	Total Na 1 1	0	0
33	C	1	Total Na 1 1	0	0
33	A	1	Total Na 1 1	0	0
33	R	2	Total Na 2 2	0	0
33	9	3	Total Na 3 3	0	0
33	L	1	Total Na 1 1	0	0
33	S	1	Total Na 1 1	0	0
33	M	1	Total Na 1 1	0	0

- Molecule 34 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	10	Total Cl 10 10	0	0
34	J	3	Total Cl 3 3	0	0
34	B	1	Total Cl 1 1	0	0
34	A	1	Total Cl 1 1	0	0
34	N	1	Total Cl 1 1	0	0
34	O	1	Total Cl 1 1	0	0
34	R	1	Total Cl 1 1	0	0
34	Y	1	Total Cl 1 1	0	0
34	L	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	3	1	Total 1	Cl 1	0	0
34	M	1	Total 1	Cl 1	0	0

- Molecule 35 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	O	1	Total 1	Cd 1	0	0
35	Z	1	Total 1	Cd 1	0	0
35	1	1	Total 1	Cd 1	0	0
35	3	1	Total 1	Cd 1	0	0
35	U	1	Total 1	Cd 1	0	0

- Molecule 36 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	2	Total 2	K 2	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	117	Total 117	O 117	0	0
37	B	146	Total 146	O 146	0	0
37	C	170	Total 170	O 170	0	0
37	D	47	Total 47	O 47	0	0
37	E	42	Total 42	O 42	0	0
37	F	24	Total 24	O 24	0	0
37	G	19	Total 19	O 19	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	H	72	Total 72	O 72	0	0
37	I	9	Total 9	O 9	0	0
37	J	51	Total 51	O 51	0	0
37	K	56	Total 56	O 56	0	0
37	L	72	Total 72	O 72	0	0
37	M	119	Total 119	O 119	0	0
37	N	65	Total 65	O 65	0	0
37	O	39	Total 39	O 39	0	0
37	P	63	Total 63	O 63	0	0
37	Q	52	Total 52	O 52	0	0
37	R	80	Total 80	O 80	0	0
37	S	33	Total 33	O 33	0	0
37	T	38	Total 38	O 38	0	0
37	U	27	Total 27	O 27	0	0
37	V	14	Total 14	O 14	0	0
37	W	66	Total 66	O 66	0	0
37	X	29	Total 29	O 29	0	0
37	Y	94	Total 94	O 94	0	0
37	Z	26	Total 26	O 26	0	0
37	1	53	Total 53	O 53	0	0
37	2	40	Total 40	O 40	0	0

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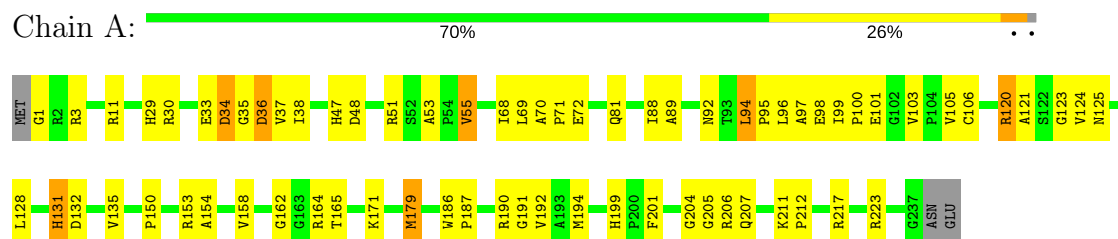
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	3	72	Total 72	O 72	0	0
37	0	5949	Total 5949	O 5949	0	0
37	9	139	Total 139	O 139	0	0

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

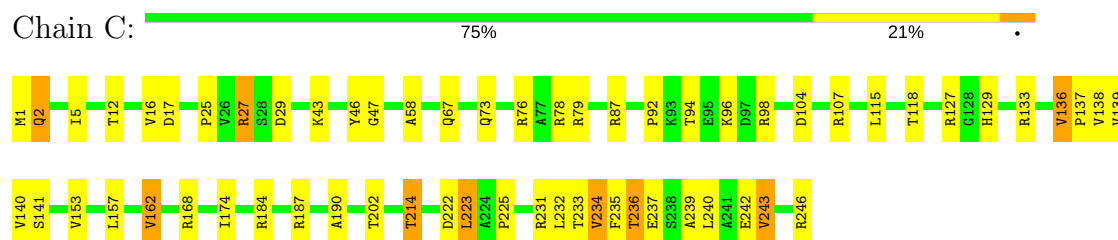
• Molecule 1: 50S ribosomal protein L2P



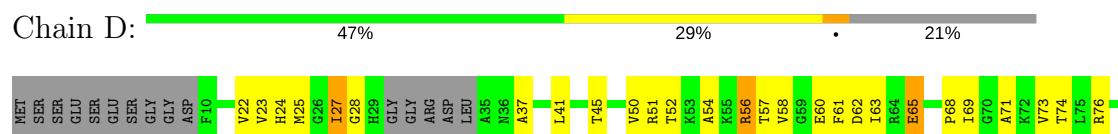
• Molecule 2: 50S ribosomal protein L3P

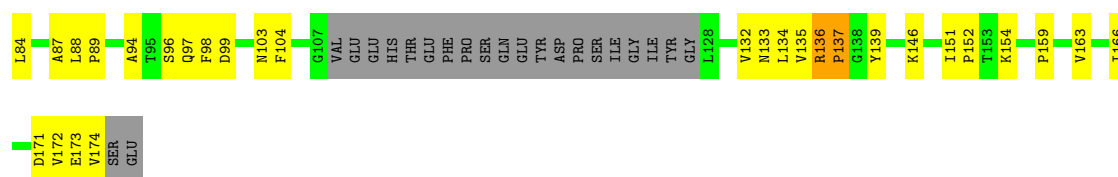


• Molecule 3: 50S ribosomal protein L4P

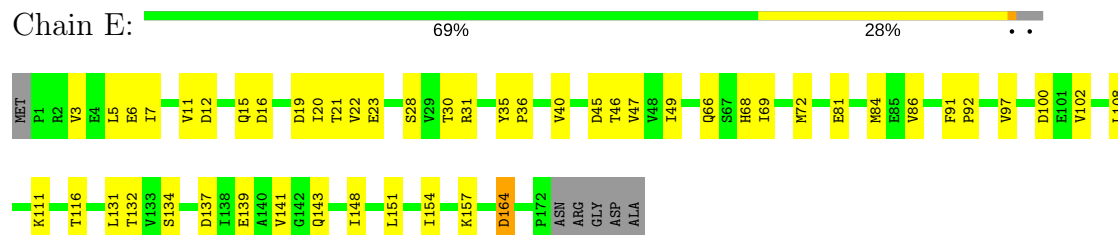


• Molecule 4: 50S ribosomal protein L5P

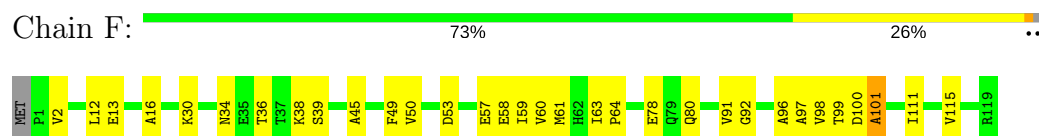




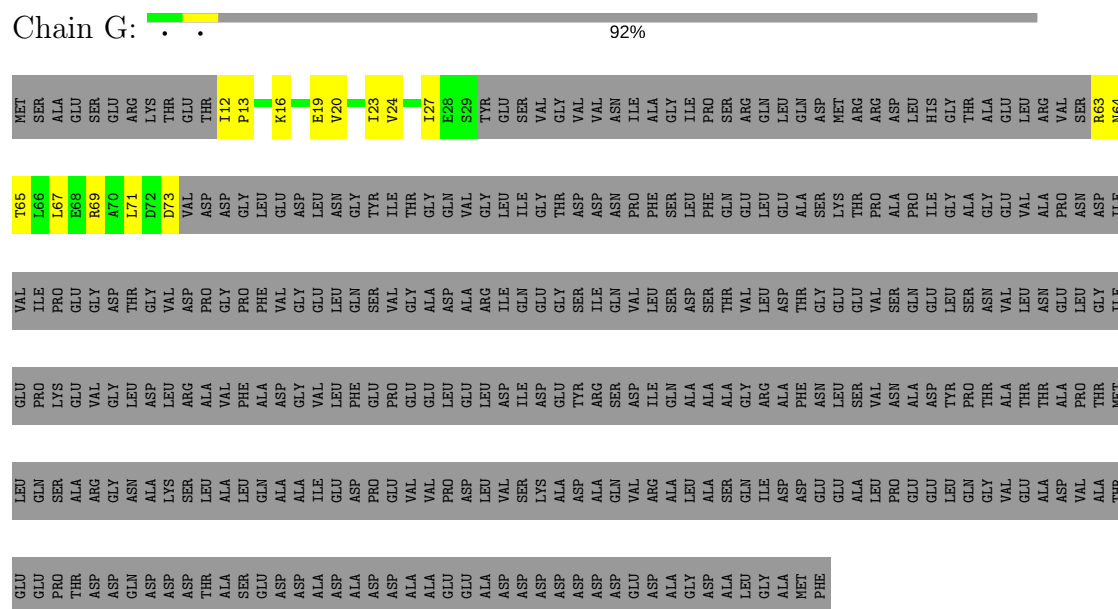
- Molecule 5: 50S ribosomal protein L6P



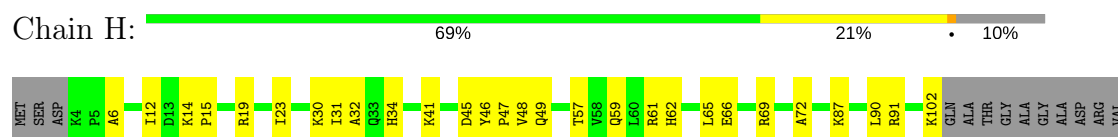
- Molecule 6: 50S ribosomal protein L7Ae



- Molecule 7: 50S ribosomal protein L10E



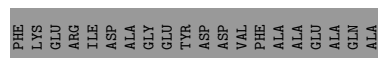
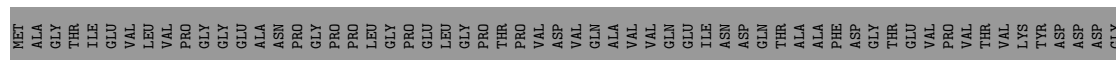
- Molecule 8: 50S ribosomal protein L10e





• Molecule 9: 50S ribosomal protein L11P

Chain I: 25% 18% 57%



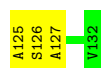
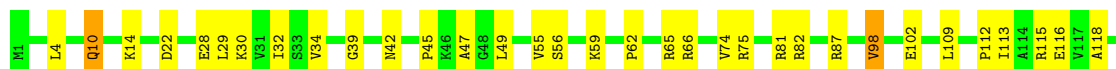
• Molecule 10: 50S ribosomal protein L13P

Chain J: 72% 23%



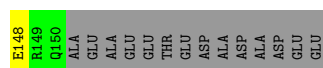
• Molecule 11: 50S ribosomal protein L14P

Chain K: 73% 26%



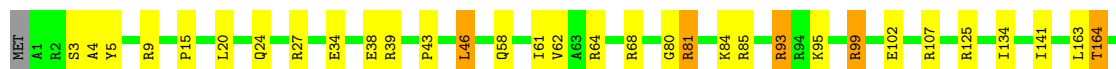
• Molecule 12: 50S ribosomal protein L15P

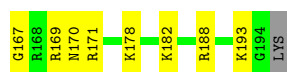
Chain L: 71% 16% 12%



• Molecule 13: 50S ribosomal protein L15e

Chain M: 79% 18%





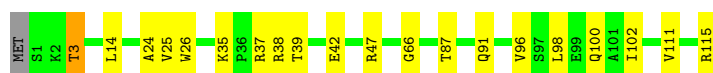
- Molecule 14: 50S ribosomal protein L18P

Chain N: 67% 31% ..



- Molecule 15: 50S ribosomal protein L18e

Chain O: 82% 16% ..



- Molecule 16: 50S ribosomal protein L19e

Chain P: 82% 14% .



- Molecule 17: 50S ribosomal protein L21e

Chain Q: 83% 14% ..



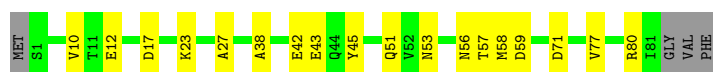
- Molecule 18: 50S ribosomal protein L22P

Chain R: 78% 17% . .



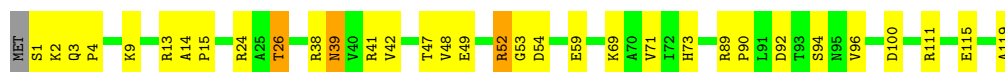
- Molecule 19: 50S ribosomal protein L23P

Chain S: 74% 21% 5%



- Molecule 20: 50S ribosomal protein L24P

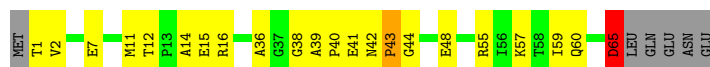
Chain T: 72% 25% . .



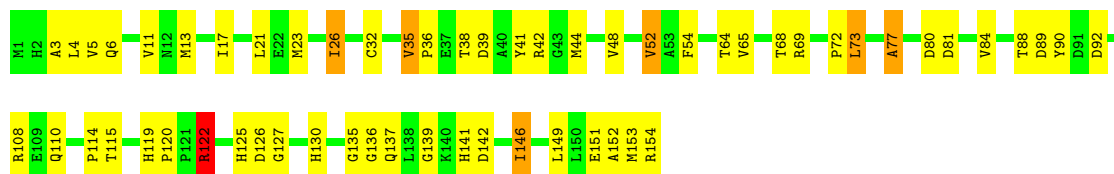
- Molecule 21: 50S ribosomal protein L24e



- Molecule 22: 50S ribosomal protein L29P



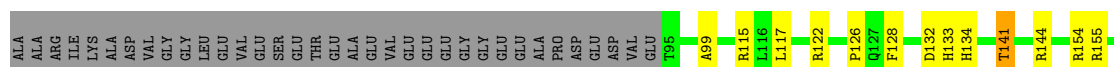
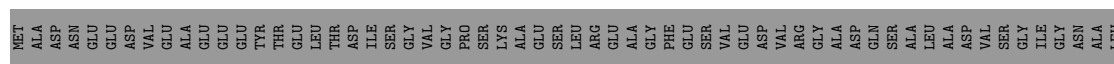
- Molecule 23: 50S ribosomal protein L30P



- Molecule 24: 50S ribosomal protein L31e

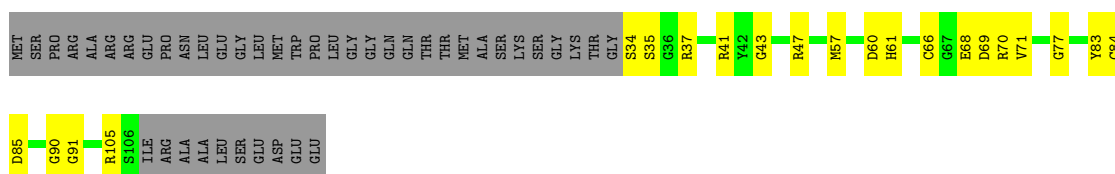


- Molecule 25: 50S ribosomal protein L32e



- Molecule 26: 50S ribosomal protein L37Ae





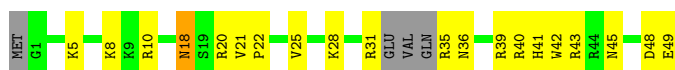
- Molecule 27: 50S ribosomal protein L37e

Chain 1: 74% 25%



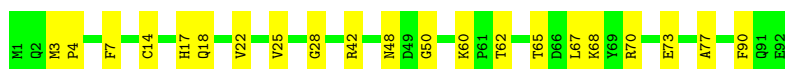
- Molecule 28: 50S ribosomal protein L39e

Chain 2: 52% 38% 8%



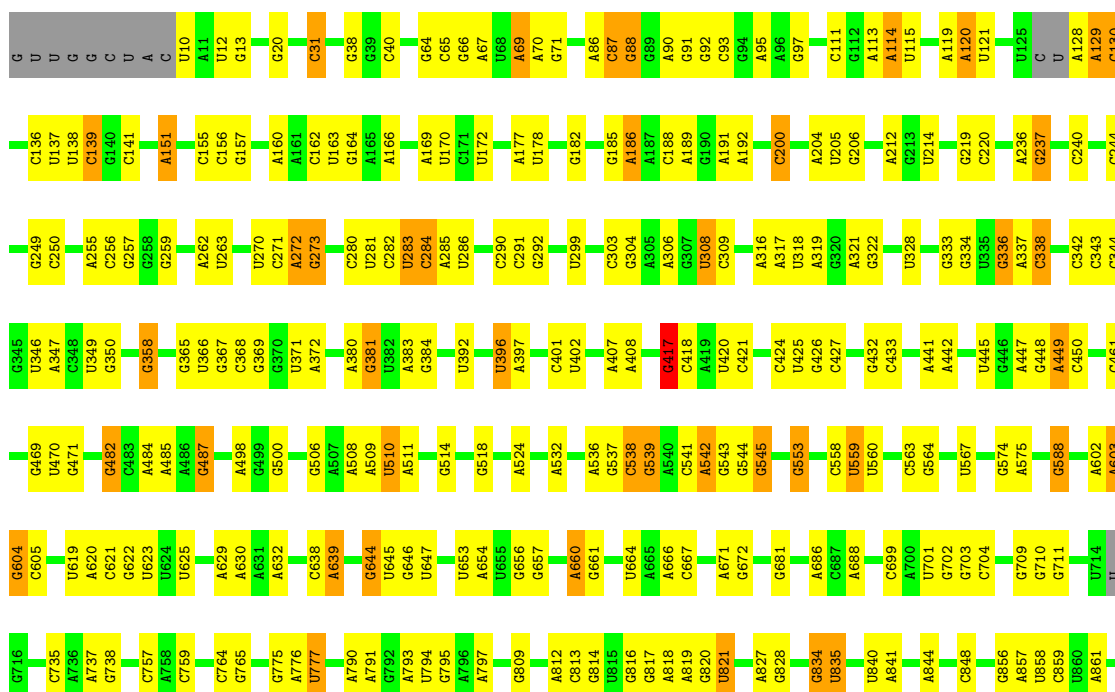
- Molecule 29: 50S ribosomal protein L44E

Chain 3: 77% 23%

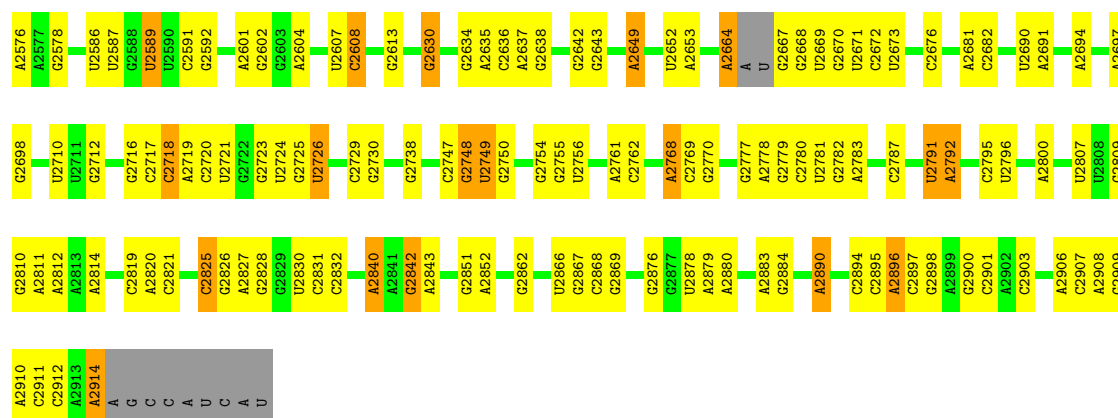


- Molecule 30: 23S RIBOSOMAL RNA

Chain 0: 62% 27% 5% 6%

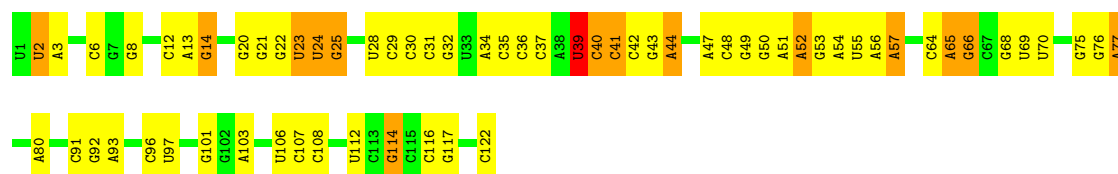


A2479	G2365	A2258	G	C2114	U1996	G1878	A1733	A1615	A1482	C1360	U1244	G1167	G1059	A867
G2480	A2369	U2265	C	U2115	A1997	U1879	C1734	A1524	C1463	A1367	C1245	C1168	C1060	G868
A2483	A2266	A2266	U	U2116	G2001	C1880	C1735	U1625	A1484	U1368	A1246	A1171	G1072	G869
C2487	A2372	C2269	G	G2128	C2002	C1881	A1736	A1626	A1485	A1369	U1249	A1172	G1076	G870
A2488	U2373	G2270	C	G2134	U2003	C1882	U1741	G1627	A1493	G1370	C1250	A1173	G1077	G871
G2489	G2386	G2271	G	A2135	U2004	G1884	A1742	A1632	G1497	U1372	C1251	A1174	G1078	G872
C2491	C2388	G2272	G	G2136	G2005	G1884	G1762	A1633	U1500	A1372	A1252	G1175	A1078	A875
C2493	U2389	U2290	C	A	U2008	A1909	U1766	G1634	G1503	U1180	C1253	A1079	A1079	A876
C2502	A2401	C2296	C	C	G2009	A1919	U1771	G1635	U1504	A1181	C1257	C1080	A1081	A877
A2503	C2402	U2289	C	G	A2010	C1920	U1772	G1636	U1505	C1182	G1258	A1082	A1082	G878
C2504	C2403	U2290	C	U	A2011	A1921	G1773	G1637	U1506	C1183	C1259	C1083	C1083	A882
G2505	G2404	U2291	C	G	U2012	A1922	C1772	A1641	U1507	C1184	U1266	C1084	C1084	U883
A2506	A2301	C2312	C	G	G2013	G1925	G1773	A1642	U1508	U1185	C1267	C1085	C1085	U884
C2507	A2302	C2313	C	U	G2014	U1926	A1778	A1643	U1509	C1186	C1268	A1086	A1086	G885
C2508	G2309	C2314	C	A	A2015	A1927	A1779	A1644	U1510	U1187	G1269	G1087	G1087	A894
A2509	A2310	C2315	A	G	U2016	A1928	U1788	U1654	U1511	A1188	U1270	A1088	A1088	G898
C2510	A2311	C2316	C	U	U2017	C1943	U1789	U1655	U1512	G1190	U1271	A1097	A1097	C899
G2511	A2312	C2317	C	G	U2018	C1944	C1787	U1656	U1513	A1192	C1289	G1099	G1099	G902
C2515	A2313	C2318	U	U	U2019	C1945	U1788	U1657	U1514	A1193	A1291	C1103	C1103	A905
G2516	G2412	C2319	C	G	U2020	G1946	G1789	U1658	U1515	A1200	A1292	U1109	U1109	G906
A2517	A2413	C2320	C	U	G2021	G1947	C1798	U1659	U1516	C1201	A1293	G1110	G1110	A907
C2518	A2414	C2321	A	A	U2022	G1948	A1815	U1660	U1517	A1202	G1295	C999	C999	A912
G2519	A2415	C2322	C	G	U2023	G1949	C1816	U1661	U1518	G1299	G1300	U1116	U1116	A912
C2520	G2416	C2323	U	U	U2024	G1950	U1826	U1662	U1519	U1205	C1204	U1117	U1117	C920
A2521	U2422	C2324	C	U	U2025	G1951	C1826	U1663	U1520	U1206	U1206	A1118	A1118	G921
G2524	G2426	C2325	C	A	U2026	U1952	C1827	U1664	U1521	A1207	U1207	G1119	G1119	A922
C2525	A2434	C2326	C	G	U2027	U1953	U1827	U1665	U1522	C1305	U1306	U1120	U1120	A923
G2526	U2435	C2327	C	U	U2028	U1954	C1828	U1666	U1523	U1307	U1307	G1121	G1121	A923
U2527	G2443	C2328	C	U	U2029	U1955	C1829	U1667	U1524	A1313	G1211	C1127	C1127	U932
C2533	U2444	C2329	C	G	U2030	U1956	C1830	U1668	U1525	U1314	G1212	U1128	U1128	C933
G2534	U2445	C2330	C	U	U2031	U1957	C1831	U1669	U1526	G1315	C1213	G1129	G1129	G940
C2535	G2446	C2331	C	G	U2032	U1958	C1832	U1670	U1527	G1316	G1214	U1130	U1130	G941
G2536	G2447	C2332	C	U	U2033	U1959	C1833	U1671	U1528	G1317	G1215	G1131	G1131	U942
C2537	G2448	C2333	C	U	U2034	U1960	C1834	U1672	U1529	G1318	G1216	A1132	A1132	U942
A2538	G2449	C2334	C	U	U2035	U1961	C1835	U1673	U1530	G1319	G1217	G1133	G1133	C946
U2541	G2450	C2335	C	G	U2036	U1962	C1836	U1674	U1531	U1328	U1218	U1134	U1134	U947
G2542	G2451	C2336	C	U	U2037	U1963	C1837	U1675	U1532	U1329	U1219	G1135	G1135	G946
C2543	G2452	C2337	C	U	U2038	U1964	C1838	U1676	U1533	A1330	A1330	U1026	U1026	G946
U2552	G2453	C2338	C	U	U2039	U1965	C1839	U1677	U1534	U1331	U1219	G1027	G1027	U947
A2553	G2454	C2339	C	G	U2040	U1966	C1840	U1678	U1535	U1332	U1219	U1028	U1028	G946
G2554	G2455	C2340	C	U	U2041	U1967	C1841	U1679	U1536	U1333	U1219	U1029	U1029	U949
C2555	G2456	C2341	C	U	U2042	U1968	C1842	U1680	U1537	U1334	U1219	G1039	G1039	G950
A2556	G2457	C2342	C	U	U2043	U1969	C1843	U1681	U1538	U1335	U1219	G1040	G1040	A951
G2557	G2458	C2343	C	U	U2044	U1970	C1844	U1682	U1539	U1336	U1219	G1041	G1041	G952
C2558	G2459	C2344	C	U	U2045	U1971	C1845	U1683	U1540	U1337	U1219	G1042	G1042	G953
U2559	G2460	C2345	C	U	U2046	U1972	C1846	U1684	U1541	U1338	U1219	G1043	G1043	G958
G2560	G2461	C2346	C	U	U2047	U1973	C1847	U1685	U1542	U1339	U1219	G1044	G1044	C959
C2561	G2462	C2347	C	U	U2048	U1974	C1848	U1686	U1543	U1340	U1219	G1045	G1045	G960
U2562	G2463	C2348	C	U	U2049	U1975	C1849	U1687	U1544	U1341	U1219	G1046	G1046	A961
A2563	G2464	C2349	C	U	U2050	U1976	C1850	U1688	U1545	U1342	U1219	G1047	G1047	C962
G2564	G2465	C2350	C	U	U2051	U1977	C1851	U1689	U1546	U1343	U1219	G1048	G1048	G963
C2565	G2466	C2351	C	U	U2052	U1978	C1852	U1690	U1547	U1344	U1219	G1049	G1049	G968
U2566	G2467	C2352	C	U	U2053	U1979	C1853	U1691	U1548	U1345	U1219	G1050	G1050	C969
G2567	G2468	C2353	C	U	U2054	U1980	C1854	U1692	U1549	U1346	U1219	G1051	G1051	A961
C2568	G2469	C2354	C	U	U2055	U1981	C1855	U1693	U1550	U1347	U1219	G1052	G1052	C962
U2569	G2470	C2355	C	U	U2056	U1982	C1856	U1694	U1551	U1348	U1219	G1053	G1053	G969
G2570	G2471	C2356	C	U	U2057	U1983	C1857	U1695	U1552	U1349	U1219	G1054	G1054	U970
C2571	G2472	C2357	C	U	U2058	U1984	C1858	U1696	U1553	U1350	U1219	G1055	G1055	A1057
U2572	G2473	C2358	C	U	U2059	U1985	C1859	U1697	U1554	U1351	U1219	G1056	G1056	A1058
C2573	G2474	C2359	C	U	U2060	U1986	C1860	U1698	U1555	U1352	U1219	G1057	G1057	G
A2574	G2475	C2360	C	U	U2061	U1987	C1861	U1699	U1556	U1353	U1219	G1058	G1058	
G2575	G2476	C2361	C	U	U2062	U1988	C1862	U1700	U1557	U1354	U1219	G1059	G1059	
C2576	G2477	C2362	C	U	U2063	U1989	C1863	U1701	U1558	U1355	U1219	G1060	G1060	
U2577	G2478	C2363	C	U	U2064	U1990	C1864	U1702	U1559	U1356	U1219	G1061	G1061	
C2578	G2479	C2364	C	U	U2065	U1991	C1865	U1703	U1560	U1357	U1219	G1062	G1062	
G2579	G2480	C2365	C	U	U2066	U1992	C1866	U1704	U1561	U1358	U1219	G1063	G1063	
A2580	G2481	C2366	C	U	U2067	U1993	C1867	U1705	U1562	U1359	U1219	G1064	G1064	
C2581	G2482	C2367	C	U	U2068	U1994	C1868	U1706	U1563	U1360	U1219	G1065	G1065	
G2582	G2483	C2368	C	U	U2069	U1995	C1869	U1707	U1564	U1361	U1219	G1066	G1066	
U2583	G2484	C2369	C	U	U2070	U1996	C1870	U1708	U1565	U1362	U1219	G1067	G1067	
C2584	G2485	C2370	C	U	U2071	U1997	C1871	U1709	U1566	U1363	U1219	G1068	G1068	
G2585	G2486	C2371	C	U	U2072	U1998	C1872	U1710	U1567	U1364	U1219	G1069	G1069	
A2586	G2487	C2372	C	U	U2073	U1999	C1873	U1711	U1568	U1365	U1219	G1070	G1070	
C2587	G2488	C2373	C	U	U2074	U2000	C1874	U1712	U1569	U1366	U1219	G1071	G1071	
U2588	G2489	C2374	C	U	U2075	U2001	C1875	U1713	U1570	U1367	U1219	G1072	G1072	
C2589	G2490	C2375	C	U	U2076	U2002	C1876	U1714	U1571	U1368	U1219	G1073	G1073	
G2590	G2491	C2376	C	U	U2077	U2003	C1877	U1715	U1572	U1369	U1219	G1074	G1074	
A2591	G2492	C2377	C	U	U2078	U2004	C1878	U1716	U1573	U1370	U1219	G1075	G1075	
C2592	G2493	C2378	C	U	U2079	U2005	C1879	U1717	U1574	U1371	U1219	G1076	G1076	
U2593	G2494	C2379	C	U	U2080	U2006	C1880	U1718	U1575	U1372	U1219	G1077	G1077	
C2594	G2495	C2380	C	U	U2081	U2007	C1881	U1719	U1576	U1373	U1219	G1078	G1078	
G2595	G2496	C2381	C	U	U2082	U2008	C1882	U1720	U1577	U1374	U1219	G1079	G1079	
A2596	G2497	C2382	C	U	U2083	U2009	C1883	U1721	U1578	U1375	U1219	G1080	G1080	
C2597	G2498	C2383	C	U	U2084	U2010	C1884	U1722	U1579	U1376	U1219	G1081	G1081	
G2598	G2499	C2384	C	U	U2085	U2011	C1885	U1723	U1580	U1377	U1219	G1082	G1082	
U2599	G2500	C2385	C	U	U2086	U2012	C1886	U1724	U1581	U1378	U1219	G1083	G1083	
C2600	G2501	C2386	C	U	U2087	U2013	C1887	U1725	U1582	U1379	U1219	G1084	G1084	
A2601	G2502	C2387	C	U	U2088	U2014	C1888	U1726	U1583	U1380	U1219	G1085	G1085	
C2602	G2503	C2388	C	U	U2089	U2015	C1889	U1727	U1584	U1381	U1219	G1086	G1086	
U2603	G2504	C2389	C											



- Molecule 31: 5S RIBOSOMAL RNA

Chain 9:  48% 40% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.65Å 299.67Å 573.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.95 – 2.40 85.47 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.5 (49.95-2.40) 90.6 (85.47-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.231 0.184 , 0.216	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	99049	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.33	0/1786	0.66	0/2408
2	B	0.32	0/2690	0.64	0/3652
3	C	0.36	0/1885	0.64	0/2552
4	D	0.32	0/1111	0.56	0/1498
5	E	0.31	0/1382	0.56	0/1880
6	F	0.32	0/901	0.54	0/1224
7	G	0.42	0/241	0.74	0/324
8	H	0.39	0/1302	0.68	0/1743
9	I	0.34	0/526	0.53	0/716
10	J	0.33	0/1136	0.58	0/1530
11	K	0.32	0/1004	0.65	0/1351
12	L	0.34	0/1130	0.65	0/1509
13	M	0.33	0/1582	0.62	0/2116
14	N	0.28	0/1474	0.61	0/1999
15	O	0.32	0/874	0.59	1/1181 (0.1%)
16	P	0.32	0/1147	0.52	0/1528
17	Q	0.33	0/749	0.67	0/1005
18	R	1.31	7/1172 (0.6%)	1.13	5/1578 (0.3%)
19	S	0.33	0/648	0.59	1/875 (0.1%)
20	T	0.31	0/958	0.62	1/1289 (0.1%)
21	U	0.36	0/417	0.60	0/562
22	V	0.36	0/502	0.68	1/675 (0.1%)
23	W	0.33	0/1219	0.65	1/1655 (0.1%)
24	X	0.36	0/664	0.59	0/895
25	Y	0.36	0/1146	0.62	0/1536
26	Z	0.34	0/584	0.66	0/781
27	1	0.42	0/438	0.65	0/578
28	2	0.33	0/401	0.56	0/529
29	3	0.36	0/771	0.59	0/1024
30	0	0.33	0/65958	0.69	21/102869 (0.0%)
31	9	0.29	0/2904	0.69	1/4526 (0.0%)
All	All	0.36	7/98702 (0.0%)	0.68	32/147588 (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
18	R	1	0
30	0	0	39
31	9	0	1
All	All	1	40

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CA-C	-29.63	0.93	1.52
18	R	150	PRO	CB-CG	16.19	2.31	1.50
18	R	150	PRO	N-CA	14.71	1.72	1.47
18	R	150	PRO	CA-CB	12.12	1.77	1.53
18	R	150	PRO	CG-CD	11.79	1.89	1.50
18	R	150	PRO	C-O	11.61	1.46	1.23
18	R	150	PRO	N-CD	9.24	1.60	1.47

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	N-CA-C	-24.01	49.68	112.10
18	R	150	PRO	CB-CA-C	-19.94	62.16	112.00
18	R	150	PRO	CA-C-O	-16.63	80.28	120.20
30	0	1942	A	C5'-C4'-C3'	8.15	129.05	116.00
18	R	150	PRO	CA-N-CD	7.93	122.80	111.70
22	V	65	ASP	CB-CG-OD1	7.92	125.43	118.30
30	0	871	G	C5'-C4'-O4'	-7.20	100.46	109.10
18	R	150	PRO	N-CA-CB	6.86	111.54	103.30
30	0	1819	G	C5'-C4'-C3'	6.74	126.79	116.00
30	0	1504	A	C1'-O4'-C4'	-6.54	104.67	109.90
31	9	39	U	N1-C1'-C2'	6.47	122.41	114.00
30	0	2316	G	C5'-C4'-C3'	-6.43	105.71	116.00
30	0	1979	G	C2'-C3'-O3'	6.36	123.87	113.70
30	0	1878	G	N9-C1'-C2'	-6.28	105.09	112.00
30	0	1942	A	C5'-C4'-O4'	6.20	116.54	109.10
30	0	2467	A	C1'-O4'-C4'	-6.18	104.95	109.90
30	0	206	G	C5'-C4'-C3'	-6.05	106.32	116.00
30	0	2291	A	N9-C1'-C2'	5.93	121.71	114.00
30	0	1829	A	N9-C1'-C2'	-5.85	105.56	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	1592	G	N9-C1'-C2'	5.66	121.36	114.00
30	0	1942	A	C4'-C3'-C2'	-5.44	97.16	102.60
30	0	1942	A	C1'-O4'-C4'	-5.30	105.66	109.90
23	W	122	ARG	NE-CZ-NH1	5.27	122.94	120.30
30	0	1504	A	N9-C1'-C2'	5.25	120.83	114.00
30	0	2313	C	C5'-C4'-O4'	5.25	115.40	109.10
30	0	841	A	C1'-O4'-C4'	-5.23	105.72	109.90
15	O	66	GLY	N-CA-C	5.16	126.01	113.10
30	0	777	U	O4'-C1'-N1	5.15	112.32	108.20
19	S	27	ALA	N-CA-C	-5.09	97.27	111.00
20	T	52	ARG	N-CA-C	5.06	124.66	111.00
30	0	1819	G	C4'-C3'-C2'	-5.05	97.55	102.60
30	0	1120	U	C5'-C4'-C3'	-5.02	107.97	116.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

All (40) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1039	G	Sidechain
30	0	1078	A	Sidechain
30	0	1237	U	Sidechain
30	0	1340	G	Sidechain
30	0	1342	C	Sidechain
30	0	1417	G	Sidechain
30	0	1450	C	Sidechain
30	0	1829	A	Sidechain
30	0	1845	A	Sidechain
30	0	1848	G	Sidechain
30	0	1863	G	Sidechain
30	0	1867	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1972	U	Sidechain
30	0	2103	A	Sidechain
30	0	2316	G	Sidechain
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain

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Mol	Chain	Res	Type	Group
30	0	2506	A	Sidechain
30	0	2543	G	Sidechain
30	0	2552	C	Sidechain
30	0	2564	G	Sidechain
30	0	2607	U	Sidechain
30	0	2630	G	Sidechain
30	0	270	U	Sidechain
30	0	2842	G	Sidechain
30	0	396	U	Sidechain
30	0	417	G	Sidechain
30	0	449	A	Sidechain
30	0	469	G	Sidechain
30	0	471	G	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	639	A	Sidechain
30	0	795	G	Sidechain
30	0	867	A	Sidechain
31	9	39	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	1753	0	1766	74	0
2	B	2625	0	2533	80	0
3	C	1860	0	1813	65	0
4	D	1094	0	1085	45	0
5	E	1357	0	1266	42	0
6	F	890	0	843	26	0
7	G	240	0	231	11	0
8	H	1282	0	1292	34	0
9	I	519	0	500	23	0
10	J	1120	0	1098	39	0
11	K	994	0	1027	40	0
12	L	1118	0	1076	26	0
13	M	1558	0	1572	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	N	1445	0	1401	55	0
15	O	865	0	873	19	0
16	P	1136	0	1123	20	0
17	Q	735	0	728	11	0
18	R	1149	0	1122	31	0
19	S	641	0	605	13	0
20	T	950	0	923	24	0
21	U	410	0	364	16	0
22	V	499	0	511	19	0
23	W	1196	0	1137	66	0
24	X	654	0	653	21	0
25	Y	1130	0	1133	30	0
26	Z	573	0	532	14	0
27	1	431	0	426	17	0
28	2	396	0	413	24	0
29	3	755	0	728	16	0
30	0	59021	0	29809	870	0
31	9	2599	0	1325	72	0
32	0	109	0	0	0	0
32	3	1	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	73	0	0	0	0
33	9	3	0	0	0	0
33	A	1	0	0	0	0
33	C	1	0	0	0	0
33	H	1	0	0	0	0
33	J	1	0	0	0	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	Q	1	0	0	0	0
33	R	2	0	0	0	0
33	S	1	0	0	0	0
34	0	10	0	0	0	0
34	3	1	0	0	0	0
34	A	1	0	0	0	0
34	B	1	0	0	0	0
34	J	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	L	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	O	1	0	0	0	0
34	R	1	0	0	0	0
34	Y	1	0	0	0	0
35	1	1	0	0	0	0
35	3	1	0	0	0	0
35	O	1	0	0	0	0
35	U	1	0	0	0	0
35	Z	1	0	0	0	0
36	0	2	0	0	0	0
37	0	5949	0	0	149	0
37	1	53	0	0	2	0
37	2	40	0	0	4	0
37	3	72	0	0	6	0
37	9	139	0	0	7	0
37	A	117	0	0	14	0
37	B	146	0	0	13	0
37	C	170	0	0	18	0
37	D	47	0	0	5	0
37	E	42	0	0	4	0
37	F	24	0	0	2	0
37	G	19	0	0	1	0
37	H	72	0	0	5	0
37	I	9	0	0	3	0
37	J	51	0	0	2	0
37	K	56	0	0	5	0
37	L	72	0	0	9	0
37	M	119	0	0	9	0
37	N	65	0	0	10	0
37	O	39	0	0	3	0
37	P	63	0	0	1	0
37	Q	52	0	0	3	0
37	R	80	0	0	2	0
37	S	33	0	0	2	0
37	T	38	0	0	2	0
37	U	27	0	0	1	0
37	V	14	0	0	1	0
37	W	66	0	0	5	0
37	X	29	0	0	5	0
37	Y	94	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	Z	26	0	0	2	0
All	All	99049	0	59908	1694	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 11.

All (1694) 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)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.89	1.50
14:N:37:ARG:NH1	31:9:6:C:H5''	1.61	1.14
30:0:871:G:C8	30:0:871:G:H5'	1.86	1.10
30:0:960:G:H4'	37:0:6980:HOH:O	1.49	1.09
18:R:150:PRO:CG	18:R:150:PRO:CB	2.30	1.08
18:R:150:PRO:CG	18:R:150:PRO:C	2.21	1.08
30:0:1160:G:C5'	30:0:1161:A:H5'	1.85	1.06
15:O:3:THR:HG22	30:0:656:G:H5'	1.38	1.06
10:J:82:THR:HG23	30:0:1242:A:H5'	1.37	1.05
13:M:171:ARG:HD3	30:0:156:C:H5''	1.37	1.05
30:0:2812:A:H2	30:0:2814:A:H62	1.08	1.02
30:0:1160:G:H5'	30:0:1161:A:H5'	1.02	1.01
31:9:56:A:H2'	31:9:57:A:H5''	1.42	1.01
30:0:1372:A:H3'	37:0:6737:HOH:O	1.60	1.00
30:0:1160:G:H5'	30:0:1161:A:C5'	1.91	1.00
30:0:2717:C:H2'	30:0:2718:C:H5''	1.43	0.99
11:K:29:LEU:HB3	11:K:55:VAL:HG11	1.44	0.99
31:9:76:G:H3'	31:9:77:A:H5''	1.44	0.98
30:0:2710:U:H1'	37:0:7172:HOH:O	1.62	0.98
30:0:1474:C:H6	30:0:1474:C:H5'	1.30	0.97
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.46	0.96
30:0:542:A:H5'	30:0:542:A:H8	1.28	0.96
30:0:871:G:H8	30:0:871:G:H5'	1.25	0.95
30:0:2717:C:C2'	30:0:2718:C:H5''	1.96	0.95
28:2:41:HIS:H	28:2:45:ASN:HD22	1.11	0.95
4:D:134:LEU:HD11	4:D:166:ILE:HD11	1.49	0.94
30:0:214:U:H5'	37:0:5687:HOH:O	1.67	0.94
30:0:541:C:H2'	30:0:542:A:H5''	1.50	0.94
11:K:10:GLN:H	11:K:10:GLN:HE21	0.96	0.93
30:0:1835:U:H5	30:0:1840:A:N7	1.66	0.93
30:0:1625:U:H4'	37:0:4207:HOH:O	1.68	0.93
3:C:236:THR:HG22	3:C:239:ALA:H	1.30	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.17	0.92
30:0:381:G:H5''	37:0:3859:HOH:O	1.67	0.92
13:M:164:THR:HG22	13:M:167:GLY:H	1.33	0.92
30:0:282:C:H1'	30:0:368:C:N4	1.85	0.91
30:0:871:G:H8	30:0:871:G:C5'	1.83	0.91
20:T:71:VAL:HG11	20:T:90:PRO:HB3	1.53	0.90
30:0:1184:C:H1'	37:0:7015:HOH:O	1.70	0.90
30:0:870:G:H2'	30:0:871:G:H5''	1.51	0.90
30:0:2291:A:C8	30:0:2309:C:H5'	2.06	0.90
21:U:52:THR:HG22	21:U:54:THR:H	1.35	0.90
30:0:1116:U:O2'	30:0:1118:A:H2	1.55	0.89
30:0:1667:A:H8	30:0:1667:A:H5'	1.36	0.89
30:0:2748:G:H2'	37:0:7089:HOH:O	1.72	0.89
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.54	0.89
30:0:1666:C:O2'	30:0:1667:A:H5''	1.70	0.89
30:0:1701:A:H4'	30:0:1702:U:H5''	1.53	0.89
30:0:236:A:H4'	30:0:237:G:H5'	1.55	0.87
30:0:541:C:C2'	30:0:542:A:H5''	2.03	0.87
2:B:140:LEU:HA	37:B:8581:HOH:O	1.74	0.87
11:K:39:GLY:HA2	37:0:4763:HOH:O	1.73	0.87
30:0:871:G:C8	30:0:871:G:C5'	2.58	0.87
30:0:1116:U:H3	30:0:1246:A:H62	1.23	0.86
16:P:115:SER:H	16:P:118:GLN:HE21	1.19	0.86
30:0:69:A:H5'	30:0:69:A:C8	2.10	0.86
4:D:154:LYS:HD2	4:D:154:LYS:H	1.38	0.86
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.19	0.86
30:0:2506:A:O2'	30:0:2507:G:H8	1.59	0.86
23:W:6:GLN:HB2	23:W:26:ILE:HD12	1.55	0.85
30:0:1300:G:H1'	37:0:4223:HOH:O	1.77	0.85
14:N:37:ARG:HH12	31:9:6:C:H5''	1.39	0.85
1:A:223:ARG:HH12	30:0:2270:G:H4'	1.42	0.85
31:9:39:U:H1'	31:9:44:A:H61	1.42	0.85
30:0:282:C:O2'	30:0:283:U:H5'	1.77	0.84
26:Z:70:ARG:HD2	26:Z:83:TYR:HB2	1.58	0.84
30:0:545:G:H8	30:0:545:G:H5'	1.40	0.84
23:W:88:THR:HB	37:W:6679:HOH:O	1.77	0.84
30:0:506:G:H22	30:0:509:A:C5'	1.91	0.83
30:0:1119:G:N2	30:0:1246:A:C2	2.46	0.83
30:0:69:A:H5'	30:0:69:A:H8	1.42	0.83
31:9:14:G:H5'	31:9:14:G:H8	1.43	0.83
2:B:206:THR:HG21	30:0:2716:G:H5''	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1730:G:H5'	30:0:1731:C:C5	2.14	0.82
26:Z:34:SER:HB2	37:Z:8414:HOH:O	1.77	0.82
30:0:1862:C:H1'	37:0:6768:HOH:O	1.80	0.82
30:0:2586:U:H3	30:0:2592:G:H22	1.28	0.82
30:0:1118:A:H3'	30:0:1118:A:H8	1.44	0.82
30:0:272:A:H3'	37:0:7079:HOH:O	1.79	0.81
30:0:2769:C:C2'	30:0:2770:G:H5'	2.10	0.81
37:I:5128:HOH:O	30:0:1168:C:H4'	1.81	0.81
25:Y:200:THR:HG22	25:Y:201:GLU:HG3	1.61	0.81
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.63	0.81
30:0:506:G:H22	30:0:509:A:H5''	1.45	0.81
30:0:564:G:H1'	37:0:5857:HOH:O	1.81	0.81
30:0:346:U:H4'	37:0:6392:HOH:O	1.80	0.81
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.26	0.81
30:0:2851:G:O2'	30:0:2852:A:H5'	1.81	0.81
11:K:10:GLN:N	11:K:10:GLN:HE21	1.79	0.81
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.63	0.81
8:H:170:ARG:HD2	37:H:8342:HOH:O	1.79	0.80
31:9:56:A:C2'	31:9:57:A:H5''	2.11	0.80
23:W:88:THR:HG23	23:W:110:GLN:HE21	1.46	0.80
21:U:46:ALA:HB1	21:U:52:THR:HG21	1.63	0.80
30:0:1474:C:C6	30:0:1474:C:H5'	2.17	0.80
30:0:1973:A:H5'	30:0:1973:A:H8	1.47	0.80
30:0:2908:A:H2'	30:0:2909:G:O4'	1.82	0.80
30:0:1118:A:H3'	30:0:1118:A:C8	2.16	0.80
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.63	0.80
30:0:2637:A:H5'	37:0:8794:HOH:O	1.80	0.79
1:A:199:HIS:HD2	1:A:201:PHE:H	1.27	0.79
2:B:238:ASN:HD22	2:B:240:GLY:H	1.26	0.79
3:C:127:ARG:NH2	3:C:225:PRO:HG2	1.98	0.79
2:B:307:ARG:HG3	2:B:307:ARG:HH11	1.47	0.79
30:0:544:G:H2'	30:0:545:G:H5''	1.65	0.78
31:9:29:C:H2'	31:9:30:C:H5'	1.66	0.78
30:0:1119:G:H22	30:0:1246:A:H2	1.32	0.78
30:0:541:C:H2'	30:0:542:A:C5'	2.14	0.78
15:O:3:THR:CG2	30:0:656:G:H5'	2.12	0.78
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.83	0.78
11:K:81:ARG:HB2	11:K:87:ARG:HH11	1.49	0.78
23:W:122:ARG:NH2	23:W:154:ARG:HB3	1.99	0.78
30:0:182:G:H5'	37:0:4697:HOH:O	1.83	0.78
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.81	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:30:LYS:H	8:H:62:HIS:HD2	1.31	0.77
30:0:1919:A:H4'	37:0:4389:HOH:O	1.85	0.77
30:0:2896:A:H5''	37:0:5645:HOH:O	1.84	0.77
3:C:1:MET:HG2	3:C:2:GLN:H	1.49	0.77
30:0:1206:U:H6	30:0:1206:U:H5'	1.50	0.76
30:0:1165:G:H4'	30:0:1174:A:O2'	1.86	0.76
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.67	0.76
30:0:1080:C:H4'	30:0:1081:A:OP1	1.84	0.76
22:V:1:THR:HG23	22:V:2:VAL:H	1.50	0.76
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.68	0.76
30:0:2004:U:H4'	37:0:4853:HOH:O	1.85	0.76
30:0:542:A:H5'	30:0:542:A:C8	2.18	0.76
14:N:144:GLY:O	14:N:147:ILE:HG22	1.85	0.76
30:0:603:A:H5''	30:0:604:G:OP1	1.86	0.75
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.66	0.75
30:0:2769:C:H2'	30:0:2770:G:H5'	1.68	0.75
30:0:2506:A:HO2'	30:0:2507:G:H8	0.81	0.75
30:0:1701:A:H4'	30:0:1702:U:C5'	2.16	0.75
10:J:19:MET:HE3	10:J:132:LEU:HD21	1.69	0.75
14:N:37:ARG:NH1	31:9:6:C:C5'	2.48	0.75
2:B:321:PRO:HA	37:B:8656:HOH:O	1.85	0.75
30:0:877:G:H5'	30:0:878:G:OP1	1.86	0.74
29:3:65:THR:HG22	29:3:67:LEU:HG	1.69	0.74
30:0:2635:A:O2'	30:0:2636:C:H5'	1.88	0.74
30:0:559:U:H5'	30:0:559:U:H6	1.53	0.74
30:0:870:G:C2'	30:0:871:G:H5''	2.18	0.74
4:D:99:ASP:HB3	4:D:103:ASN:H	1.53	0.74
31:9:39:U:H1'	31:9:44:A:N6	2.03	0.74
2:B:86:ALA:HA	37:B:8581:HOH:O	1.87	0.73
30:0:1603:A:H5'	30:0:1605:G:O4'	1.88	0.73
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.69	0.73
37:B:8634:HOH:O	30:0:2672:C:H1'	1.87	0.73
30:0:2323:G:H5''	37:0:4318:HOH:O	1.88	0.73
5:E:143:GLN:NE2	30:0:2779:G:H21	1.86	0.73
30:0:558:C:O2'	30:0:559:U:H5''	1.89	0.73
14:N:113:SER:HB2	37:N:8558:HOH:O	1.87	0.73
30:0:1497:G:H4'	30:0:1627:G:O2'	1.88	0.72
9:I:73:LEU:HD12	9:I:107:LYS:HZ2	1.53	0.72
30:0:1666:C:H2'	30:0:1667:A:H5'	1.70	0.72
1:A:35:GLY:O	1:A:36:ASP:HB3	1.90	0.72
30:0:1130:U:H5'	37:0:7223:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.71	0.72
30:0:2505:G:O2'	30:0:2506:A:H5'	1.89	0.72
3:C:174:ILE:CD1	30:0:338:C:H4'	2.19	0.72
15:O:3:THR:HG22	30:0:656:G:C5'	2.18	0.72
30:0:2507:G:H2'	30:0:2510:C:H42	1.55	0.72
30:0:1180:U:H1'	37:0:9766:HOH:O	1.90	0.71
4:D:25:MET:HE3	4:D:37:ALA:HB1	1.71	0.71
14:N:23:ARG:HD3	37:N:8546:HOH:O	1.90	0.71
9:I:127:CYS:HB3	9:I:132:VAL:HB	1.71	0.71
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.71	0.71
11:K:10:GLN:H	11:K:10:GLN:NE2	1.80	0.71
30:0:2756:U:H3	30:0:2896:A:H2	1.34	0.71
1:A:211:LYS:HB2	37:A:8612:HOH:O	1.91	0.71
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.71	0.71
21:U:9:CYS:HA	21:U:52:THR:HG23	1.73	0.71
26:Z:34:SER:OG	30:0:797:A:H4'	1.90	0.71
1:A:51:ARG:HB2	37:A:8599:HOH:O	1.91	0.71
30:0:1667:A:C8	30:0:1667:A:H5'	2.25	0.70
30:0:299:U:H5'	37:0:6885:HOH:O	1.91	0.70
28:2:41:HIS:N	28:2:45:ASN:HD22	1.88	0.70
30:0:1835:U:C5	30:0:1840:A:N7	2.56	0.70
30:0:1634:G:H3'	37:0:3430:HOH:O	1.90	0.70
30:0:1166:A:H61	30:0:1180:U:H3	1.38	0.70
30:0:1183:C:N4	30:0:1184:C:H41	1.90	0.70
30:0:558:C:C2'	30:0:559:U:H5''	2.21	0.70
31:9:14:G:H5'	31:9:14:G:C8	2.26	0.70
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.73	0.70
16:P:59:ARG:NH2	16:P:66:GLN:HE22	1.90	0.70
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.74	0.70
13:M:171:ARG:CD	30:0:156:C:H5''	2.19	0.69
18:R:128:ARG:NH2	30:0:2054:A:N3	2.40	0.69
30:0:2426:G:H1'	37:0:5638:HOH:O	1.92	0.69
30:0:2533:C:H5'	30:0:2533:C:H6	1.57	0.69
28:2:39:ARG:HG2	37:2:3143:HOH:O	1.92	0.69
13:M:178:LYS:HB2	37:0:6424:HOH:O	1.90	0.69
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.07	0.69
2:B:41:PHE:CD1	2:B:79:MET:HE2	2.27	0.69
30:0:281:U:H2'	30:0:282:C:O4'	1.91	0.69
30:0:951:A:C2'	30:0:952:G:H5'	2.22	0.69
1:A:191:GLY:HA2	1:A:194:MET:CE	2.22	0.69
10:J:76:ASP:HA	37:J:5907:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1603:A:H5''	30:0:1605:G:H5'	1.75	0.69
30:0:536:A:H3'	37:0:4588:HOH:O	1.92	0.69
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.74	0.69
30:0:558:C:H2'	30:0:559:U:C5'	2.23	0.69
30:0:1058:A:H2'	30:0:1060:C:H5''	1.74	0.68
30:0:1632:A:H2'	30:0:1633:C:H5'	1.74	0.68
30:0:2812:A:C2	30:0:2814:A:N6	2.59	0.68
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.74	0.68
30:0:2756:U:N3	30:0:2896:A:C2	2.59	0.68
2:B:211:THR:HG21	37:0:7003:HOH:O	1.92	0.68
30:0:2769:C:H2'	30:0:2770:G:C5'	2.23	0.68
30:0:2787:C:H5	37:0:4174:HOH:O	1.76	0.68
30:0:1166:A:H1'	30:0:1192:A:C2	2.28	0.68
30:0:1730:G:C5'	30:0:1731:C:C6	2.77	0.68
28:2:41:HIS:H	28:2:45:ASN:ND2	1.89	0.68
3:C:76:ARG:HG2	3:C:78:ARG:NH1	2.08	0.68
1:A:191:GLY:HA2	1:A:194:MET:HE3	1.76	0.68
30:0:1766:U:O2	30:0:1778:A:H5'	1.94	0.68
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.94	0.67
30:0:1701:A:H5'	37:0:5830:HOH:O	1.93	0.67
30:0:1730:G:H5'	30:0:1731:C:H5	1.58	0.67
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.76	0.67
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.76	0.67
30:0:1189:A:H3'	37:0:7231:HOH:O	1.93	0.67
30:0:1878:G:H1'	37:0:5667:HOH:O	1.94	0.67
19:S:57:THR:HG22	19:S:59:ASP:H	1.58	0.67
30:0:1441:G:O2'	30:0:1442:A:H5'	1.94	0.67
30:0:272:A:H5'	30:0:273:G:OP2	1.94	0.67
18:R:98:ASN:HD21	30:0:500:G:H21	1.41	0.67
23:W:125:HIS:HD2	23:W:127:GLY:H	1.42	0.67
3:C:140:VAL:HB	37:C:8449:HOH:O	1.93	0.67
30:0:2064:U:H5'	30:0:2652:U:O3'	1.94	0.67
30:0:1377:C:H6	30:0:1377:C:H5'	1.60	0.67
30:0:1187:U:O2'	30:0:1189:A:H2	1.77	0.67
10:J:74:ARG:HB3	10:J:74:ARG:HH11	1.58	0.67
30:0:1819:G:H2'	30:0:1820:G:H4'	1.76	0.67
29:3:48:ASN:HD21	30:0:2468:A:H61	1.41	0.67
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.10	0.67
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.09	0.66
30:0:2827:A:H2'	30:0:2828:G:O4'	1.95	0.66
30:0:31:C:H4'	37:0:6974:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:856:G:H2'	37:0:4975:HOH:O	1.94	0.66
1:A:199:HIS:CD2	1:A:201:PHE:H	2.11	0.66
23:W:141:HIS:HB2	23:W:146:ILE:HG12	1.78	0.66
6:F:91:VAL:HG12	6:F:92:GLY:H	1.60	0.66
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.78	0.66
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.11	0.66
30:0:545:G:C8	30:0:545:G:H5'	2.27	0.66
23:W:21:LEU:HD22	23:W:26:ILE:HD11	1.77	0.66
10:J:52:GLN:HE22	30:0:1119:G:H8	1.42	0.66
30:0:711:G:H1'	37:0:6640:HOH:O	1.95	0.66
30:0:1205:U:H2'	30:0:1206:U:C5'	2.25	0.66
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.77	0.66
3:C:139:VAL:HG13	37:C:8446:HOH:O	1.95	0.66
30:0:1209:C:H2'	30:0:1210:G:H8	1.61	0.66
30:0:2783:A:H3'	37:0:4774:HOH:O	1.95	0.66
3:C:236:THR:HG21	37:C:8373:HOH:O	1.96	0.66
30:0:1185:U:H2'	30:0:1186:C:C6	2.31	0.66
30:0:544:G:C2'	30:0:545:G:H5''	2.24	0.66
3:C:236:THR:HG22	3:C:239:ALA:N	2.08	0.66
4:D:135:VAL:HG22	4:D:136:ARG:H	1.60	0.66
30:0:1205:U:H2'	30:0:1206:U:H5''	1.76	0.65
12:L:30:ARG:HD3	30:0:164:G:H4'	1.78	0.65
22:V:1:THR:HB	30:0:93:C:H5''	1.76	0.65
23:W:6:GLN:HB2	23:W:26:ILE:CD1	2.26	0.65
30:0:2414:A:H2'	30:0:2415:A:C8	2.31	0.65
30:0:856:G:C8	37:0:4975:HOH:O	2.48	0.65
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.78	0.65
23:W:122:ARG:HH11	23:W:122:ARG:CG	2.08	0.65
23:W:21:LEU:HD22	23:W:26:ILE:CD1	2.26	0.65
31:9:64:C:H2'	31:9:65:A:H5'	1.79	0.65
30:0:1741:U:H5'	30:0:1742:A:OP1	1.96	0.65
14:N:5:ARG:NH1	30:0:962:C:H1'	2.10	0.65
31:9:54:A:O2'	31:9:55:U:H5'	1.96	0.65
3:C:5:ILE:HD11	3:C:16:VAL:HG23	1.78	0.65
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.78	0.65
18:R:29:LYS:HE2	30:0:524:A:C5'	2.26	0.65
3:C:5:ILE:HD11	3:C:16:VAL:CG2	2.27	0.65
6:F:96:ALA:HA	37:F:3111:HOH:O	1.97	0.65
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.42	0.65
23:W:88:THR:HG23	23:W:110:GLN:NE2	2.11	0.65
30:0:1878:G:O2'	30:0:1879:U:C6	2.48	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:185:GLY:HA2	37:B:8633:HOH:O	1.97	0.65
16:P:117:SER:HB3	30:0:1593:C:OP1	1.98	0.64
30:0:2608:C:H2'	37:0:3110:HOH:O	1.96	0.64
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.78	0.64
5:E:97:VAL:HG12	37:E:4191:HOH:O	1.97	0.64
12:L:133:VAL:HA	37:L:8562:HOH:O	1.95	0.64
12:L:18:HIS:HD2	30:0:902:G:N7	1.95	0.64
22:V:42:ASN:HB3	37:V:7247:HOH:O	1.97	0.64
30:0:1632:A:C2'	30:0:1633:C:H5'	2.28	0.64
27:1:16:HIS:HD2	30:0:470:U:O2'	1.81	0.64
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.09	0.64
30:0:31:C:H2'	37:0:7238:HOH:O	1.97	0.64
30:0:1666:C:C2'	30:0:1667:A:H5''	2.27	0.64
8:H:49:GLN:HE21	8:H:140:TYR:HE2	1.46	0.64
30:0:1666:C:H2'	30:0:1667:A:C5'	2.27	0.64
14:N:4:PRO:HG3	31:9:69:U:OP1	1.98	0.63
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.12	0.63
30:0:1641:A:H2'	30:0:1642:A:H5'	1.79	0.63
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.34	0.63
2:B:41:PHE:HB3	2:B:190:MET:HE3	1.80	0.63
19:S:51:GLN:HE21	19:S:53:ASN:HD21	1.45	0.63
30:0:2649:A:H5'	30:0:2649:A:H8	1.63	0.63
30:0:2717:C:H2'	30:0:2718:C:C5'	2.24	0.63
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.78	0.63
13:M:99:ARG:HH21	13:M:170:ASN:HD22	1.45	0.63
30:0:1330:A:H2	37:0:4223:HOH:O	1.81	0.63
30:0:2769:C:O2'	30:0:2770:G:H5'	1.97	0.63
5:E:139:GLU:OE2	30:0:2781:U:H1'	1.99	0.63
25:Y:141:THR:HG23	37:Y:8586:HOH:O	1.99	0.63
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.81	0.63
25:Y:187:VAL:HG12	25:Y:205:ILE:HA	1.81	0.63
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.81	0.63
30:0:281:U:O2'	30:0:282:C:H5'	1.99	0.63
30:0:558:C:H2'	30:0:559:U:H5'	1.81	0.63
30:0:506:G:H22	30:0:509:A:H5'	1.64	0.62
18:R:39:THR:HG23	18:R:107:GLU:O	1.98	0.62
20:T:9:LYS:HB2	37:0:6974:HOH:O	1.98	0.62
27:1:20:ARG:HG2	30:0:111:C:O2'	1.99	0.62
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.34	0.62
27:1:25:LYS:HE2	37:2:7213:HOH:O	1.98	0.62
30:0:2832:C:H5	37:0:6762:HOH:O	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:185:VAL:HG12	37:Y:8567:HOH:O	1.99	0.62
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.64	0.62
9:I:120:ALA:O	9:I:124:VAL:HG23	1.99	0.62
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.80	0.62
1:A:192:VAL:HB	37:A:8587:HOH:O	1.99	0.62
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.65	0.62
30:0:138:U:H5''	30:0:139:C:OP2	1.99	0.62
30:0:1666:C:C2'	30:0:1667:A:C5'	2.78	0.62
30:0:2717:C:O2'	30:0:2718:C:H5''	1.99	0.62
30:0:2768:A:H2'	30:0:2769:C:O4'	1.99	0.62
2:B:195:ARG:HG2	2:B:323:LEU:HD22	1.81	0.62
4:D:57:THR:HG23	4:D:63:ILE:HA	1.82	0.62
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.80	0.62
10:J:47:THR:HB	37:0:4375:HOH:O	2.00	0.62
30:0:1730:G:H5''	30:0:1731:C:H6	1.65	0.62
2:B:145:HIS:HD2	2:B:146:THR:O	1.83	0.62
4:D:99:ASP:HA	37:0:5842:HOH:O	2.00	0.62
30:0:1118:A:C8	30:0:1118:A:C3'	2.79	0.61
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.82	0.61
29:3:73:GLU:HB3	37:3:8559:HOH:O	2.00	0.61
31:9:2:U:OP2	31:9:3:A:H5'	2.00	0.61
31:9:29:C:C2'	31:9:30:C:H5'	2.30	0.61
30:0:1130:U:H2'	30:0:1131:G:O4'	2.00	0.61
2:B:211:THR:HG23	30:0:2840:A:OP1	2.00	0.61
30:0:396:U:O2'	30:0:418:C:H4'	2.00	0.61
2:B:179:LEU:O	2:B:183:GLU:HG2	1.99	0.61
6:F:91:VAL:HG12	6:F:92:GLY:N	2.14	0.61
12:L:136:ALA:HB3	37:L:8562:HOH:O	1.99	0.61
13:M:80:GLY:O	13:M:81:ARG:HD3	1.99	0.61
30:0:1778:A:H2'	30:0:1779:A:H5'	1.82	0.61
30:0:2346:C:O5'	30:0:2346:C:H6	1.83	0.61
30:0:2533:C:C6	30:0:2533:C:H5'	2.34	0.61
3:C:236:THR:H	3:C:239:ALA:HB3	1.65	0.61
18:R:39:THR:HG22	18:R:42:GLU:H	1.65	0.61
30:0:1189:A:H1'	30:0:1209:C:H1'	1.83	0.61
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.83	0.61
2:B:16:ARG:NH1	37:B:8617:HOH:O	2.34	0.61
3:C:96:LYS:NZ	30:0:1351:G:OP1	2.33	0.61
30:0:1201:C:H2'	30:0:1202:A:H5'	1.82	0.61
30:0:951:A:O2'	30:0:952:G:H5'	2.01	0.61
30:0:960:G:H2'	30:0:960:G:N3	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1189:A:H1'	30:0:1209:C:C1'	2.30	0.61
30:0:2502:C:C2'	30:0:2503:A:H5'	2.30	0.61
15:O:42:GLU:HB2	37:O:2176:HOH:O	2.00	0.61
31:9:13:A:O2'	31:9:14:G:H5''	2.00	0.61
26:Z:35:SER:HB3	26:Z:47:ARG:HB2	1.81	0.61
10:J:82:THR:HG23	30:0:1242:A:C5'	2.24	0.60
2:B:238:ASN:HD22	2:B:240:GLY:N	1.98	0.60
12:L:143:THR:HG22	12:L:144:ASP:N	2.16	0.60
4:D:163:VAL:HA	37:D:6326:HOH:O	2.02	0.60
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.81	0.60
23:W:21:LEU:HB3	23:W:26:ILE:HG12	1.82	0.60
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.67	0.60
13:M:61:ILE:HG13	37:M:8617:HOH:O	1.99	0.60
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.46	0.60
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.65	0.60
30:0:2587:OMU:H2'	30:0:2589:U:H5''	1.83	0.60
1:A:105:VAL:CG1	1:A:154:ALA:HB1	2.31	0.60
1:A:48:ASP:HB3	37:A:8599:HOH:O	2.02	0.60
12:L:4:LYS:HE2	30:0:645:U:OP2	2.01	0.60
30:0:2415:A:H2'	30:0:2416:G:H5'	1.82	0.60
9:I:110:ASP:O	30:0:1163:G:H5'	2.02	0.60
14:N:37:ARG:NH1	31:9:6:C:OP1	2.34	0.60
30:0:2768:A:O2'	30:0:2769:C:H5'	2.01	0.60
30:0:1528:A:H2'	30:0:1529:G:O4'	2.01	0.60
30:0:1172:G:H5''	37:0:6809:HOH:O	2.01	0.60
30:0:1377:C:H5'	30:0:1377:C:C6	2.37	0.60
30:0:1559:A:H1'	37:0:5413:HOH:O	2.02	0.60
18:R:117:HIS:HD2	30:0:20:G:H21	1.50	0.60
2:B:267:LYS:HD3	37:B:8526:HOH:O	2.01	0.60
23:W:88:THR:HG22	23:W:89:ASP:N	2.17	0.60
25:Y:235:GLU:H	25:Y:235:GLU:CD	2.05	0.60
30:0:1205:U:C2'	30:0:1206:U:H5''	2.32	0.59
30:0:1350:U:H4'	37:0:4662:HOH:O	2.02	0.59
30:0:2670:G:O2'	30:0:2671:U:H5'	2.02	0.59
30:0:2578:G:H5'	30:0:2578:G:H8	1.67	0.59
2:B:212:GLN:HB2	2:B:257:THR:CG2	2.29	0.59
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.02	0.59
25:Y:133:HIS:HD2	37:Y:8579:HOH:O	1.85	0.59
30:0:1175:G:H1'	30:0:1193:A:H2'	1.84	0.59
30:0:2488:A:H2	37:0:6826:HOH:O	1.84	0.59
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:49:G:O2'	31:9:50:G:H5'	2.01	0.59
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.35	0.59
23:W:4:LEU:O	23:W:32:CYS:HA	2.03	0.59
23:W:88:THR:HG22	23:W:89:ASP:H	1.67	0.59
30:0:2756:U:N3	30:0:2896:A:H2	1.98	0.59
31:9:23:U:O2'	31:9:24:U:H4'	2.02	0.59
23:W:84:VAL:HG12	37:W:6679:HOH:O	2.02	0.59
30:0:567:U:H5''	37:0:5949:HOH:O	2.01	0.59
30:0:2420:G:O2'	30:0:2421:G:H5'	2.02	0.59
3:C:27:ARG:NH2	30:0:657:G:OP1	2.31	0.59
10:J:107:ASN:HD21	10:J:109:TYR:HB2	1.68	0.59
23:W:139:GLY:O	23:W:141:HIS:HD2	1.85	0.59
30:0:1159:G:H1	30:0:1208:C:H42	1.50	0.59
30:0:204:A:C2'	30:0:205:U:H5'	2.32	0.59
30:0:2649:A:H5'	30:0:2649:A:C8	2.38	0.59
30:0:1120:U:H5''	30:0:1120:U:C6	2.37	0.58
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.85	0.58
9:I:112:LEU:HD11	30:0:1162:G:H1'	1.84	0.58
11:K:109:LEU:HD13	11:K:113:ILE:HD11	1.85	0.58
23:W:122:ARG:HH11	23:W:122:ARG:HG2	1.68	0.58
30:0:1182:C:H1'	30:0:1192:A:H8	1.68	0.58
30:0:1667:A:H2'	30:0:1668:U:C6	2.38	0.58
30:0:2316:G:H4'	37:0:5638:HOH:O	2.03	0.58
31:9:64:C:C2'	31:9:65:A:H5'	2.33	0.58
18:R:17:MET:SD	37:R:8542:HOH:O	2.57	0.58
31:9:75:G:H1	31:9:106:U:H3	1.51	0.58
8:H:48:VAL:HA	8:H:170:ARG:O	2.03	0.58
18:R:29:LYS:HE2	30:0:524:A:H5'	1.85	0.58
30:0:1730:G:C5'	30:0:1731:C:H6	2.16	0.58
30:0:2604:A:H5'	37:0:5339:HOH:O	2.04	0.58
3:C:236:THR:CG2	3:C:239:ALA:H	2.11	0.58
18:R:99:ALA:HB1	18:R:109:MET:CE	2.32	0.58
20:T:52:ARG:HD2	30:0:317:A:H5''	1.84	0.58
1:A:211:LYS:HB3	1:A:212:PRO:HD2	1.84	0.58
3:C:76:ARG:HD3	37:C:8366:HOH:O	2.04	0.58
5:E:100:ASP:HB2	37:E:2789:HOH:O	2.03	0.58
23:W:64:THR:O	23:W:68:THR:HG22	2.04	0.58
23:W:80:ASP:O	23:W:84:VAL:HG23	2.02	0.58
30:0:2320:U:H4'	30:0:2321:A:O4'	2.03	0.58
30:0:2718:C:H6	30:0:2718:C:H5'	1.69	0.58
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:134:HIS:HE1	30:0:538:C:OP2	1.87	0.58
14:N:80:SER:HB2	37:N:8535:HOH:O	2.02	0.58
19:S:51:GLN:NE2	19:S:53:ASN:HD21	2.02	0.58
30:0:1118:A:H8	30:0:1119:G:H5''	1.67	0.58
31:9:92:G:H2'	31:9:93:A:C8	2.39	0.58
12:L:148:GLU:HA	37:L:8561:HOH:O	2.04	0.58
14:N:43:VAL:HG13	14:N:118:ILE:HD11	1.84	0.58
30:0:2064:U:H4'	30:0:2653:A:OP1	2.04	0.57
29:3:60:LYS:HG3	37:0:7104:HOH:O	2.04	0.57
31:9:20:G:O2'	31:9:21:G:H5'	2.04	0.57
10:J:107:ASN:ND2	10:J:109:TYR:H	2.01	0.57
30:0:2878:U:H2'	30:0:2879:A:O4'	2.04	0.57
31:9:35:C:H5''	37:9:8455:HOH:O	2.04	0.57
3:C:78:ARG:HG3	3:C:78:ARG:HH11	1.67	0.57
16:P:10:ALA:HA	16:P:13:VAL:HG12	1.86	0.57
18:R:29:LYS:HE2	30:0:524:A:H5''	1.87	0.57
3:C:76:ARG:HG2	3:C:78:ARG:HH12	1.68	0.57
4:D:103:ASN:ND2	4:D:134:LEU:H	2.02	0.57
30:0:1119:G:N2	30:0:1246:A:H2	1.95	0.57
31:9:28:U:H2'	31:9:29:C:C6	2.39	0.57
2:B:162:MET:HE2	2:B:310:ARG:HD3	1.87	0.57
19:S:57:THR:HG22	19:S:59:ASP:N	2.18	0.57
30:0:1819:G:H5'	37:0:4250:HOH:O	2.05	0.57
30:0:1972:U:H2'	30:0:1973:A:H5''	1.85	0.57
23:W:38:THR:HG22	37:W:3580:HOH:O	2.03	0.57
30:0:1679:C:H5'	37:0:8846:HOH:O	2.04	0.57
30:0:1701:A:H5''	30:0:1702:U:H3'	1.86	0.57
30:0:1834:C:H2'	30:0:1840:A:N6	2.18	0.57
30:0:432:G:O2'	30:0:433:C:H5'	2.05	0.57
30:0:1289:C:O2'	30:0:1290:G:H5'	2.05	0.57
30:0:2064:U:H5'	30:0:2652:U:H4'	1.85	0.57
12:L:6:ARG:HD3	30:0:1299:G:O6	2.04	0.57
30:0:1730:G:C5'	30:0:1731:C:C5	2.87	0.57
30:0:558:C:C2'	30:0:559:U:C5'	2.82	0.57
3:C:115:LEU:HD21	3:C:243:VAL:HG13	1.87	0.57
23:W:125:HIS:CD2	23:W:127:GLY:H	2.23	0.57
30:0:558:C:H2'	30:0:559:U:H5''	1.86	0.56
30:0:681:G:N3	30:0:681:G:H5'	2.20	0.56
1:A:121:ALA:O	1:A:124:VAL:HG22	2.04	0.56
6:F:50:VAL:CG1	6:F:60:VAL:HG11	2.35	0.56
13:M:182:LYS:HE2	30:0:392:U:O2'	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:24:GLN:NE2	13:M:27:ARG:HH11	2.03	0.56
25:Y:144:ARG:NH1	37:Y:8573:HOH:O	2.37	0.56
30:0:1181:A:C2'	30:0:1182:C:H5'	2.36	0.56
30:0:2467:A:H1'	37:0:4272:HOH:O	2.04	0.56
30:0:282:C:O2'	30:0:283:U:C5'	2.51	0.56
27:1:42:SER:HB2	37:1:8409:HOH:O	2.05	0.56
30:0:703:G:O2'	30:0:704:C:H5'	2.06	0.56
13:M:24:GLN:HE21	13:M:27:ARG:HH11	1.53	0.56
14:N:7:LYS:HE3	17:Q:21:ARG:O	2.05	0.56
21:U:14:GLU:O	21:U:17:THR:HB	2.05	0.56
25:Y:204:ARG:HH22	30:0:553:G:P	2.28	0.56
30:0:1878:G:O2'	30:0:1879:U:H6	1.89	0.56
30:0:2435:U:H1'	37:0:4978:HOH:O	2.06	0.56
1:A:192:VAL:HG13	37:A:8553:HOH:O	2.05	0.56
10:J:103:VAL:HG12	37:J:5907:HOH:O	2.04	0.56
19:S:43:GLU:HB3	37:S:7106:HOH:O	2.05	0.56
30:0:2488:A:H61	30:0:2534:C:H42	1.53	0.56
30:0:2851:G:C2'	30:0:2852:A:H5'	2.35	0.56
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.86	0.56
3:C:1:MET:HG2	3:C:2:GLN:N	2.20	0.56
30:0:2300:A:H4'	30:0:2301:A:O5'	2.06	0.56
16:P:143:ALA:HA	37:P:184:HOH:O	2.03	0.56
30:0:1118:A:H62	30:0:1244:U:H3	1.54	0.56
6:F:38:LYS:HE3	30:0:244:C:OP2	2.06	0.56
30:0:282:C:H1'	30:0:368:C:H42	1.70	0.56
1:A:153:ARG:HH11	1:A:153:ARG:HB2	1.71	0.56
10:J:107:ASN:HD22	10:J:109:TYR:H	1.53	0.56
30:0:1278:A:H4'	30:0:1279:U:C4	2.41	0.56
2:B:139:ASP:HB2	2:B:165:ARG:HE	1.70	0.56
11:K:34:VAL:CG2	11:K:47:ALA:HB2	2.36	0.56
22:V:39:ALA:N	22:V:40:PRO:HD2	2.21	0.56
30:0:1477:C:H5'	30:0:1868:G:C5'	2.35	0.56
30:0:899:C:H5'	37:0:9733:HOH:O	2.05	0.56
30:0:2251:G:H2'	30:0:2252:A:C8	2.41	0.56
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.04	0.56
1:A:223:ARG:HG3	37:A:8595:HOH:O	2.05	0.56
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.71	0.56
11:K:55:VAL:HG12	11:K:56:SER:N	2.21	0.56
13:M:95:LYS:HE2	30:0:157:G:H4'	1.88	0.56
14:N:37:ARG:NE	37:N:8533:HOH:O	2.39	0.56
30:0:2502:C:H2'	30:0:2503:A:H5'	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:50:VAL:HG22	31:9:41:C:O4'	2.05	0.56
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.70	0.56
30:0:1120:U:H5'	30:0:1121:G:OP2	2.05	0.55
30:0:1250:C:O2'	30:0:1251:C:H5'	2.05	0.55
30:0:2825:C:H4'	30:0:2826:G:O5'	2.06	0.55
30:0:396:U:H1'	37:0:7180:HOH:O	2.06	0.55
31:9:91:C:H2'	31:9:92:G:O4'	2.05	0.55
20:T:53:GLY:HA3	37:T:6384:HOH:O	2.05	0.55
16:P:120:ARG:HD2	30:0:1594:C:OP2	2.07	0.55
30:0:2361:A:H5''	37:0:8523:HOH:O	2.07	0.55
37:N:8545:HOH:O	31:9:49:G:H5''	2.05	0.55
1:A:96:LEU:HD22	1:A:128:LEU:HD13	1.87	0.55
5:E:68:HIS:O	5:E:72:MET:HG3	2.06	0.55
5:E:81:GLU:HG2	5:E:134:SER:HB3	1.86	0.55
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.35	0.55
21:U:37:GLU:HB3	37:U:408:HOH:O	2.06	0.55
4:D:25:MET:CE	4:D:37:ALA:HB1	2.36	0.55
14:N:110:THR:HB	14:N:113:SER:OG	2.06	0.55
14:N:141:ARG:HH21	31:9:48:C:H4'	1.71	0.55
30:0:1783:A:O2'	30:0:1784:U:H5'	2.06	0.55
30:0:88:G:H5'	30:0:88:G:H8	1.72	0.55
23:W:115:THR:HG23	37:W:5420:HOH:O	2.06	0.55
23:W:21:LEU:HD21	23:W:48:VAL:CG1	2.36	0.55
13:M:188:ARG:HD3	30:0:155:C:OP2	2.06	0.55
30:0:204:A:H2'	30:0:205:U:H5'	1.88	0.55
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.87	0.55
18:R:25:PHE:CE2	18:R:29:LYS:HE3	2.41	0.55
30:0:1636:G:O2'	30:0:1637:A:H5'	2.07	0.55
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.42	0.55
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.07	0.55
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.87	0.55
23:W:122:ARG:HG3	23:W:152:ALA:O	2.06	0.55
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.41	0.55
22:V:39:ALA:C	22:V:41:GLU:H	2.09	0.55
30:0:1595:G:O2'	30:0:1596:U:H5'	2.07	0.55
27:1:16:HIS:HE1	30:0:775:G:OP1	1.90	0.55
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.88	0.55
2:B:17:LYS:O	2:B:260:HIS:HD2	1.90	0.55
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.36	0.55
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.89	0.55
30:0:1135:G:H5'	37:0:5475:HOH:O	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1165:G:O2'	30:0:1174:A:H1'	2.07	0.54
30:0:661:G:C5	30:0:686:A:C2	2.95	0.54
13:M:84:LYS:HE2	37:M:8571:HOH:O	2.06	0.54
14:N:11:ARG:HG3	14:N:14:ARG:NH1	2.22	0.54
14:N:41:LYS:HD3	37:9:8439:HOH:O	2.08	0.54
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.43	0.54
30:0:1972:U:H2'	30:0:1973:A:C5'	2.37	0.54
30:0:2467:A:O2'	30:0:2468:A:H2'	2.06	0.54
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.72	0.54
30:0:1181:A:H2'	30:0:1182:C:H5'	1.89	0.54
30:0:2419:U:H5''	30:0:2420:G:H5'	1.89	0.54
30:0:485:A:N3	30:0:487:G:H5''	2.22	0.54
2:B:125:GLU:O	2:B:129:ARG:HG3	2.07	0.54
30:0:1158:G:O2'	30:0:1159:G:H5'	2.08	0.54
30:0:2712:G:H5'	37:0:4763:HOH:O	2.07	0.54
3:C:79:ARG:O	3:C:87:ARG:HG2	2.08	0.54
9:I:100:VAL:HG11	9:I:124:VAL:HG22	1.89	0.54
11:K:29:LEU:HB3	11:K:55:VAL:CG1	2.28	0.54
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.88	0.54
18:R:17:MET:HE1	37:0:3769:HOH:O	2.06	0.54
30:0:1299:G:H5'	37:0:3611:HOH:O	2.06	0.54
30:0:1926:G:H2'	30:0:1927:A:C8	2.43	0.54
30:0:2524:G:H21	30:0:2526:C:N4	2.05	0.54
30:0:343:C:O2'	30:0:344:C:H5'	2.06	0.54
31:9:76:G:C3'	31:9:77:A:H5''	2.28	0.54
2:B:18:ARG:HG3	2:B:256:GLN:HG3	1.89	0.54
2:B:254:GLN:HG3	37:0:9223:HOH:O	2.08	0.54
9:I:69:PRO:HA	30:0:1164:U:OP1	2.08	0.54
30:0:1615:A:H5'	37:0:3722:HOH:O	2.06	0.54
30:0:200:C:H2'	37:0:9976:HOH:O	2.08	0.54
3:C:115:LEU:O	3:C:118:THR:HB	2.08	0.54
4:D:159:PRO:O	4:D:163:VAL:HG23	2.07	0.54
25:Y:187:VAL:HG22	25:Y:192:ASP:HB2	1.89	0.54
30:0:1279:U:O2	30:0:1279:U:H2'	2.06	0.54
30:0:644:G:N3	30:0:644:G:H5'	2.22	0.54
4:D:23:VAL:HG21	4:D:45:THR:HG21	1.88	0.54
11:K:82:ARG:NH2	11:K:115:ARG:HG2	2.23	0.54
30:0:1268:C:O2'	30:0:1269:G:H5'	2.07	0.54
30:0:1973:A:H5'	30:0:1973:A:C8	2.35	0.54
30:0:2638:G:H5'	37:0:4469:HOH:O	2.08	0.54
24:X:43:VAL:HG12	24:X:44:ASP:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1972:U:C2'	30:0:1973:A:H5''	2.37	0.54
30:0:280:C:H2'	30:0:281:U:O4'	2.08	0.54
17:Q:95:GLU:HA	30:0:949:U:H4'	1.89	0.54
2:B:51:VAL:CG2	2:B:327:VAL:HG13	2.38	0.54
4:D:54:ALA:CB	4:D:69:ILE:HD12	2.38	0.54
12:L:80:ASP:HB2	12:L:90:ARG:O	2.08	0.54
9:I:87:PRO:C	9:I:89:GLU:H	2.10	0.53
2:B:336:GLN:O	30:0:2862:G:H4'	2.07	0.53
24:X:25:ARG:HD2	37:X:3861:HOH:O	2.07	0.53
3:C:184:ARG:HD2	30:0:1306:U:OP1	2.08	0.53
14:N:160:SER:HB3	31:9:51:A:H5'	1.89	0.53
14:N:4:PRO:HD2	37:0:6319:HOH:O	2.08	0.53
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.89	0.53
9:I:113:SER:HB2	9:I:118:ASN:HB2	1.89	0.53
13:M:169:ARG:HD2	37:M:8587:HOH:O	2.08	0.53
30:0:1730:G:H5''	30:0:1731:C:C6	2.41	0.53
30:0:2001:G:O2'	30:0:2002:C:H5'	2.08	0.53
30:0:95:A:H5''	30:0:97:G:O4'	2.08	0.53
1:A:36:ASP:O	1:A:38:ILE:N	2.34	0.53
5:E:11:VAL:HG12	5:E:12:ASP:N	2.23	0.53
20:T:1:SER:HB2	30:0:447:A:OP2	2.08	0.53
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.89	0.53
2:B:329:TYR:CE2	21:U:15:PRO:HG2	2.44	0.53
30:0:814:G:H4'	37:0:9664:HOH:O	2.08	0.53
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.48	0.53
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.90	0.53
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.73	0.53
1:A:105:VAL:HG11	1:A:154:ALA:HB1	1.90	0.53
21:U:39:ASN:ND2	21:U:44:ARG:HH11	2.06	0.53
30:0:1116:U:O2'	30:0:1118:A:C2	2.40	0.53
30:0:172:U:H5'	37:0:3697:HOH:O	2.09	0.53
31:9:24:U:H3'	31:9:25:G:H5'	1.90	0.53
1:A:97:ALA:HB2	1:A:150:PRO:HB2	1.91	0.53
2:B:51:VAL:HG23	2:B:329:TYR:O	2.09	0.53
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.43	0.53
5:E:69:ILE:HA	5:E:72:MET:HE3	1.90	0.53
6:F:101:ALA:HA	37:F:5413:HOH:O	2.09	0.53
13:M:81:ARG:HG3	13:M:85:ARG:HB2	1.91	0.53
30:0:2563:U:H2'	30:0:2565:C:O5'	2.08	0.52
13:M:58:GLN:NE2	30:0:259:G:H21	2.08	0.52
31:9:107:C:H5	37:9:8435:HOH:O	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:73:HIS:HE1	30:0:1789:G:O6	1.91	0.52
30:0:1189:A:H1'	30:0:1209:C:O4'	2.09	0.52
30:0:1525:G:H5'	30:0:1526:A:OP2	2.09	0.52
29:3:17:HIS:O	29:3:18:GLN:HG3	2.10	0.52
2:B:307:ARG:HG3	2:B:307:ARG:NH1	2.20	0.52
6:F:58:GLU:HA	6:F:61:MET:HE2	1.90	0.52
14:N:163:PHE:HZ	14:N:171:HIS:HD1	1.55	0.52
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.74	0.52
30:0:2866:U:H4'	30:0:2867:G:H5'	1.90	0.52
6:F:39:SER:HB3	6:F:45:ALA:HB2	1.91	0.52
7:G:64:ASN:N	7:G:64:ASN:HD22	2.06	0.52
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.09	0.52
16:P:83:LYS:HG2	30:0:793:A:H5''	1.92	0.52
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.92	0.52
30:0:2256:G:H2'	30:0:2257:G:C5'	2.39	0.52
1:A:81:GLN:HB2	1:A:92:ASN:ND2	2.23	0.52
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.09	0.52
16:P:41:ARG:HH22	30:0:1500:U:P	2.32	0.52
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.90	0.52
30:0:2241:C:O2'	30:0:2242:U:H5'	2.09	0.52
30:0:794:U:H3	30:0:819:A:H61	1.57	0.52
4:D:135:VAL:HG22	4:D:136:ARG:N	2.24	0.52
30:0:1211:G:O2'	30:0:1212:C:H5'	2.10	0.52
13:M:163:LEU:HD21	30:0:188:C:H5''	1.91	0.52
1:A:123:GLY:HA3	1:A:162:GLY:HA2	1.92	0.52
3:C:246:ARG:NH1	37:C:8369:HOH:O	2.42	0.52
17:Q:25:PRO:HB2	37:Q:4350:HOH:O	2.10	0.52
23:W:151:GLU:O	23:W:154:ARG:HB2	2.09	0.52
1:A:95:PRO:HG2	1:A:98:GLU:HG2	1.91	0.52
15:O:47:ARG:HG3	15:O:47:ARG:HH11	1.75	0.52
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.10	0.52
5:E:69:ILE:HA	5:E:72:MET:CE	2.40	0.52
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.92	0.52
23:W:130:HIS:O	23:W:136:GLY:HA3	2.10	0.52
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.10	0.52
30:0:319:A:H4'	30:0:338:C:C4	2.45	0.52
20:T:1:SER:HB2	30:0:447:A:P	2.50	0.52
30:0:65:C:O2'	30:0:66:G:H5'	2.09	0.52
30:0:820:G:O2'	30:0:856:G:H4'	2.10	0.52
14:N:11:ARG:NH1	31:9:8:G:O6	2.42	0.52
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:MET:HG2	1:A:186:TRP:CB	2.40	0.51
9:I:108:HIS:N	9:I:109:PRO:HD2	2.25	0.51
30:0:1118:A:C8	30:0:1119:G:H5''	2.45	0.51
30:0:1120:U:H6	30:0:1120:U:H5''	1.75	0.51
30:0:2329:C:O2'	30:0:2330:U:H5'	2.10	0.51
30:0:291:C:H2'	30:0:292:G:O4'	2.11	0.51
10:J:19:MET:HE2	10:J:132:LEU:HD11	1.92	0.51
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.91	0.51
30:0:1406:A:H4'	30:0:1407:A:H5''	1.92	0.51
30:0:2507:G:H2'	30:0:2510:C:N4	2.23	0.51
30:0:256:C:H2'	30:0:257:G:O4'	2.11	0.51
15:O:25:VAL:HG12	30:0:709:G:O2'	2.10	0.51
2:B:305:ASP:O	2:B:306:LYS:HB2	2.11	0.51
8:H:66:GLU:HA	37:H:8381:HOH:O	2.09	0.51
17:Q:11:ARG:HD3	37:Q:5620:HOH:O	2.09	0.51
19:S:51:GLN:HE21	19:S:53:ASN:ND2	2.08	0.51
24:X:71:ARG:HD3	37:X:2171:HOH:O	2.10	0.51
25:Y:187:VAL:HB	25:Y:203:VAL:HG22	1.91	0.51
30:0:1165:G:O2'	30:0:1174:A:C1'	2.59	0.51
30:0:1942:A:H3'	37:0:6896:HOH:O	2.11	0.51
30:0:1996:U:O2'	30:0:1997:A:H5'	2.11	0.51
30:0:2769:C:H2'	30:0:2770:G:O4'	2.11	0.51
30:0:951:A:H2'	30:0:952:G:H5'	1.92	0.51
28:2:31:ARG:NH2	37:2:7177:HOH:O	2.43	0.51
3:C:236:THR:HA	37:C:8449:HOH:O	2.10	0.51
9:I:124:VAL:O	9:I:124:VAL:HG12	2.11	0.51
25:Y:169:ARG:HB2	30:0:1268:C:O2'	2.11	0.51
30:0:2795:C:O2'	30:0:2796:U:H5'	2.09	0.51
30:0:920:C:H5'	30:0:921:G:C4	2.45	0.51
8:H:12:ILE:HG23	8:H:129:ARG:CZ	2.41	0.51
14:N:48:VAL:HG11	14:N:55:ASP:HB3	1.93	0.51
30:0:1527:A:H1'	30:0:1528:A:C8	2.45	0.51
30:0:2072:G:C6	30:0:2533:C:H1'	2.46	0.51
30:0:969:G:H1	30:0:999:C:H42	1.59	0.51
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.91	0.51
1:A:191:GLY:HA2	1:A:194:MET:HE2	1.93	0.51
19:S:10:VAL:HG11	22:V:36:ALA:HA	1.92	0.51
30:0:1342:C:O2'	30:0:1343:C:H5'	2.10	0.51
30:0:2830:U:H3'	37:0:4770:HOH:O	2.09	0.51
30:0:90:A:H2'	30:0:91:G:O4'	2.11	0.51
29:3:48:ASN:ND2	29:3:50:GLY:H	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:23:VAL:HG21	4:D:45:THR:CG2	2.41	0.51
30:0:2301:A:H5''	30:0:2302:A:H5'	1.91	0.51
30:0:2591:C:H2'	30:0:2592:G:O4'	2.11	0.51
24:X:15:ARG:NH1	30:0:2896:A:OP1	2.44	0.51
30:0:848:C:H5'	37:0:6823:HOH:O	2.10	0.51
31:9:49:G:H2'	31:9:50:G:O4'	2.11	0.51
4:D:104:PHE:CE2	4:D:132:VAL:HB	2.46	0.51
4:D:84:LEU:HA	4:D:87:ALA:HB3	1.93	0.51
5:E:23:GLU:HG2	5:E:28:SER:HB3	1.93	0.51
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.41	0.51
12:L:30:ARG:HD2	37:0:8538:HOH:O	2.11	0.51
22:V:55:ARG:O	22:V:59:ILE:HG12	2.11	0.51
1:A:53:ALA:HB3	37:A:8599:HOH:O	2.10	0.51
23:W:65:VAL:HA	23:W:68:THR:HG22	1.92	0.51
30:0:1180:U:H2'	30:0:1181:A:C8	2.46	0.51
30:0:2478:U:O2'	30:0:2479:A:H5'	2.10	0.51
11:K:30:LYS:O	11:K:55:VAL:HG13	2.11	0.51
21:U:33:SER:O	21:U:37:GLU:HG3	2.10	0.51
30:0:1333:U:H2'	30:0:1334:C:C6	2.46	0.50
30:0:1503:U:H2'	30:0:1504:A:O4'	2.12	0.50
30:0:2445:U:H2'	30:0:2446:G:C8	2.46	0.50
30:0:2756:U:C2	30:0:2896:A:H2	2.28	0.50
30:0:960:G:N3	30:0:960:G:C2'	2.74	0.50
31:9:56:A:C3'	31:9:57:A:H5''	2.40	0.50
3:C:214:THR:HG23	37:C:8435:HOH:O	2.10	0.50
4:D:25:MET:HE2	4:D:41:LEU:HG	1.93	0.50
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.46	0.50
30:0:2265:U:H2'	30:0:2266:A:C8	2.47	0.50
28:2:35:ARG:HB2	37:2:2691:HOH:O	2.11	0.50
2:B:264:GLU:HG2	2:B:267:LYS:CE	2.41	0.50
30:0:1741:U:O2'	30:0:2723:G:H4'	2.11	0.50
2:B:288:GLY:HA2	30:0:2898:G:H4'	1.93	0.50
27:1:28:HIS:HE1	30:0:776:A:OP1	1.94	0.50
2:B:212:GLN:HA	30:0:1733:A:H4'	1.92	0.50
7:G:16:LYS:O	7:G:20:VAL:HG23	2.12	0.50
8:H:41:LYS:HE2	8:H:45:ASP:HB3	1.93	0.50
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.10	0.50
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.94	0.50
30:0:2415:A:C2'	30:0:2416:G:H5'	2.41	0.50
30:0:2472:C:O2'	30:0:2634:G:H4'	2.12	0.50
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1603:A:C5'	30:0:1605:G:O4'	2.60	0.50
30:0:1921:A:C6	30:0:1922:A:C2	3.00	0.50
30:0:2842:G:H2'	30:0:2843:A:H5'	1.93	0.50
30:0:447:A:O2'	30:0:448:G:H5'	2.12	0.50
4:D:76:ARG:NE	31:9:44:A:O4'	2.45	0.50
2:B:214:PRO:HD2	37:B:8521:HOH:O	2.12	0.50
5:E:15:GLN:HG2	5:E:19:ASP:O	2.12	0.50
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.94	0.50
23:W:122:ARG:NH2	37:0:4835:HOH:O	2.45	0.50
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.74	0.50
3:C:174:ILE:HD11	30:0:338:C:H4'	1.94	0.50
10:J:45:VAL:HG21	10:J:129:PHE:CD1	2.46	0.50
20:T:24:ARG:HH21	20:T:39:ASN:ND2	2.09	0.50
30:0:1342:C:C2'	30:0:1343:C:H5'	2.42	0.50
30:0:1419:U:H5'	30:0:1420:C:OP2	2.11	0.50
30:0:861:A:C8	37:0:5228:HOH:O	2.55	0.50
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.43	0.50
29:3:62:THR:HB	37:3:8549:HOH:O	2.10	0.50
20:T:38:ARG:NH1	37:T:6217:HOH:O	2.44	0.50
25:Y:187:VAL:HG23	37:Y:8567:HOH:O	2.11	0.50
30:0:2505:G:C2'	30:0:2506:A:H5'	2.41	0.50
30:0:308:U:C4	30:0:342:C:H1'	2.46	0.50
30:0:702:G:O2'	30:0:703:G:H5'	2.12	0.50
2:B:254:GLN:HG2	2:B:255:GLY:N	2.25	0.50
22:V:44:GLY:HA3	30:0:92:G:H4'	1.94	0.50
6:F:59:ILE:HD13	30:0:263:U:O4'	2.11	0.50
29:3:3:MET:O	29:3:90:PHE:HA	2.12	0.50
8:H:14:LYS:HE2	37:0:3382:HOH:O	2.11	0.50
8:H:49:GLN:HG3	8:H:140:TYR:CE2	2.47	0.50
11:K:62:PRO:HG3	11:K:65:ARG:NH2	2.26	0.50
26:Z:77:GLY:HA2	26:Z:91:GLY:O	2.12	0.50
10:J:52:GLN:NE2	30:0:1119:G:H8	2.06	0.49
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.93	0.49
1:A:179:MET:HA	1:A:179:MET:CE	2.42	0.49
1:A:3:ARG:HD3	30:0:870:G:OP2	2.11	0.49
37:R:8545:HOH:O	30:0:1370:G:H5''	2.12	0.49
30:0:2256:G:H2'	30:0:2257:G:H5'	1.95	0.49
2:B:102:THR:HG21	2:B:182:VAL:O	2.11	0.49
3:C:98:ARG:NH1	37:C:8355:HOH:O	2.44	0.49
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.94	0.49
14:N:179:LEU:HA	14:N:184:ILE:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:13:MET:CE	23:W:17:ILE:HG22	2.42	0.49
30:0:185:G:H4'	30:0:186:A:H4'	1.94	0.49
30:0:2061:C:C2'	30:0:2062:A:H5'	2.42	0.49
30:0:542:A:H2'	30:0:543:G:O4'	2.13	0.49
1:A:128:LEU:HG	37:A:8568:HOH:O	2.11	0.49
2:B:102:THR:HG23	2:B:182:VAL:HG12	1.95	0.49
7:G:20:VAL:O	7:G:24:VAL:HG23	2.12	0.49
13:M:164:THR:HG22	13:M:167:GLY:N	2.14	0.49
23:W:11:VAL:HG11	30:0:1086:A:C6	2.46	0.49
30:0:1127:C:C5	30:0:1128:U:C4	3.00	0.49
25:Y:115:ARG:HH21	30:0:1266:U:H4'	1.76	0.49
27:1:16:HIS:CD2	30:0:470:U:O2'	2.65	0.49
30:0:602:A:O2'	30:0:605:C:H4'	2.11	0.49
30:0:941:G:O2'	30:0:942:U:H5'	2.12	0.49
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.47	0.49
15:O:24:ALA:HB3	30:0:710:G:OP1	2.11	0.49
20:T:49:GLU:HB3	20:T:59:GLU:HG2	1.95	0.49
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.94	0.49
30:0:1137:G:H1'	37:0:3414:HOH:O	2.12	0.49
30:0:1206:U:H2'	30:0:1207:A:O4'	2.13	0.49
30:0:858:U:C6	37:0:4975:HOH:O	2.66	0.49
3:C:43:LYS:HG2	30:0:449:A:N7	2.27	0.49
4:D:154:LYS:H	4:D:154:LYS:CD	2.18	0.49
22:V:16:ARG:NH1	22:V:65:ASP:O	2.46	0.49
30:0:1189:A:O2'	30:0:1208:C:H2'	2.11	0.49
30:0:1819:G:H2'	30:0:1820:G:C4'	2.43	0.49
30:0:2010:A:H2'	37:0:5505:HOH:O	2.11	0.49
30:0:1787:C:H4'	30:0:2883:A:O4'	2.12	0.49
3:C:233:THR:HG22	3:C:234:VAL:N	2.26	0.49
1:A:211:LYS:O	30:0:1943:C:H4'	2.13	0.49
30:0:407:A:H5'	37:0:5572:HOH:O	2.13	0.49
4:D:23:VAL:HG22	4:D:73:VAL:HB	1.95	0.49
26:Z:37:ARG:NH1	37:Z:8419:HOH:O	2.45	0.49
30:0:1205:U:H2'	30:0:1206:U:H5'	1.95	0.49
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.42	0.49
4:D:65:GLU:HG3	37:D:6752:HOH:O	2.12	0.49
30:0:1641:A:C2'	30:0:1642:A:H5'	2.43	0.49
28:2:5:LYS:HD2	30:0:1675:C:H5''	1.95	0.49
30:0:2289:G:N2	30:0:2291:A:C2	2.71	0.49
30:0:441:A:H1'	30:0:442:A:N7	2.28	0.49
31:9:20:G:H3'	37:9:8434:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1167:G:H2'	30:0:1168:C:O4'	2.13	0.49
30:0:2089:A:O2'	30:0:2090:G:H5'	2.13	0.49
30:0:2896:A:N3	30:0:2896:A:H2'	2.28	0.49
30:0:482:G:H4'	30:0:508:A:N1	2.28	0.49
22:V:1:THR:CB	30:0:93:C:H5''	2.43	0.49
1:A:194:MET:SD	30:0:875:A:C2	3.06	0.49
2:B:221:GLN:HE22	11:K:42:ASN:ND2	2.03	0.49
3:C:78:ARG:HG3	3:C:78:ARG:NH1	2.27	0.49
8:H:49:GLN:NE2	8:H:140:TYR:HE2	2.11	0.49
10:J:88:PRO:O	10:J:94:GLY:HA3	2.13	0.49
30:0:1314:U:H5''	30:0:1316:G:O4'	2.13	0.48
30:0:559:U:H2'	30:0:560:U:O4'	2.13	0.48
30:0:871:G:H4'	37:0:3951:HOH:O	2.12	0.48
24:X:80:GLU:HB3	37:X:5564:HOH:O	2.12	0.48
30:0:1291:A:H2	37:0:4838:HOH:O	1.96	0.48
10:J:19:MET:CE	10:J:132:LEU:HD11	2.43	0.48
30:0:1730:G:H5'	30:0:1731:C:C6	2.43	0.48
30:0:737:A:H2'	30:0:738:G:O4'	2.13	0.48
2:B:154:VAL:HG12	2:B:156:LYS:HG2	1.96	0.48
30:0:1014:A:H2'	30:0:1015:C:H5'	1.95	0.48
30:0:1506:U:H6	30:0:1506:U:H5'	1.79	0.48
12:L:18:HIS:CD2	30:0:902:G:N7	2.79	0.48
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.29	0.48
2:B:62:ARG:HA	2:B:65:MET:CE	2.43	0.48
3:C:129:HIS:HE1	3:C:231:ARG:HA	1.79	0.48
7:G:12:ILE:N	7:G:13:PRO:HD3	2.28	0.48
30:0:1339:G:C6	30:0:1340:G:N1	2.80	0.48
30:0:1667:A:H2'	30:0:1668:U:H6	1.77	0.48
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.78	0.48
30:0:2911:C:H2'	30:0:2912:C:C6	2.49	0.48
2:B:264:GLU:HG2	2:B:267:LYS:HE2	1.95	0.48
2:B:297:VAL:HB	37:B:8606:HOH:O	2.12	0.48
13:M:107:ARG:NH1	37:M:8573:HOH:O	2.46	0.48
16:P:81:LYS:HG2	37:0:9060:HOH:O	2.14	0.48
30:0:1044:C:H3'	30:0:1045:G:H5''	1.95	0.48
30:0:1377:C:C5'	30:0:1377:C:H6	2.25	0.48
30:0:1588:G:C6	30:0:1589:G:N1	2.82	0.48
30:0:2314:G:C2'	30:0:2315:C:H5'	2.43	0.48
1:A:125:ASN:HB3	1:A:158:VAL:HG12	1.95	0.48
14:N:58:LEU:N	14:N:58:LEU:HD12	2.29	0.48
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:39:ALA:N	22:V:40:PRO:CD	2.77	0.48
30:0:1159:G:H21	30:0:1189:A:H8	1.62	0.48
30:0:1772:C:H5'	30:0:1773:G:C5	2.49	0.48
30:0:2421:G:H4'	37:0:4318:HOH:O	2.13	0.48
30:0:871:G:H8	30:0:871:G:H5''	1.74	0.48
31:9:2:U:OP2	31:9:2:U:H4'	2.14	0.48
2:B:82:VAL:HG12	2:B:82:VAL:O	2.12	0.48
2:B:85:ARG:NH1	37:B:8634:HOH:O	2.46	0.48
4:D:166:ILE:HD12	37:D:6326:HOH:O	2.13	0.48
13:M:99:ARG:HH21	13:M:170:ASN:ND2	2.11	0.48
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.96	0.48
30:0:1409:G:H5'	37:0:3263:HOH:O	2.14	0.48
30:0:255:A:H2'	30:0:256:C:C6	2.49	0.48
30:0:2754:G:C2'	30:0:2755:G:H5'	2.44	0.48
31:9:55:U:H4'	31:9:56:A:C8	2.48	0.48
1:A:29:HIS:HB2	1:A:153:ARG:HH12	1.79	0.48
2:B:268:ARG:NH2	2:B:325:PRO:HG3	2.28	0.48
3:C:12:THR:HB	37:C:8439:HOH:O	2.13	0.48
4:D:137:PRO:O	31:9:30:C:OP1	2.32	0.48
10:J:74:ARG:NH1	10:J:76:ASP:HB2	2.28	0.48
12:L:67:ARG:HB2	12:L:112:GLY:HA3	1.95	0.48
13:M:15:PRO:HA	13:M:20:LEU:HD23	1.95	0.48
23:W:108:ARG:HE	23:W:114:PRO:HG3	1.78	0.48
24:X:25:ARG:HG2	37:X:5356:HOH:O	2.13	0.48
30:0:1202:A:C2'	30:0:1203:G:H5'	2.44	0.48
30:0:1419:U:H2'	30:0:1685:A:C2	2.49	0.48
30:0:2134:G:C6	30:0:2258:A:C8	3.01	0.48
30:0:236:A:C4'	30:0:237:G:H5'	2.38	0.48
30:0:2909:G:H2'	30:0:2910:A:H8	1.78	0.48
14:N:11:ARG:HD3	31:9:114:G:O6	2.13	0.48
3:C:27:ARG:HG3	3:C:29:ASP:OD1	2.14	0.48
18:R:29:LYS:HD3	37:0:4262:HOH:O	2.14	0.48
30:0:1484:G:H2'	37:0:8620:HOH:O	2.14	0.48
11:K:87:ARG:NH2	30:0:2720:C:O2	2.47	0.48
13:M:125:ARG:HD3	37:0:4520:HOH:O	2.13	0.48
23:W:154:ARG:NH1	30:0:588:G:O6	2.46	0.48
23:W:38:THR:HG22	23:W:39:ASP:N	2.29	0.48
26:Z:35:SER:CB	26:Z:47:ARG:HB2	2.44	0.48
30:0:10:U:O4	30:0:532:A:OP2	2.31	0.47
30:0:2668:G:H2'	30:0:2669:U:C6	2.49	0.47
30:0:2768:A:H5''	37:0:3966:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:PRO:HB2	37:A:8556:HOH:O	2.14	0.47
3:C:87:ARG:NH2	30:0:894:A:C2	2.82	0.47
14:N:4:PRO:HB2	30:0:1010:C:H4'	1.96	0.47
30:0:1202:A:H2'	30:0:1203:G:H5'	1.96	0.47
30:0:1735:C:O2'	30:0:1736:A:H5'	2.12	0.47
30:0:1883:U:O2'	30:0:1884:G:H5'	2.13	0.47
30:0:2487:C:H5	37:0:4427:HOH:O	1.97	0.47
30:0:764:C:H2'	30:0:765:G:O4'	2.14	0.47
5:E:111:LYS:HE3	30:0:2690:U:O2'	2.14	0.47
8:H:6:ALA:CA	8:H:61:ARG:HH12	2.26	0.47
14:N:132:ASN:O	14:N:135:VAL:HG12	2.13	0.47
16:P:115:SER:OG	16:P:118:GLN:HG3	2.15	0.47
23:W:149:LEU:HG	23:W:153:MET:CE	2.44	0.47
30:0:1474:C:C5'	30:0:1474:C:H6	2.15	0.47
30:0:1878:G:O2'	30:0:1879:U:P	2.73	0.47
30:0:285:A:H2'	30:0:286:U:O4'	2.14	0.47
30:0:920:C:H5''	30:0:921:G:O5'	2.14	0.47
9:I:84:SER:HB3	9:I:92:VAL:CG2	2.44	0.47
10:J:45:VAL:HG23	10:J:130:VAL:O	2.14	0.47
10:J:131:THR:HG22	10:J:134:GLU:H	1.79	0.47
17:Q:66:LYS:HB2	17:Q:70:ALA:O	2.14	0.47
23:W:38:THR:O	23:W:42:ARG:HB2	2.14	0.47
23:W:4:LEU:HD22	23:W:52:VAL:CG2	2.40	0.47
23:W:72:PRO:HG2	23:W:77:ALA:HB3	1.97	0.47
30:0:1450:C:H4'	30:0:1493:A:C5	2.49	0.47
30:0:407:A:H8	37:0:4000:HOH:O	1.96	0.47
30:0:816:G:C6	30:0:817:G:N1	2.82	0.47
1:A:164:ARG:NE	37:A:8580:HOH:O	2.47	0.47
23:W:38:THR:HG22	23:W:39:ASP:H	1.79	0.47
30:0:2724:U:H2'	30:0:2725:G:O4'	2.14	0.47
30:0:426:G:H2'	30:0:427:C:O4'	2.14	0.47
30:0:834:G:H4'	30:0:835:U:OP2	2.15	0.47
29:3:70:ARG:HD3	37:3:8571:HOH:O	2.14	0.47
18:R:14:ALA:HB3	18:R:147:LEU:HB2	1.97	0.47
21:U:17:THR:HG22	21:U:18:GLY:N	2.29	0.47
30:0:1006:A:N1	30:0:2311:A:H1'	2.29	0.47
30:0:1116:U:HO2'	30:0:1118:A:H2	0.72	0.47
30:0:1187:U:HO2'	30:0:1188:A:H8	1.60	0.47
30:0:1132:A:N6	30:0:1229:C:H2'	2.30	0.47
30:0:603:A:H4'	30:0:604:G:O5'	2.15	0.47
1:A:211:LYS:HD3	37:A:8604:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:87:ARG:NH1	37:K:4066:HOH:O	2.47	0.47
15:O:14:LEU:HD23	15:O:102:ILE:HD11	1.96	0.47
22:V:12:THR:HG23	22:V:14:ALA:H	1.80	0.47
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.94	0.47
30:0:506:G:N2	30:0:509:A:H5''	2.22	0.47
5:E:84:MET:HE1	5:E:148:ILE:HD12	1.97	0.47
13:M:107:ARG:HH11	13:M:107:ARG:HG3	1.80	0.47
13:M:61:ILE:HA	37:M:8617:HOH:O	2.15	0.47
25:Y:144:ARG:NE	37:Y:8610:HOH:O	2.47	0.47
30:0:1056:U:H2'	30:0:1057:A:O4'	2.15	0.47
30:0:162:C:H2'	30:0:163:U:H5'	1.96	0.47
30:0:1681:G:H5''	30:0:1682:A:H5'	1.96	0.47
30:0:2900:G:H2'	30:0:2901:C:O4'	2.15	0.47
3:C:214:THR:HB	37:0:9200:HOH:O	2.13	0.47
4:D:94:ALA:HB3	4:D:97:GLN:HG3	1.96	0.47
25:Y:122:ARG:NH2	37:Y:8535:HOH:O	2.48	0.47
30:0:2291:A:N9	30:0:2309:C:H5'	2.29	0.47
30:0:2831:C:C2'	30:0:2832:C:H5'	2.45	0.47
5:E:132:THR:HB	37:E:2227:HOH:O	2.14	0.47
5:E:35:TYR:HA	10:J:127:ILE:HD12	1.96	0.47
14:N:1:ALA:HB2	31:9:14:G:O2'	2.15	0.47
20:T:71:VAL:HG11	20:T:90:PRO:CB	2.36	0.47
30:0:1181:A:H2'	30:0:1182:C:C5'	2.45	0.47
30:0:2019:A:H5'	37:0:4079:HOH:O	2.15	0.47
30:0:2506:A:O2'	30:0:2507:G:O5'	2.33	0.47
10:J:75:PRO:HD3	10:J:136:SER:OG	2.15	0.47
30:0:1562:C:O2	30:0:1562:C:H2'	2.14	0.47
30:0:1657:A:H2'	30:0:1658:A:C8	2.50	0.47
11:K:66:ARG:HD2	30:0:1992:U:OP2	2.15	0.47
30:0:417:G:P	37:0:6968:HOH:O	2.71	0.47
31:9:24:U:H3'	31:9:25:G:C5'	2.45	0.47
30:0:1205:U:C2'	30:0:1206:U:C5'	2.93	0.46
30:0:1213:C:O2'	30:0:1214:G:H5'	2.15	0.46
30:0:1353:C:P	37:0:4219:HOH:O	2.73	0.46
30:0:2361:A:H2'	30:0:2362:A:C8	2.50	0.46
4:D:172:VAL:HG12	4:D:173:GLU:N	2.30	0.46
14:N:38:LYS:HE2	14:N:107:ASN:ND2	2.30	0.46
30:0:2256:G:C2'	30:0:2257:G:H5'	2.44	0.46
30:0:2419:U:H5''	30:0:2420:G:C5'	2.45	0.46
30:0:920:C:H4'	30:0:921:G:C2	2.49	0.46
31:9:31:C:H2'	31:9:32:G:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.76	0.46
2:B:27:ASN:HB2	37:0:3602:HOH:O	2.16	0.46
6:F:30:LYS:HE2	6:F:99:THR:HG21	1.97	0.46
20:T:54:ASP:OD2	30:0:316:A:H5'	2.16	0.46
20:T:92:ASP:OD1	20:T:94:SER:HB3	2.16	0.46
25:Y:189:ASN:ND2	25:Y:192:ASP:H	2.14	0.46
26:Z:41:ARG:NH1	30:0:821:U:H4'	2.31	0.46
30:0:1441:G:H1'	37:0:7314:HOH:O	2.15	0.46
12:L:73:VAL:HG21	12:L:116:HIS:CD2	2.50	0.46
14:N:147:ILE:HB	37:N:8545:HOH:O	2.14	0.46
21:U:14:GLU:OE1	21:U:15:PRO:HD2	2.16	0.46
30:0:1200:A:H4'	37:0:6890:HOH:O	2.14	0.46
30:0:2112:A:H2'	30:0:2113:G:C8	2.51	0.46
30:0:2456:A:H5'	37:0:5242:HOH:O	2.15	0.46
30:0:445:U:H1'	37:0:6885:HOH:O	2.14	0.46
4:D:27:ILE:HD11	4:D:37:ALA:HB3	1.98	0.46
7:G:19:GLU:O	7:G:23:ILE:HG13	2.15	0.46
15:O:87:THR:O	15:O:91:GLN:HG3	2.16	0.46
20:T:111:ARG:HB3	20:T:119:ALA:HB2	1.98	0.46
30:0:1044:C:H5	37:0:6150:HOH:O	1.96	0.46
30:0:1174:A:C5	30:0:1201:C:H4'	2.50	0.46
30:0:136:C:H2'	30:0:137:U:O4'	2.15	0.46
30:0:1625:U:H5''	37:0:5568:HOH:O	2.15	0.46
30:0:69:A:H8	30:0:69:A:C5'	2.20	0.46
31:9:31:C:C2	31:9:50:G:N2	2.84	0.46
12:L:61:ALA:HA	37:L:8553:HOH:O	2.15	0.46
16:P:41:ARG:NH2	30:0:1500:U:OP2	2.48	0.46
19:S:56:ASN:O	28:2:8:LYS:NZ	2.46	0.46
20:T:9:LYS:HE3	20:T:13:ARG:NH1	2.30	0.46
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.97	0.46
30:0:2010:A:C2'	37:0:5505:HOH:O	2.62	0.46
30:0:2256:G:O2'	30:0:2257:G:H5'	2.16	0.46
30:0:284:C:H4'	30:0:285:A:H8	1.80	0.46
30:0:538:C:H5''	30:0:539:G:C8	2.50	0.46
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.62	0.46
31:9:55:U:H4'	31:9:56:A:H8	1.78	0.46
7:G:23:ILE:O	7:G:27:ILE:HG13	2.15	0.46
30:0:1181:A:N1	30:0:1192:A:O2'	2.48	0.46
30:0:1252:A:H2'	30:0:1253:C:O4'	2.15	0.46
30:0:1947:G:H2'	30:0:1948:G:H8	1.81	0.46
30:0:821:U:H5''	37:0:9582:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:118:THR:O	3:C:136:VAL:HG13	2.16	0.46
24:X:30:MET:HG2	30:0:1384:C:H5'	1.98	0.46
30:0:1393:A:H2'	30:0:1394:C:C6	2.51	0.46
5:E:143:GLN:HE22	30:0:2779:G:H21	1.59	0.46
30:0:876:A:N3	30:0:876:A:H2'	2.31	0.46
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.15	0.46
20:T:69:LYS:O	20:T:71:VAL:HG23	2.16	0.46
25:Y:220:GLU:HG3	37:Y:8546:HOH:O	2.15	0.46
30:0:1592:G:O2'	30:0:1593:C:O5'	2.34	0.46
30:0:2570:G:H5''	37:0:4452:HOH:O	2.15	0.46
30:0:304:G:H1'	30:0:347:A:N6	2.31	0.46
31:9:36:C:C5	31:9:37:C:C5	3.04	0.46
1:A:88:ILE:HG22	1:A:88:ILE:O	2.16	0.46
3:C:104:ASP:HA	3:C:107:ARG:NH1	2.31	0.46
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.96	0.46
8:H:102:LYS:HD3	8:H:122:LYS:HD3	1.97	0.46
5:E:36:PRO:HD3	10:J:127:ILE:HD12	1.97	0.46
11:K:81:ARG:HD3	11:K:87:ARG:NH1	2.31	0.46
23:W:3:ALA:O	23:W:54:PHE:HA	2.16	0.46
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.96	0.46
30:0:1249:U:H2'	30:0:1250:C:C6	2.51	0.46
30:0:2672:C:O2'	30:0:2673:U:H5'	2.16	0.46
30:0:2831:C:H2'	30:0:2832:C:H5'	1.97	0.46
30:0:1314:U:H2'	37:0:5422:HOH:O	2.15	0.45
30:0:2726:U:O2	30:0:2749:U:O5'	2.34	0.45
30:0:574:G:O2'	30:0:575:A:H5'	2.16	0.45
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.46	0.45
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.46	0.45
14:N:164:ASP:OD1	14:N:167:ASP:HA	2.15	0.45
30:0:119:A:H2'	30:0:120:A:H5''	1.96	0.45
30:0:138:U:OP2	30:0:139:C:H5	1.98	0.45
30:0:2716:G:O2'	30:0:2717:C:H5'	2.17	0.45
2:B:98:THR:HG22	30:0:2820:A:OP1	2.16	0.45
30:0:69:A:C8	30:0:69:A:C5'	2.92	0.45
31:9:52:A:H2'	31:9:53:G:O4'	2.16	0.45
14:N:154:LEU:C	14:N:156:GLU:H	2.19	0.45
19:S:45:TYR:HD2	37:S:4527:HOH:O	1.99	0.45
20:T:3:GLN:HA	20:T:4:PRO:HD3	1.82	0.45
30:0:1119:G:C6	30:0:1244:U:C5	3.04	0.45
30:0:1559:A:C1'	37:0:5413:HOH:O	2.62	0.45
30:0:2061:C:H2'	30:0:2062:A:H5'	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:168:ARG:NH2	3:C:190:ALA:O	2.49	0.45
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.98	0.45
37:C:8357:HOH:O	15:O:3:THR:HG21	2.15	0.45
30:0:1183:C:H42	30:0:1184:C:H41	1.62	0.45
30:0:130:C:H5'	37:0:4755:HOH:O	2.16	0.45
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.81	0.45
5:E:31:ARG:NH1	37:E:5919:HOH:O	2.49	0.45
14:N:164:ASP:CG	14:N:167:ASP:HA	2.37	0.45
19:S:38:ALA:O	19:S:42:GLU:HG3	2.15	0.45
28:2:41:HIS:HE1	30:0:1439:C:OP1	1.99	0.45
30:0:1878:G:O2'	30:0:1879:U:C5	2.67	0.45
20:T:2:LYS:HG2	30:0:447:A:OP1	2.17	0.45
30:0:844:A:C6	30:0:882:A:C5	3.04	0.45
5:E:7:ILE:HG22	5:E:45:ASP:O	2.16	0.45
8:H:69:ARG:HD3	37:H:8381:HOH:O	2.16	0.45
14:N:108:SER:HA	14:N:109:PRO:HD3	1.76	0.45
15:O:35:LYS:HD3	37:0:4157:HOH:O	2.17	0.45
16:P:16:VAL:CG1	16:P:20:ARG:HB2	2.46	0.45
30:0:1505:U:H1'	37:0:7139:HOH:O	2.16	0.45
13:M:171:ARG:NH2	30:0:189:A:OP1	2.49	0.45
30:0:1925:G:O2'	30:0:1926:G:H5'	2.17	0.45
30:0:2289:G:N2	30:0:2291:A:H2	2.13	0.45
30:0:2326:C:H4'	30:0:2412:G:H4'	1.99	0.45
14:N:127:LEU:HD13	37:N:8556:HOH:O	2.16	0.45
16:P:115:SER:H	16:P:118:GLN:NE2	2.00	0.45
26:Z:84:CYS:O	26:Z:85:ASP:HB2	2.15	0.45
30:0:1188:A:N7	30:0:1189:A:C2	2.85	0.45
30:0:1545:C:H2'	30:0:1546:G:O4'	2.17	0.45
30:0:2526:C:H5'	30:0:2526:C:C6	2.51	0.45
30:0:816:G:H5'	30:0:1598:A:H4'	1.98	0.45
3:C:104:ASP:HA	3:C:107:ARG:HH12	1.80	0.45
5:E:5:LEU:HD21	5:E:66:GLN:HG3	1.99	0.45
10:J:107:ASN:C	10:J:107:ASN:HD22	2.20	0.45
30:0:1060:C:H6	30:0:1060:C:H5'	1.82	0.45
30:0:1200:A:H3'	37:0:5302:HOH:O	2.16	0.45
30:0:1596:U:H2'	30:0:1598:A:OP2	2.16	0.45
18:R:80:TYR:O	30:0:2050:G:H5''	2.17	0.45
30:0:2667:G:H1'	30:0:2914:A:N3	2.31	0.45
1:A:100:PRO:HG2	1:A:103:VAL:CG2	2.44	0.45
2:B:72:THR:HB	37:B:8606:HOH:O	2.16	0.45
3:C:127:ARG:CZ	3:C:225:PRO:HG2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:133:THR:HG22	9:I:134:ILE:N	2.32	0.45
15:O:96:VAL:HG13	15:O:100:GLN:HB2	1.98	0.45
16:P:13:VAL:HG21	16:P:41:ARG:HG2	1.99	0.45
30:0:1183:C:H2'	37:0:5790:HOH:O	2.17	0.45
1:A:1:GLY:HA2	30:0:2114:C:OP1	2.17	0.45
4:D:52:THR:HG21	30:0:2346:C:O2'	2.16	0.45
30:0:2361:A:H8	30:0:2361:A:H5'	1.82	0.45
30:0:2509:A:OP2	30:0:2510:C:H5	2.00	0.45
30:0:2515:C:H2'	30:0:2516:G:O4'	2.16	0.45
30:0:2781:U:C2'	30:0:2782:G:H5'	2.46	0.45
30:0:484:A:N1	30:0:506:G:H4'	2.32	0.45
30:0:541:C:C2'	30:0:542:A:C5'	2.82	0.45
1:A:33:GLU:CD	1:A:33:GLU:H	2.20	0.45
6:F:60:VAL:HG12	6:F:60:VAL:O	2.17	0.45
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.47	0.45
15:O:39:THR:O	15:O:115:ARG:NH2	2.49	0.45
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.99	0.45
30:0:1209:C:H2'	30:0:1210:G:C8	2.48	0.45
12:L:14:GLY:O	30:0:1295:G:H5''	2.17	0.45
30:0:2883:A:H2'	30:0:2884:G:O4'	2.17	0.45
30:0:999:C:O2'	30:0:1000:C:H5'	2.18	0.44
30:0:1979:G:O2'	30:0:1980:U:OP1	2.29	0.44
27:1:10:LYS:HG3	37:1:8431:HOH:O	2.17	0.44
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.16	0.44
4:D:51:ARG:HH11	4:D:68:PRO:HB3	1.81	0.44
6:F:16:ALA:HA	6:F:111:ILE:HD13	1.99	0.44
8:H:23:ILE:HG23	8:H:123:ILE:HD11	1.99	0.44
8:H:61:ARG:HH11	8:H:61:ARG:HG3	1.82	0.44
11:K:74:VAL:HG13	11:K:113:ILE:HG23	1.98	0.44
30:0:1044:C:H5''	37:0:8543:HOH:O	2.17	0.44
30:0:1058:A:H2'	30:0:1060:C:C5'	2.44	0.44
37:I:5128:HOH:O	30:0:1168:C:C5'	2.64	0.44
28:2:42:TRP:HB3	30:0:1418:U:OP1	2.18	0.44
30:0:1942:A:O2'	30:0:1943:C:H5'	2.18	0.44
30:0:2553:A:H2'	30:0:2553:A:N3	2.31	0.44
30:0:2781:U:H2'	30:0:2782:G:H5'	2.00	0.44
30:0:316:A:N3	30:0:336:G:O2'	2.43	0.44
30:0:292:G:H2'	30:0:358:G:N2	2.33	0.44
29:3:70:ARG:HG2	29:3:77:ALA:HB2	1.99	0.44
3:C:16:VAL:HG12	3:C:17:ASP:H	1.81	0.44
11:K:75:ARG:HD3	11:K:112:PRO:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:164:THR:HB	37:M:8519:HOH:O	2.17	0.44
13:M:167:GLY:O	13:M:171:ARG:HG3	2.17	0.44
15:O:37:ARG:HD2	30:O:656:G:OP2	2.17	0.44
30:O:1477:C:H5'	30:O:1868:G:H5''	1.98	0.44
30:O:2090:G:H2'	30:O:2091:G:C8	2.51	0.44
30:O:2103:A:N7	30:O:2538:A:N6	2.65	0.44
30:O:212:A:O4'	30:O:214:U:C6	2.71	0.44
30:O:2135:A:O2'	30:O:2136:G:H5'	2.16	0.44
30:O:2642:G:H2'	30:O:2643:G:O4'	2.17	0.44
30:O:2712:G:P	37:O:4763:HOH:O	2.75	0.44
30:O:2791:U:H1'	30:O:2792:A:H5''	1.99	0.44
30:O:958:G:H2'	30:O:959:C:C6	2.52	0.44
27:1:25:LYS:HD2	28:2:48:ASP:HA	1.98	0.44
31:9:57:A:N6	37:9:8441:HOH:O	2.47	0.44
3:C:25:PRO:HG2	37:C:8322:HOH:O	2.17	0.44
8:H:59:GLN:HE21	8:H:129:ARG:NE	2.00	0.44
18:R:128:ARG:HH22	30:O:2054:A:H2	1.61	0.44
30:O:2812:A:N7	37:O:7067:HOH:O	2.36	0.44
31:9:2:U:C4'	37:9:8480:HOH:O	2.66	0.44
3:C:236:THR:HG22	3:C:239:ALA:CB	2.47	0.44
4:D:88:LEU:HB2	4:D:89:PRO:HD3	1.98	0.44
5:E:3:VAL:CG2	5:E:49:ILE:HB	2.48	0.44
10:J:90:LYS:HB2	34:J:8502:CL:CL	2.54	0.44
10:J:93:ARG:HH11	10:J:93:ARG:HB3	1.81	0.44
12:L:21:ARG:N	37:L:8524:HOH:O	2.50	0.44
15:O:14:LEU:CD2	15:O:102:ILE:HD11	2.48	0.44
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.17	0.44
18:R:111:ILE:HG23	18:R:145:LEU:CD1	2.48	0.44
25:Y:144:ARG:NH2	37:Y:8610:HOH:O	2.49	0.44
30:O:2115:U:H2'	30:O:2116:U:C6	2.53	0.44
30:O:281:U:H3'	37:O:6755:HOH:O	2.17	0.44
2:B:244:PRO:HB3	30:O:1234:U:N3	2.32	0.44
3:C:2:GLN:HB3	37:C:8333:HOH:O	2.17	0.44
3:C:2:GLN:HB3	37:C:8384:HOH:O	2.18	0.44
4:D:50:VAL:O	4:D:71:ALA:HA	2.18	0.44
4:D:56:ARG:N	37:D:6752:HOH:O	2.50	0.44
8:H:62:HIS:HA	8:H:65:LEU:HD23	1.99	0.44
12:L:133:VAL:HB	37:L:8547:HOH:O	2.17	0.44
18:R:106:GLY:HA2	18:R:109:MET:CE	2.47	0.44
30:O:1014:A:H5''	31:9:101:G:O2'	2.18	0.44
30:O:1940:C:H4'	37:O:6896:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1948:G:H2'	30:0:1949:G:O4'	2.18	0.44
30:0:2004:U:H2'	30:0:2005:G:OP1	2.16	0.44
30:0:559:U:H5'	30:0:559:U:C6	2.42	0.44
30:0:834:G:H3'	30:0:835:U:H4'	1.99	0.44
29:3:28:GLY:HA3	30:0:2434:A:O3'	2.17	0.44
2:B:57:GLU:HA	2:B:58:PRO:HD2	1.89	0.44
3:C:153:VAL:O	3:C:157:LEU:HG	2.18	0.44
5:E:116:THR:HG22	5:E:151:LEU:HD22	2.00	0.44
13:M:193:LYS:HB3	30:0:392:U:C5'	2.48	0.44
22:V:7:GLU:O	22:V:11:MET:HG3	2.18	0.44
30:0:1423:C:O2'	30:0:1424:A:H5'	2.18	0.44
30:0:2353:A:H4'	30:0:2354:A:O5'	2.17	0.44
30:0:737:A:H2	37:0:6249:HOH:O	1.98	0.44
27:1:28:HIS:CD2	27:1:30:LYS:HB2	2.52	0.44
2:B:71:VAL:HG11	2:B:296:LEU:HD22	1.99	0.44
3:C:140:VAL:HG12	3:C:141:SER:N	2.33	0.44
7:G:63:ARG:NH1	30:0:1151:G:OP1	2.50	0.44
11:K:45:PRO:HB2	37:0:6920:HOH:O	2.17	0.44
21:U:13:ILE:HG12	21:U:32:CYS:HB3	1.99	0.44
30:0:113:A:OP2	30:0:114:A:H2'	2.17	0.44
30:0:1299:G:N2	37:0:4223:HOH:O	2.49	0.44
3:C:184:ARG:NH2	30:0:450:C:OP1	2.35	0.44
30:0:660:A:H4'	30:0:661:G:O5'	2.18	0.44
14:N:160:SER:CB	31:9:51:A:H5'	2.48	0.44
3:C:237:GLU:HB2	37:C:8428:HOH:O	2.16	0.44
3:C:235:PHE:HE2	3:C:243:VAL:HG21	1.82	0.44
5:E:31:ARG:NH1	5:E:68:HIS:CG	2.86	0.44
8:H:172:GLU:HB3	37:H:8392:HOH:O	2.18	0.44
12:L:143:THR:HG22	12:L:144:ASP:H	1.78	0.44
30:0:2403:C:H2'	30:0:2404:G:O5'	2.17	0.44
29:3:14:CYS:SG	37:3:8559:HOH:O	2.62	0.44
31:9:34:A:H2'	31:9:35:C:O4'	2.18	0.44
30:0:2031:C:H2'	30:0:2032:U:O4'	2.17	0.43
30:0:2326:C:H4'	30:0:2412:G:C4'	2.48	0.43
30:0:2401:A:H5'	37:0:9014:HOH:O	2.18	0.43
30:0:240:C:O2	30:0:240:C:H2'	2.18	0.43
1:A:171:LYS:HB2	30:0:820:G:C5	2.53	0.43
31:9:49:G:C2'	31:9:50:G:H5'	2.48	0.43
8:H:41:LYS:HE2	8:H:45:ASP:CB	2.47	0.43
14:N:139:TRP:HA	14:N:139:TRP:CE3	2.53	0.43
14:N:169:PRO:O	14:N:172:PHE:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:12:THR:HG22	22:V:15:GLU:CG	2.46	0.43
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.99	0.43
30:0:1592:G:O2'	30:0:1593:C:O4'	2.34	0.43
30:0:2820:A:H2'	30:0:2821:C:O4'	2.18	0.43
30:0:653:U:H2'	30:0:654:A:C8	2.53	0.43
12:L:27:ARG:HD2	30:0:757:C:OP1	2.18	0.43
28:2:20:ARG:HG2	28:2:21:VAL:N	2.33	0.43
2:B:41:PHE:CD2	2:B:190:MET:HE3	2.53	0.43
3:C:107:ARG:NH1	37:C:8429:HOH:O	2.51	0.43
5:E:20:ILE:CD1	5:E:40:VAL:HG11	2.44	0.43
22:V:44:GLY:O	22:V:48:GLU:HG2	2.18	0.43
23:W:125:HIS:HE1	37:W:3071:HOH:O	2.01	0.43
23:W:5:VAL:HG11	23:W:153:MET:HE3	1.98	0.43
24:X:74:ALA:HB2	24:X:85:VAL:HG13	2.00	0.43
30:0:1825:U:O2'	30:0:1826:C:H5'	2.18	0.43
30:0:2073:G:OP2	30:0:2490:A:H5'	2.19	0.43
30:0:2508:C:H2'	37:0:6301:HOH:O	2.17	0.43
30:0:2697:A:H2'	30:0:2698:G:O4'	2.18	0.43
30:0:333:G:O2'	30:0:334:G:H5'	2.19	0.43
30:0:510:U:H6	37:0:6987:HOH:O	2.01	0.43
2:B:14:GLY:HA3	37:B:8609:HOH:O	2.17	0.43
2:B:62:ARG:HA	2:B:65:MET:HE2	2.01	0.43
13:M:64:ARG:HD2	37:M:8581:HOH:O	2.17	0.43
14:N:116:PHE:HB3	14:N:136:LEU:HD23	2.00	0.43
30:0:1367:A:H2'	30:0:1368:U:O4'	2.18	0.43
30:0:1684:A:O2'	30:0:1685:A:H5''	2.18	0.43
30:0:2754:G:O2'	30:0:2755:G:H5'	2.17	0.43
30:0:2768:A:H3'	37:0:3966:HOH:O	2.17	0.43
28:2:48:ASP:O	28:2:49:GLU:HB2	2.18	0.43
31:9:80:A:C2	31:9:103:A:C4	3.07	0.43
31:9:65:A:N6	31:9:112:U:C6	2.86	0.43
2:B:30:PRO:HB2	2:B:39:GLN:NE2	2.33	0.43
3:C:242:GLU:HG3	37:C:8381:HOH:O	2.19	0.43
7:G:12:ILE:HA	37:0:5006:HOH:O	2.17	0.43
15:O:38:ARG:NH1	37:O:7674:HOH:O	2.50	0.43
21:U:9:CYS:CA	21:U:52:THR:HG23	2.47	0.43
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.82	0.43
30:0:2464:C:H5''	30:0:2465:A:OP1	2.18	0.43
30:0:941:G:C5	30:0:942:U:C4	3.06	0.43
31:9:39:U:HO2'	31:9:42:C:H5	1.58	0.43
1:A:33:GLU:O	1:A:34:ASP:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:74:ARG:O	10:J:78:ILE:HG12	2.18	0.43
13:M:39:ARG:NH2	37:M:8617:HOH:O	2.51	0.43
18:R:111:ILE:HG23	18:R:145:LEU:HD11	2.01	0.43
20:T:41:ARG:NH1	20:T:42:VAL:O	2.51	0.43
30:0:1406:A:H4'	30:0:1407:A:C5'	2.49	0.43
30:0:2072:G:H3'	30:0:2073:G:C5'	2.49	0.43
30:0:2269:C:C2'	30:0:2270:G:H5'	2.49	0.43
1:A:206:ARG:NH2	30:0:2630:G:O6	2.48	0.43
30:0:380:A:H4'	30:0:381:G:OP1	2.19	0.43
30:0:876:A:N3	30:0:876:A:C2'	2.82	0.43
1:A:153:ARG:HD3	37:A:8528:HOH:O	2.18	0.43
2:B:314:ALA:HB3	2:B:317:PRO:HG3	2.00	0.43
5:E:137:ASP:O	5:E:141:VAL:HG23	2.19	0.43
13:M:9:ARG:HD2	30:0:380:A:OP2	2.18	0.43
14:N:11:ARG:NH2	37:N:8519:HOH:O	2.51	0.43
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.48	0.43
23:W:119:HIS:HD2	23:W:120:PRO:O	2.01	0.43
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.32	0.43
25:Y:117:LEU:HA	25:Y:174:VAL:HG11	2.01	0.43
26:Z:37:ARG:HD3	30:0:818:A:O2'	2.19	0.43
30:0:1535:G:H2'	30:0:1536:C:C6	2.54	0.43
30:0:249:G:O2'	30:0:250:C:H5'	2.18	0.43
6:F:59:ILE:CD1	30:0:263:U:C2	3.01	0.43
5:E:31:ARG:HH12	5:E:68:HIS:CG	2.36	0.43
9:I:84:SER:HB2	9:I:90:ASP:HB2	1.99	0.43
11:K:28:GLU:HB3	11:K:59:LYS:HB2	2.00	0.43
19:S:57:THR:CG2	19:S:58:MET:N	2.82	0.43
23:W:108:ARG:HE	23:W:114:PRO:CG	2.32	0.43
23:W:126:ASP:HB3	23:W:135:GLY:O	2.18	0.43
24:X:25:ARG:HD3	24:X:64:ALA:O	2.18	0.43
30:0:1556:G:O2'	30:0:1557:G:H5'	2.18	0.43
30:0:1701:A:H1'	37:0:5924:HOH:O	2.18	0.43
30:0:2456:A:H2'	30:0:2457:U:C6	2.53	0.43
30:0:567:U:C5'	37:0:5949:HOH:O	2.65	0.43
1:A:105:VAL:HG12	1:A:106:CYS:N	2.33	0.43
6:F:36:THR:HG23	6:F:97:ALA:HB2	2.00	0.43
18:R:132:ARG:HG2	18:R:133:ALA:N	2.34	0.43
22:V:1:THR:HG23	22:V:2:VAL:N	2.28	0.43
30:0:1098:A:H2'	30:0:1099:G:O4'	2.19	0.43
30:0:1163:G:H2'	30:0:1164:U:C5	2.54	0.43
30:0:1771:U:O2'	30:0:1773:G:N7	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2842:G:C2'	30:0:2843:A:H5'	2.48	0.43
30:0:2868:C:H2'	30:0:2869:G:O4'	2.19	0.43
30:0:303:C:H2'	30:0:304:G:O4'	2.19	0.43
5:E:11:VAL:HG13	5:E:23:GLU:O	2.19	0.43
20:T:14:ALA:HA	20:T:15:PRO:HD3	1.91	0.43
30:0:1883:U:C2'	30:0:1884:G:H5'	2.49	0.43
30:0:407:A:H2'	30:0:408:A:C8	2.54	0.43
27:1:28:HIS:HD2	27:1:30:LYS:H	1.65	0.43
1:A:171:LYS:HB2	30:0:820:G:C6	2.54	0.43
1:A:186:TRP:CG	1:A:187:PRO:HA	2.54	0.43
2:B:36:PRO:HA	2:B:168:GLY:CA	2.46	0.43
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.48	0.43
6:F:50:VAL:CG2	6:F:63:ILE:HG21	2.49	0.43
8:H:149:VAL:HG22	37:H:8378:HOH:O	2.18	0.43
11:K:125:ALA:C	11:K:127:ALA:H	2.23	0.43
12:L:50:GLY:C	30:0:2453:G:H4'	2.39	0.43
17:Q:45:PRO:O	30:0:2365:G:H4'	2.18	0.43
37:Q:5998:HOH:O	30:0:2296:C:H5	2.01	0.42
30:0:283:U:C5	30:0:284:C:N3	2.87	0.42
30:0:559:U:C5'	30:0:559:U:H6	2.28	0.42
30:0:818:A:H5''	37:0:6135:HOH:O	2.18	0.42
28:2:28:LYS:O	30:0:87:C:H2'	2.19	0.42
28:2:40:ARG:HG3	28:2:45:ASN:CB	2.49	0.42
1:A:55:VAL:HG22	1:A:68:ILE:O	2.19	0.42
2:B:190:MET:HE1	2:B:194:PHE:CD1	2.54	0.42
2:B:49:THR:HG21	2:B:331:SER:O	2.19	0.42
9:I:129:SER:O	9:I:130:LEU:HD23	2.19	0.42
12:L:143:THR:CG2	12:L:144:ASP:N	2.80	0.42
14:N:62:HIS:HB3	14:N:65:ASP:OD1	2.19	0.42
37:I:3512:HOH:O	30:0:1163:G:N2	2.52	0.42
30:0:1165:G:H1'	30:0:1174:A:H1'	2.01	0.42
30:0:1202:A:H2'	30:0:1203:G:C5'	2.50	0.42
30:0:128:A:O2'	30:0:129:A:H5'	2.19	0.42
30:0:1427:A:H61	30:0:1440:U:H1'	1.84	0.42
30:0:1562:C:H42	30:0:2738:G:H1	1.67	0.42
30:0:946:C:H2'	30:0:947:U:C6	2.54	0.42
27:1:28:HIS:CD2	27:1:31:LYS:HG3	2.53	0.42
29:3:3:MET:HG3	29:3:4:PRO:HD2	2.01	0.42
1:A:11:ARG:HD3	37:0:8736:HOH:O	2.19	0.42
12:L:72:ASN:HB2	37:L:8570:HOH:O	2.17	0.42
13:M:81:ARG:HD2	30:0:160:A:O3'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:119:HIS:HE1	37:0:9078:HOH:O	2.02	0.42
24:X:74:ALA:CB	24:X:85:VAL:HG22	2.49	0.42
23:W:23:MET:O	30:0:1025:C:H5'	2.19	0.42
30:0:1641:A:H2'	30:0:1642:A:C5'	2.48	0.42
30:0:907:A:H4'	30:0:1328:A:C2	2.54	0.42
4:D:173:GLU:HG3	4:D:174:VAL:HG23	2.02	0.42
6:F:91:VAL:HG11	30:0:262:A:OP2	2.19	0.42
6:F:49:PHE:HE1	6:F:98:VAL:HG23	1.84	0.42
8:H:34:HIS:HD2	8:H:90:LEU:O	2.01	0.42
30:0:1183:C:N4	30:0:1184:C:N4	2.64	0.42
30:0:1980:U:O2	30:0:2008:U:H4'	2.19	0.42
30:0:2290:U:H2'	37:0:6681:HOH:O	2.18	0.42
30:0:2372:A:H2'	30:0:2373:U:C6	2.55	0.42
30:0:2493:C:O2	30:0:2493:C:H2'	2.17	0.42
30:0:2526:C:O2'	30:0:2527:U:H5'	2.19	0.42
4:D:76:ARG:NH1	31:9:42:C:O2	2.51	0.42
5:E:21:THR:HG23	5:E:30:THR:OG1	2.19	0.42
14:N:32:PRO:HD2	14:N:99:GLU:O	2.20	0.42
17:Q:33:PHE:HE2	17:Q:93:ARG:HG3	1.83	0.42
23:W:11:VAL:HG11	30:0:1086:A:N6	2.34	0.42
30:0:1462:C:O2'	30:0:1463:U:H5'	2.19	0.42
30:0:1701:A:H4'	30:0:1702:U:O5'	2.18	0.42
1:A:187:PRO:HB2	30:0:1845:A:O3'	2.20	0.42
5:E:6:GLU:HG2	5:E:46:THR:HG22	2.01	0.42
10:J:130:VAL:HG12	10:J:131:THR:N	2.35	0.42
23:W:41:TYR:HA	23:W:44:MET:HE3	2.01	0.42
23:W:73:LEU:HA	23:W:73:LEU:HD12	1.77	0.42
24:X:18:ARG:NH1	37:X:4132:HOH:O	2.52	0.42
30:0:1433:G:O2'	30:0:1434:A:H5'	2.20	0.42
30:0:2243:C:H5''	37:0:3288:HOH:O	2.19	0.42
30:0:2323:G:H5'	37:0:6566:HOH:O	2.19	0.42
37:3:8515:HOH:O	30:0:2408:A:H2	2.02	0.42
30:0:2421:G:H3'	30:0:2422:U:C5'	2.50	0.42
30:0:2769:C:C2'	30:0:2770:G:C5'	2.86	0.42
30:0:349:U:O2'	30:0:350:G:H5'	2.20	0.42
30:0:366:U:H2'	30:0:367:G:O4'	2.19	0.42
30:0:912:A:C4	30:0:1294:A:C2	3.08	0.42
29:3:18:GLN:HG2	37:3:8514:HOH:O	2.19	0.42
31:9:116:C:O2'	31:9:117:G:H5'	2.20	0.42
31:9:39:U:C2'	31:9:40:C:OP1	2.68	0.42
4:D:166:ILE:HB	37:D:6326:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:43:PRO:HG3	13:M:62:VAL:HG21	2.00	0.42
24:X:43:VAL:HG12	24:X:44:ASP:H	1.84	0.42
24:X:72:VAL:HG22	24:X:85:VAL:HG12	2.01	0.42
25:Y:208:LYS:O	30:0:1313:A:H5'	2.19	0.42
30:0:1482:A:O2'	30:0:1483:C:H5'	2.20	0.42
30:0:1624:A:H4'	30:0:1625:U:H5'	2.02	0.42
30:0:177:A:H2'	30:0:178:U:O4'	2.19	0.42
30:0:1878:G:O2'	30:0:1879:U:OP2	2.37	0.42
30:0:2271:G:N3	30:0:2271:G:H2'	2.34	0.42
30:0:2831:C:H2'	30:0:2832:C:C5'	2.49	0.42
30:0:2894:C:O2'	30:0:2895:C:H5'	2.19	0.42
30:0:790:A:H2'	30:0:791:A:O4'	2.20	0.42
2:B:258:GLY:H	2:B:260:HIS:CE1	2.36	0.42
3:C:133:ARG:NH1	37:C:8406:HOH:O	2.51	0.42
3:C:202:THR:HG22	30:0:328:U:O4'	2.20	0.42
9:I:101:LYS:O	9:I:105:GLU:HG3	2.19	0.42
13:M:5:TYR:HE2	13:M:46:LEU:HD13	1.84	0.42
14:N:23:ARG:NH1	37:N:8546:HOH:O	2.52	0.42
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.49	0.42
30:0:1042:U:O2'	30:0:1043:C:H5'	2.20	0.42
30:0:1565:C:O4'	30:0:2738:G:H1'	2.20	0.42
30:0:1589:G:N2	30:0:1605:G:H1'	2.35	0.42
16:P:88:GLN:HE22	30:0:1799:G:H21	1.67	0.42
30:0:282:C:O2'	30:0:283:U:C4'	2.68	0.42
30:0:420:U:H2'	30:0:421:C:C6	2.55	0.42
30:0:441:A:H8	30:0:441:A:O5'	2.03	0.42
1:A:132:ASP:HB3	1:A:135:VAL:H	1.85	0.42
1:A:199:HIS:HE1	30:0:1881:A:OP1	2.02	0.42
5:E:84:MET:HB2	5:E:131:LEU:HB2	2.01	0.42
8:H:46:TYR:HA	8:H:47:PRO:HD3	1.76	0.42
8:H:30:LYS:N	8:H:62:HIS:HD2	2.07	0.42
10:J:131:THR:HG22	10:J:133:GLY:N	2.35	0.42
30:0:1119:G:N2	30:0:1246:A:N1	2.67	0.42
30:0:1304:U:H2'	30:0:1305:C:C6	2.55	0.42
30:0:1453:G:N2	30:0:1675:C:C2	2.88	0.42
30:0:2909:G:O2'	30:0:2910:A:H5'	2.20	0.42
30:0:870:G:C3'	30:0:871:G:H5''	2.50	0.42
30:0:883:U:C2'	30:0:883:U:O2	2.68	0.42
31:9:65:A:O2'	31:9:66:G:P	2.78	0.42
2:B:115:VAL:HA	2:B:116:PRO:HD3	1.87	0.42
12:L:134:GLU:HG3	37:L:8547:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:84:ALA:O	18:R:88:PHE:HD1	2.02	0.42
30:0:1218:U:H2'	30:0:1219:U:C6	2.54	0.42
30:0:12:U:H2'	30:0:13:G:H5'	2.02	0.42
30:0:1634:G:H2'	30:0:1635:U:C6	2.54	0.42
30:0:2070:G:H5''	37:0:3318:HOH:O	2.20	0.42
30:0:2403:C:C2'	30:0:2404:G:O5'	2.68	0.42
37:L:8533:HOH:O	30:0:2453:G:H5''	2.19	0.42
30:0:2491:G:H1'	37:0:6418:HOH:O	2.19	0.42
30:0:2559:C:H4'	37:0:6805:HOH:O	2.19	0.42
30:0:2664:A:OP1	30:0:2664:A:H8	2.03	0.42
21:U:50:GLU:HB3	30:0:2866:U:C4	2.55	0.42
30:0:2879:A:H2'	30:0:2880:A:O4'	2.20	0.42
30:0:290:C:O2'	30:0:291:C:H5'	2.20	0.42
30:0:151:A:C2	30:0:442:A:C8	3.08	0.42
3:C:118:THR:CG2	3:C:137:PRO:HB3	2.50	0.42
20:T:26:THR:HA	20:T:39:ASN:HB3	2.01	0.42
21:U:31:PHE:CG	21:U:37:GLU:HG2	2.55	0.42
30:0:1131:G:C6	30:0:1230:A:C4	3.07	0.41
30:0:1613:C:H2'	30:0:1614:G:O4'	2.19	0.41
30:0:1615:A:H4'	37:0:5434:HOH:O	2.20	0.41
30:0:1697:G:O2'	30:0:1698:U:H5'	2.20	0.41
30:0:1947:G:H2'	30:0:1948:G:C8	2.54	0.41
30:0:1993:C:C4	30:0:1994:A:C6	3.08	0.41
30:0:2777:G:O2'	30:0:2778:A:H5'	2.19	0.41
30:0:383:A:H2'	30:0:384:G:O4'	2.20	0.41
30:0:638:C:H2'	30:0:639:A:C8	2.54	0.41
27:1:28:HIS:HD2	27:1:31:LYS:H	1.68	0.41
28:2:18:ASN:HD21	28:2:40:ARG:H	1.68	0.41
28:2:36:ASN:HB3	28:2:39:ARG:HG3	2.01	0.41
1:A:11:ARG:HA	37:0:6768:HOH:O	2.20	0.41
2:B:294:TYR:HE2	37:B:8649:HOH:O	2.02	0.41
3:C:133:ARG:NE	3:C:138:VAL:HG22	2.35	0.41
7:G:67:LEU:O	7:G:71:LEU:HG	2.20	0.41
12:L:56:LYS:HE3	30:0:2443:C:O3'	2.20	0.41
13:M:93:ARG:HD2	30:0:1470:A:OP1	2.20	0.41
30:0:1842:A:C4	30:0:1979:G:C6	3.09	0.41
30:0:1946:C:H2'	30:0:1971:G:C8	2.55	0.41
30:0:1985:U:C2	30:0:1996:U:O4'	2.73	0.41
30:0:1909:A:N1	30:0:2128:G:H1'	2.34	0.41
30:0:2356:A:H2'	30:0:2357:G:O4'	2.19	0.41
30:0:2385:G:H2'	30:0:2386:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2388:C:O2'	30:0:2389:U:H5'	2.21	0.41
30:0:284:C:N4	37:0:6734:HOH:O	2.52	0.41
31:9:47:A:C2	31:9:48:C:C2	3.08	0.41
11:K:4:LEU:HD22	11:K:116:GLU:HB3	2.02	0.41
30:0:1103:C:C2	30:0:1241:G:N2	2.88	0.41
30:0:2312:G:H2'	30:0:2313:C:H5'	2.02	0.41
5:E:143:GLN:NE2	30:0:2780:C:H1'	2.34	0.41
30:0:283:U:H5	30:0:284:C:N3	2.18	0.41
30:0:321:A:O2'	30:0:322:G:H5'	2.20	0.41
30:0:542:A:C5'	30:0:542:A:C8	2.99	0.41
30:0:629:A:H2'	30:0:630:A:O4'	2.21	0.41
30:0:827:A:H2'	30:0:828:G:O4'	2.20	0.41
30:0:932:U:H2'	30:0:933:C:C6	2.55	0.41
31:9:65:A:C2'	31:9:66:G:OP2	2.67	0.41
1:A:153:ARG:NH1	1:A:153:ARG:HB2	2.35	0.41
1:A:89:ALA:HB3	37:A:8616:HOH:O	2.19	0.41
23:W:21:LEU:HD13	23:W:26:ILE:HD11	2.02	0.41
30:0:1257:C:H2'	30:0:1258:G:O4'	2.20	0.41
30:0:1819:G:H2'	30:0:1820:G:C5'	2.51	0.41
30:0:2518:C:H2'	30:0:2519:C:O4'	2.20	0.41
30:0:2809:G:H2'	30:0:2810:G:O4'	2.21	0.41
18:R:98:ASN:ND2	30:0:500:G:H21	2.14	0.41
30:0:664:U:O4	30:0:681:G:H5'	2.20	0.41
28:2:18:ASN:ND2	28:2:40:ARG:H	2.17	0.41
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.50	0.41
5:E:108:LEU:HD11	5:E:164:ASP:HB2	2.02	0.41
7:G:65:THR:O	7:G:69:ARG:HB2	2.19	0.41
18:R:119:VAL:HG21	18:R:142:ASP:CG	2.40	0.41
30:0:1171:A:H2'	30:0:1172:G:H5'	2.02	0.41
30:0:1926:G:H2'	30:0:1927:A:H8	1.82	0.41
30:0:2003:U:H4'	30:0:2004:U:H5	1.84	0.41
27:1:2:GLY:O	27:1:6:PRO:HG2	2.20	0.41
7:G:63:ARG:N	37:G:2569:HOH:O	2.53	0.41
20:T:2:LYS:HE2	37:0:6955:HOH:O	2.20	0.41
23:W:81:ASP:OD1	23:W:92:ASP:HB2	2.19	0.41
30:0:1185:U:H2'	30:0:1186:C:H6	1.82	0.41
30:0:1413:A:H2'	30:0:1414:A:O4'	2.20	0.41
12:L:48:LYS:HE2	30:0:220:C:C2	2.56	0.41
1:A:204:GLY:N	30:0:2634:G:OP2	2.41	0.41
30:0:2729:C:O2'	30:0:2730:G:H5'	2.20	0.41
30:0:2897:C:H2'	30:0:2898:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:371:U:H2'	30:0:372:A:H8	1.86	0.41
30:0:666:A:H2'	30:0:667:C:O4'	2.21	0.41
29:3:7:PHE:HE2	29:3:22:VAL:HG21	1.86	0.41
31:9:107:C:H2'	31:9:108:C:C6	2.55	0.41
31:9:68:G:C6	31:9:69:U:C4	3.08	0.41
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.20	0.41
2:B:217:ARG:HG3	2:B:257:THR:HG22	2.01	0.41
5:E:154:ILE:HD11	5:E:157:LYS:HE2	2.03	0.41
9:I:94:ASP:OD1	9:I:133:THR:HB	2.21	0.41
10:J:52:GLN:NE2	30:0:1119:G:C8	2.87	0.41
11:K:65:ARG:HD3	37:K:5358:HOH:O	2.20	0.41
16:P:59:ARG:HH22	16:P:66:GLN:NE2	2.16	0.41
22:V:38:GLY:C	22:V:40:PRO:HD2	2.41	0.41
25:Y:186:ARG:HG2	25:Y:186:ARG:HH11	1.86	0.41
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.21	0.41
30:0:940:G:C5	30:0:1027:G:C2	3.08	0.41
30:0:1172:G:H1'	37:0:4513:HOH:O	2.20	0.41
30:0:2015:A:H2'	30:0:2016:U:O4'	2.21	0.41
30:0:255:A:H2'	30:0:256:C:H6	1.84	0.41
30:0:401:C:H2'	30:0:402:U:C6	2.55	0.41
30:0:558:C:H5'	37:0:4803:HOH:O	2.20	0.41
30:0:625:U:H5''	30:0:1044:C:N4	2.35	0.41
1:A:95:PRO:HA	1:A:153:ARG:HA	2.02	0.41
4:D:96:SER:C	4:D:98:PHE:H	2.23	0.41
5:E:47:VAL:HG11	5:E:69:ILE:HD13	2.03	0.41
15:O:25:VAL:HG23	15:O:26:TRP:N	2.36	0.41
30:0:1529:G:H5'	37:0:6937:HOH:O	2.20	0.41
30:0:1626:A:H2'	30:0:1627:G:O4'	2.20	0.41
30:0:1815:A:H2'	30:0:1816:C:O4'	2.21	0.41
30:0:368:C:H2'	30:0:369:G:H5'	2.02	0.41
30:0:646:G:H2'	30:0:647:U:C6	2.56	0.41
3:C:214:THR:HG21	37:C:8399:HOH:O	2.20	0.41
4:D:151:ILE:HA	4:D:152:PRO:HD3	1.95	0.41
12:L:121:ILE:HG12	12:L:141:GLU:HB2	2.01	0.41
30:0:1023:C:H2'	30:0:1024:G:O4'	2.20	0.41
30:0:2718:C:H5'	30:0:2718:C:C6	2.53	0.41
2:B:28:SER:HB2	30:0:2807:U:OP2	2.21	0.41
30:0:2756:U:O2	30:0:2896:A:H2	2.03	0.41
30:0:2906:A:H5'	30:0:2907:C:O4'	2.21	0.41
30:0:38:G:N2	37:0:6885:HOH:O	2.54	0.41
30:0:424:C:H2'	30:0:425:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:THR:HG22	37:A:8611:HOH:O	2.21	0.41
3:C:46:TYR:CE2	3:C:98:ARG:NH1	2.89	0.41
6:F:111:ILE:O	6:F:115:VAL:HG23	2.20	0.41
6:F:34:ASN:HA	13:M:4:ALA:HB2	2.03	0.41
9:I:133:THR:HG22	9:I:134:ILE:H	1.86	0.41
13:M:169:ARG:NH2	37:M:8548:HOH:O	2.51	0.41
20:T:47:THR:HB	20:T:100:ASP:HB3	2.01	0.41
37:K:7438:HOH:O	21:U:20:MET:HE1	2.21	0.41
30:0:1611:G:O2'	30:0:1612:A:H5'	2.21	0.41
30:0:1883:U:H5'	30:0:2012:U:OP2	2.20	0.41
30:0:282:C:C2'	30:0:283:U:H5'	2.51	0.41
30:0:290:C:H1'	37:0:5650:HOH:O	2.20	0.41
30:0:365:G:C6	30:0:366:U:C4	3.09	0.41
30:0:603:A:H1'	30:0:605:C:C2	2.56	0.41
1:A:205:GLY:HA3	37:0:5905:HOH:O	2.21	0.41
10:J:26:VAL:HG13	10:J:36:VAL:HG11	2.02	0.41
10:J:63:ILE:HD11	30:0:1236:A:C8	2.56	0.41
11:K:22:ASP:HB2	37:K:5264:HOH:O	2.21	0.41
14:N:171:HIS:CE1	37:N:8566:HOH:O	2.74	0.41
20:T:38:ARG:HH21	30:0:306:A:P	2.44	0.41
30:0:1139:U:H2'	30:0:1140:C:C6	2.56	0.41
30:0:1159:G:H1	30:0:1208:C:N4	2.18	0.41
30:0:1429:U:C2'	30:0:1430:G:H5'	2.51	0.41
30:0:2362:A:H2'	30:0:2363:G:C8	2.56	0.41
30:0:661:G:C6	30:0:686:A:C2	3.08	0.41
31:9:96:C:H2'	31:9:97:U:C6	2.56	0.41
8:H:31:ILE:HA	8:H:66:GLU:OE1	2.20	0.41
6:F:38:LYS:NZ	13:M:3:SER:HA	2.36	0.41
25:Y:99:ALA:HB2	25:Y:233:TYR:CZ	2.55	0.41
1:A:72:GLU:HG3	26:Z:90:GLY:HA2	2.03	0.41
30:0:1080:C:O5'	30:0:1080:C:H6	2.03	0.40
30:0:2237:G:H1'	37:0:4393:HOH:O	2.20	0.40
30:0:2691:A:OP1	30:0:2691:A:H8	2.04	0.40
30:0:812:A:H2'	30:0:813:C:O4'	2.20	0.40
30:0:999:C:H2'	30:0:1000:C:O4'	2.21	0.40
31:9:12:C:H5'	31:9:70:U:O4'	2.21	0.40
1:A:211:LYS:HB3	1:A:212:PRO:CD	2.50	0.40
2:B:116:PRO:HG3	30:0:2821:C:H4'	2.03	0.40
9:I:87:PRO:C	9:I:89:GLU:N	2.75	0.40
10:J:80:LYS:HE2	10:J:98:PHE:CE1	2.56	0.40
15:O:26:TRP:HB2	37:O:3062:HOH:O	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:149:LEU:HG	23:W:153:MET:HE1	2.03	0.40
25:Y:155:ARG:NH1	37:Y:8556:HOH:O	2.53	0.40
30:0:1076:G:C2	30:0:1084:C:C2	3.09	0.40
30:0:1191:A:H2'	30:0:1193:A:H5'	2.03	0.40
30:0:1976:G:O2'	30:0:1977:U:H5'	2.21	0.40
30:0:2103:A:O2'	30:0:2104:C:H5'	2.21	0.40
30:0:2819:C:H2'	30:0:2820:A:C8	2.56	0.40
30:0:40:C:H6	30:0:40:C:O5'	2.04	0.40
11:K:115:ARG:NH2	37:K:3160:HOH:O	2.53	0.40
11:K:62:PRO:HG3	11:K:65:ARG:HH21	1.85	0.40
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.77	0.40
23:W:125:HIS:CE1	30:0:1097:A:H5''	2.55	0.40
30:0:1181:A:O2'	30:0:1182:C:H5'	2.20	0.40
28:2:10:ARG:NH2	30:0:121:U:OP2	2.40	0.40
30:0:1632:A:H2'	30:0:1633:C:C5'	2.46	0.40
30:0:1714:C:O2'	30:0:1715:C:H5'	2.21	0.40
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.56	0.40
30:0:383:A:C2	30:0:407:A:C4	3.09	0.40
30:0:64:G:H2'	30:0:65:C:O4'	2.22	0.40
30:0:858:U:H2'	30:0:859:C:C6	2.56	0.40
31:9:107:C:O2'	31:9:108:C:H5'	2.22	0.40
1:A:69:LEU:HD21	1:A:120:ARG:HB3	2.03	0.40
2:B:141:ARG:HG2	2:B:165:ARG:HA	2.03	0.40
2:B:56:ASP:OD1	2:B:322:ARG:HB3	2.21	0.40
4:D:58:VAL:HB	4:D:62:ASP:HB3	2.02	0.40
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.92	0.40
8:H:12:ILE:HD12	8:H:57:THR:HG22	2.03	0.40
23:W:35:VAL:HA	23:W:36:PRO:HD3	1.78	0.40
23:W:5:VAL:HG11	23:W:153:MET:CE	2.51	0.40
24:X:78:GLU:HG2	24:X:79:GLU:H	1.86	0.40
25:Y:184:GLU:OE1	25:Y:204:ARG:NH1	2.55	0.40
30:0:1046:G:N3	30:0:1082:A:H2	2.19	0.40
30:0:1434:A:H2'	30:0:1436:C:C5	2.56	0.40
30:0:2314:G:H2'	30:0:2315:C:H5'	2.03	0.40
30:0:10:U:C4	30:0:532:A:N7	2.89	0.40
28:2:40:ARG:HG3	28:2:45:ASN:HB2	2.04	0.40
31:9:2:U:H4'	37:9:8480:HOH:O	2.20	0.40
1:A:153:ARG:CB	1:A:153:ARG:HH11	2.33	0.40
2:B:53:LEU:HD11	2:B:327:VAL:HG22	2.03	0.40
6:F:91:VAL:CG1	6:F:92:GLY:N	2.84	0.40
9:I:70:THR:OG1	9:I:107:LYS:HE2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:37:ARG:HH12	31:9:6:C:C5'	2.23	0.40
14:N:78:MET:HB2	14:N:79:PRO:HD3	2.02	0.40
24:X:30:MET:CE	24:X:58:ALA:HB3	2.52	0.40
30:0:553:G:O4'	30:0:1325:G:H5'	2.20	0.40
30:0:1333:U:H2'	30:0:1334:C:H6	1.86	0.40
30:0:1571:G:C2'	30:0:1626:A:H61	2.34	0.40
30:0:1656:A:H2'	30:0:1657:A:O4'	2.21	0.40
30:0:2002:C:H2'	30:0:2003:U:H5'	2.03	0.40
30:0:2575:C:H2'	30:0:2576:A:O4'	2.21	0.40
30:0:563:C:H2'	30:0:564:G:O4'	2.22	0.40
30:0:622:G:O2'	30:0:623:U:H5'	2.21	0.40
15:O:38:ARG:HD3	30:0:654:A:OP2	2.22	0.40
30:0:671:A:O2'	30:0:672:G:H2'	2.22	0.40
2:B:36:PRO:HG3	2:B:169:GLY:H	1.86	0.40
2:B:275:GLY:O	2:B:291:ASP:HA	2.21	0.40
2:B:41:PHE:CZ	2:B:79:MET:HG3	2.56	0.40
3:C:138:VAL:O	3:C:234:VAL:HA	2.21	0.40
5:E:22:VAL:O	5:E:28:SER:HA	2.22	0.40
14:N:21:HIS:HD2	37:0:4268:HOH:O	2.05	0.40
14:N:38:LYS:HB2	14:N:38:LYS:HE3	1.81	0.40
19:S:77:VAL:O	19:S:80:ARG:HG2	2.22	0.40
23:W:88:THR:CG2	23:W:89:ASP:H	2.34	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	
1	A	235/240 (98%)	220 (94%)	13 (6%)	2 (1%)	19	27
2	B	335/338 (99%)	315 (94%)	17 (5%)	3 (1%)	19	27
3	C	244/246 (99%)	231 (95%)	13 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	134/177 (76%)	115 (86%)	15 (11%)	4 (3%)	5	4
5	E	170/178 (96%)	165 (97%)	5 (3%)	0	100	100
6	F	117/120 (98%)	106 (91%)	9 (8%)	2 (2%)	10	13
7	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
8	H	156/177 (88%)	148 (95%)	8 (5%)	0	100	100
9	I	68/162 (42%)	57 (84%)	11 (16%)	0	100	100
10	J	140/145 (97%)	132 (94%)	7 (5%)	1 (1%)	24	35
11	K	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	21	31
12	L	141/165 (86%)	126 (89%)	14 (10%)	1 (1%)	24	35
13	M	192/196 (98%)	187 (97%)	5 (3%)	0	100	100
14	N	184/187 (98%)	170 (92%)	11 (6%)	3 (2%)	11	14
15	O	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
16	P	141/149 (95%)	140 (99%)	1 (1%)	0	100	100
17	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
18	R	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
19	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
20	T	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
21	U	51/67 (76%)	48 (94%)	2 (4%)	1 (2%)	8	9
22	V	63/71 (89%)	60 (95%)	2 (3%)	1 (2%)	11	14
23	W	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	24	35
24	X	80/92 (87%)	74 (92%)	5 (6%)	1 (1%)	13	18
25	Y	140/241 (58%)	140 (100%)	0	0	100	100
26	Z	71/116 (61%)	63 (89%)	6 (8%)	2 (3%)	5	5
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	42 (100%)	0	0	100	100
29	3	90/92 (98%)	87 (97%)	3 (3%)	0	100	100
All	All	3705/4472 (83%)	3505 (95%)	177 (5%)	23 (1%)	27	39

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
6	F	101	ALA

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Mol	Chain	Res	Type
10	J	5	GLU
12	L	80	ASP
14	N	154	LEU
14	N	184	ILE
4	D	27	ILE
14	N	183	ASP
22	V	43	PRO
23	W	77	ALA
26	Z	105	ARG
2	B	185	GLY
4	D	56	ARG
4	D	65	GLU
21	U	55	ALA
26	Z	66	CYS
1	A	34	ASP
4	D	171	ASP
2	B	169	GLY
11	K	126	SER
6	F	100	ASP
2	B	2	GLN
24	X	70	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/182 (98%)	171 (96%)	8 (4%)	30	47
2	B	282/283 (100%)	268 (95%)	14 (5%)	27	43
3	C	193/193 (100%)	179 (93%)	14 (7%)	15	24
4	D	117/148 (79%)	112 (96%)	5 (4%)	32	49
5	E	152/156 (97%)	148 (97%)	4 (3%)	49	70
6	F	93/94 (99%)	92 (99%)	1 (1%)	76	88
7	G	27/282 (10%)	26 (96%)	1 (4%)	37	56
8	H	134/145 (92%)	129 (96%)	5 (4%)	37	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	58/130 (45%)	57 (98%)	1 (2%)	63	80
10	J	118/121 (98%)	110 (93%)	8 (7%)	17	27
11	K	106/106 (100%)	103 (97%)	3 (3%)	47	67
12	L	113/127 (89%)	110 (97%)	3 (3%)	48	68
13	M	158/160 (99%)	152 (96%)	6 (4%)	36	55
14	N	149/150 (99%)	146 (98%)	3 (2%)	58	77
15	O	93/94 (99%)	90 (97%)	3 (3%)	42	62
16	P	113/117 (97%)	111 (98%)	2 (2%)	62	79
17	Q	79/80 (99%)	75 (95%)	4 (5%)	26	42
18	R	117/122 (96%)	115 (98%)	2 (2%)	63	80
19	S	71/74 (96%)	69 (97%)	2 (3%)	47	67
20	T	105/106 (99%)	98 (93%)	7 (7%)	18	28
21	U	44/53 (83%)	44 (100%)	0	100	100
22	V	51/57 (90%)	49 (96%)	2 (4%)	35	54
23	W	130/130 (100%)	123 (95%)	7 (5%)	24	38
24	X	66/74 (89%)	60 (91%)	6 (9%)	10	15
25	Y	120/196 (61%)	112 (93%)	8 (7%)	18	28
26	Z	60/94 (64%)	58 (97%)	2 (3%)	41	61
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	52	72
29	3	79/79 (100%)	78 (99%)	1 (1%)	71	86
All	All	3095/3646 (85%)	2972 (96%)	123 (4%)	34	53

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	36	ASP
1	A	55	VAL
1	A	94	LEU
1	A	120	ARG
1	A	131	HIS
1	A	179	MET
1	A	217	ARG
2	B	7	ARG

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Mol	Chain	Res	Type
2	B	11	LEU
2	B	27	ASN
2	B	49	THR
2	B	53	LEU
2	B	56	ASP
2	B	97	LEU
2	B	98	THR
2	B	162	MET
2	B	174	ARG
2	B	190	MET
2	B	254	GLN
2	B	264	GLU
2	B	312	ARG
3	C	2	GLN
3	C	27	ARG
3	C	67	GLN
3	C	94	THR
3	C	136	VAL
3	C	162	VAL
3	C	187	ARG
3	C	214	THR
3	C	222	ASP
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	240	LEU
3	C	243	VAL
4	D	24	HIS
4	D	61	PHE
4	D	133	ASN
4	D	136	ARG
4	D	137	PRO
5	E	16	ASP
5	E	86	VAL
5	E	102	VAL
5	E	164	ASP
6	F	12	LEU
7	G	73	ASP
8	H	87	LYS
8	H	91	ARG
8	H	149	VAL
8	H	157	TYR

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Mol	Chain	Res	Type
8	H	174	LEU
9	I	135	GLU
10	J	7	ASP
10	J	39	VAL
10	J	46	ILE
10	J	52	GLN
10	J	74	ARG
10	J	79	PHE
10	J	107	ASN
10	J	127	ILE
11	K	10	GLN
11	K	49	LEU
11	K	98	VAL
12	L	35	ARG
12	L	80	ASP
12	L	140	VAL
13	M	46	LEU
13	M	68	ARG
13	M	81	ARG
13	M	93	ARG
13	M	99	ARG
13	M	164	THR
14	N	17	ARG
14	N	26	LEU
14	N	127	LEU
15	O	3	THR
15	O	98	LEU
15	O	111	VAL
16	P	91	LYS
16	P	98	ILE
17	Q	11	ARG
17	Q	16	ASN
17	Q	57	ASP
17	Q	95	GLU
18	R	13	THR
18	R	39	THR
19	S	12	GLU
19	S	71	ASP
20	T	26	THR
20	T	39	ASN
20	T	48	VAL
20	T	73	HIS

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Mol	Chain	Res	Type
20	T	89	ARG
20	T	96	VAL
20	T	115	GLU
22	V	43	PRO
22	V	65	ASP
23	W	26	ILE
23	W	35	VAL
23	W	52	VAL
23	W	73	LEU
23	W	122	ARG
23	W	142	ASP
23	W	146	ILE
24	X	15	ARG
24	X	27	ASP
24	X	49	ARG
24	X	72	VAL
24	X	82	GLU
24	X	88	GLU
25	Y	141	THR
25	Y	154	ARG
25	Y	172	THR
25	Y	187	VAL
25	Y	189	ASN
25	Y	200	THR
25	Y	203	VAL
25	Y	220	GLU
26	Z	57	MET
26	Z	68	GLU
28	2	18	ASN
29	3	42	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	HIS
2	B	27	ASN
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	256	GLN
2	B	260	HIS
2	B	320	GLN

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Mol	Chain	Res	Type
2	B	332	ASN
3	C	39	GLN
3	C	73	GLN
3	C	129	HIS
3	C	151	GLN
3	C	163	HIS
4	D	103	ASN
4	D	133	ASN
5	E	106	ASN
5	E	119	HIS
5	E	143	GLN
7	G	17	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
8	H	73	ASN
10	J	52	GLN
10	J	107	ASN
10	J	126	ASN
11	K	10	GLN
11	K	44	HIS
12	L	18	HIS
12	L	41	HIS
13	M	24	GLN
13	M	58	GLN
13	M	137	ASN
13	M	170	ASN
14	N	21	HIS
14	N	107	ASN
16	P	50	GLN
16	P	66	GLN
16	P	73	HIS
16	P	88	GLN
16	P	118	GLN
17	Q	40	HIS
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS
18	R	117	HIS
19	S	9	HIS

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Mol	Chain	Res	Type
19	S	51	GLN
20	T	39	ASN
21	U	39	ASN
21	U	48	ASN
22	V	60	GLN
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	23	HIS
25	Y	133	HIS
25	Y	134	HIS
25	Y	149	GLN
25	Y	189	ASN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	16	ASN
28	2	18	ASN
28	2	41	HIS
28	2	45	ASN
29	3	2	GLN
29	3	15	ASN
29	3	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	224 (8%)	32 (1%)
31	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3045 (94%)	240 (8%)	33 (1%)

All (240) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G
30	0	86	A

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Mol	Chain	Res	Type
30	0	87	C
30	0	88	G
30	0	114	A
30	0	115	U
30	0	120	A
30	0	130	C
30	0	139	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	170	U
30	0	186	A
30	0	191	A
30	0	192	A
30	0	200	C
30	0	219	G
30	0	237	G
30	0	271	C
30	0	272	A
30	0	273	G
30	0	283	U
30	0	284	C
30	0	308	U
30	0	309	C
30	0	318	U
30	0	336	G
30	0	337	A
30	0	358	G
30	0	381	G
30	0	397	A
30	0	417	G
30	0	461	C
30	0	487	G
30	0	498	A
30	0	510	U
30	0	511	A
30	0	514	G
30	0	537	G
30	0	538	C
30	0	539	G
30	0	542	A
30	0	545	G

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Mol	Chain	Res	Type
30	0	553	G
30	0	559	U
30	0	588	G
30	0	604	G
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	701	U
30	0	735	C
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U
30	0	835	U
30	0	840	U
30	0	868	G
30	0	869	G
30	0	871	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	884	C
30	0	885	G
30	0	898	G
30	0	905	C
30	0	921	G
30	0	923	A
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1029	U
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G
30	0	1081	A
30	0	1087	G

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Mol	Chain	Res	Type
30	0	1088	A
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	U
30	0	1137	G
30	0	1164	U
30	0	1165	G
30	0	1166	A
30	0	1174	A
30	0	1175	G
30	0	1185	U
30	0	1192	A
30	0	1193	A
30	0	1206	U
30	0	1216	G
30	0	1238	C
30	0	1239	G
30	0	1279	U
30	0	1289	C
30	0	1342	C
30	0	1353	C
30	0	1360	C
30	0	1377	C
30	0	1407	A
30	0	1409	G
30	0	1474	C
30	0	1485	A
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1528	A
30	0	1592	G
30	0	1603	A
30	0	1625	U
30	0	1626	A
30	0	1634	G
30	0	1656	A
30	0	1667	A
30	0	1682	A

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Mol	Chain	Res	Type
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1701	A
30	0	1722	U
30	0	1723	G
30	0	1725	C
30	0	1731	C
30	0	1752	G
30	0	1778	A
30	0	1779	A
30	0	1798	C
30	0	1820	G
30	0	1829	A
30	0	1856	C
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1943	C
30	0	1971	G
30	0	1973	A
30	0	1978	A
30	0	1979	G
30	0	1980	U
30	0	1996	U
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G
30	0	2033	G
30	0	2034	U
30	0	2064	U
30	0	2072	G
30	0	2073	G
30	0	2074	A
30	0	2096	A
30	0	2101	A
30	0	2102	G
30	0	2103	A
30	0	2104	C
30	0	2110	G
30	0	2243	C

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Mol	Chain	Res	Type
30	0	2258	A
30	0	2271	G
30	0	2272	G
30	0	2291	A
30	0	2317	C
30	0	2321	A
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2422	U
30	0	2462	G
30	0	2469	A
30	0	2476	C
30	0	2480	G
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2533	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2613	G
30	0	2649	A
30	0	2664	A
30	0	2681	A
30	0	2682	C
30	0	2719	A
30	0	2726	U
30	0	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2792	A
30	0	2800	A

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Mol	Chain	Res	Type
30	0	2811	A
30	0	2825	C
30	0	2840	A
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A
31	9	2	U
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	40	C
31	9	41	C
31	9	43	G
31	9	44	A
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A
30	0	129	A
30	0	169	A
30	0	338	C
30	0	603	A
30	0	699	C
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G
30	0	1080	C
30	0	1232	A
30	0	1237	U
30	0	1246	A

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Mol	Chain	Res	Type
30	0	1352	A
30	0	1377	C
30	0	1506	U
30	0	1692	C
30	0	1856	C
30	0	1942	A
30	0	1979	G
30	0	2011	A
30	0	2103	A
30	0	2313	C
30	0	2467	A
30	0	2526	C
30	0	2536	C
30	0	2649	A
30	0	2718	C
30	0	2726	U
30	0	2761	A
30	0	2791	U
31	9	65	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
30	OMU	0	2587	30	14,22,23	0.98	1 (7%)	18,31,34	3.64	2 (11%)
30	OMG	0	2588	30	19,26,27	1.04	2 (10%)	22,38,41	2.48	4 (18%)
30	UR3	0	2619	30	13,22,23	0.74	0	15,32,35	0.74	0
30	PSU	0	2621	30	16,21,22	1.58	3 (18%)	20,30,33	5.42	4 (20%)
30	1MA	0	628	33,30	16,25,26	1.00	1 (6%)	12,37,40	1.26	1 (8%)

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
30	OMU	0	2587	30	-	0/5/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/3/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	1MA	0	628	33,30	-	0/3/25/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-4.79	1.48	1.52
30	0	2588	OMG	C8-N7	-2.07	1.30	1.34
30	0	2621	PSU	C2-N1	2.52	1.43	1.38
30	0	2587	OMU	C4-N3	2.70	1.37	1.33
30	0	2621	PSU	C4-N3	2.75	1.38	1.33
30	0	628	1MA	C6-N6	2.78	1.33	1.27
30	0	2588	OMG	C6-N1	3.39	1.39	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-17.31	114.50	128.41
30	0	2588	OMG	C5-C6-N1	-8.37	111.57	123.47
30	0	2621	PSU	C5-C4-N3	-8.15	114.85	125.36
30	0	628	1MA	C2-N3-C4	-3.83	110.65	116.51
30	0	2587	OMU	C5-C4-N3	-3.66	114.66	123.17
30	0	2588	OMG	C2-N3-C4	-2.87	111.81	115.16
30	0	2588	OMG	N3-C2-N1	-2.37	123.94	127.41
30	0	2621	PSU	C6-N1-C2	2.97	120.12	115.36
30	0	2588	OMG	C6-N1-C2	6.39	125.25	116.06
30	0	2621	PSU	C4-N3-C2	14.14	127.18	115.14
30	0	2587	OMU	C4-N3-C2	14.90	126.96	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 231 ligands modelled in this entry, 231 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.