



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:15 am BST

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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

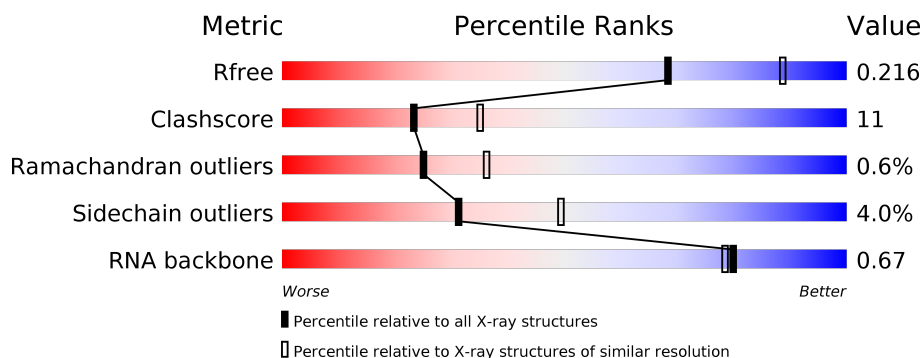
1 Overall quality at a glance

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.

















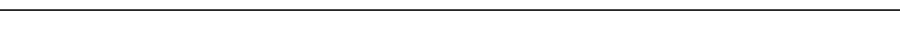




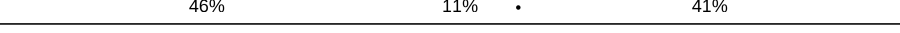
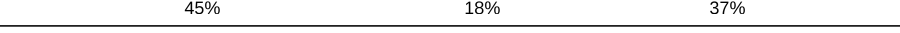




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

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	 92%
8	H	177	 69% 21% 10%
9	I	162	 25% 18% 57%
10	J	145	 72% 23%
11	K	132	 73% 26%
12	L	165	 71% 16% 12%
13	M	196	 79% 18%
14	N	187	 67% 31%
15	O	116	 82% 16%
16	P	149	 82% 14%
17	Q	96	 83% 14%
18	R	155	 78% 17%
19	S	85	 74% 21% 5%
20	T	120	 72% 25%
21	U	67	 51% 28% 21%
22	V	71	 61% 28% 8%
23	W	154	 62% 33%
24	X	92	 62% 25% 11%
25	Y	241	 46% 11% 41%
26	Z	116	 45% 18% 37%
27	1	57	 74% 25%
28	2	50	 52% 38% 8%
29	3	92	 77% 23%
30	0	2923	 62% 27% 5% 6%
31	9	122	 48% 40% 11%

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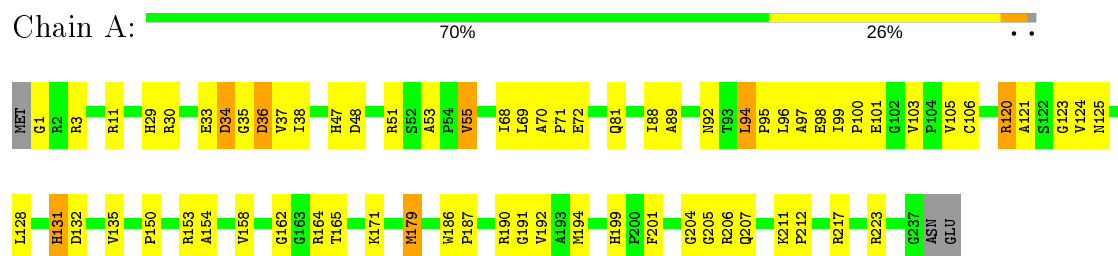
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	3	72	Total 72	O 72	0	0
37	0	5949	Total 5949	O 5949	0	0
37	9	139	Total 139	O 139	0	0

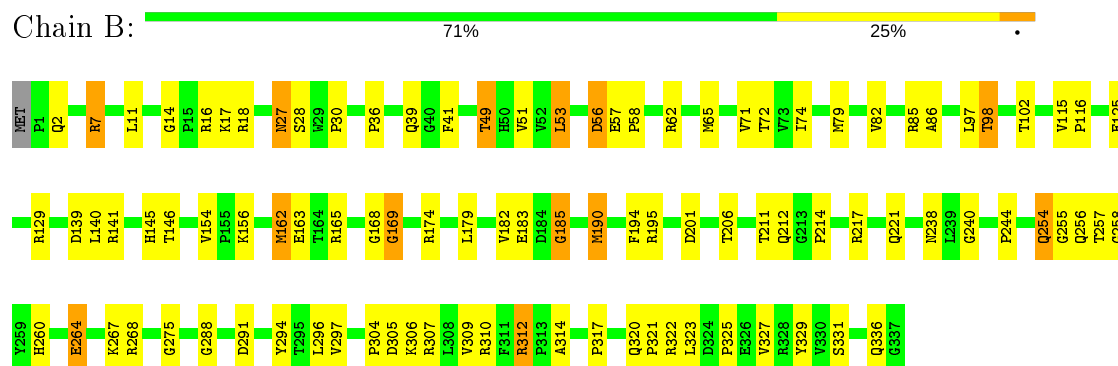
3 Residue-property plots [i](#)

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.

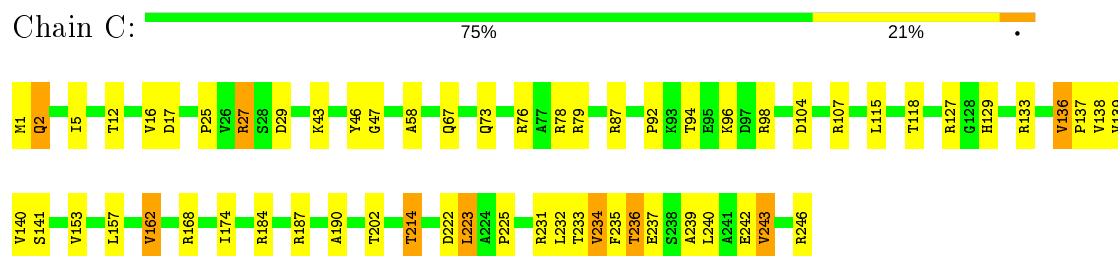
- Molecule 1: 50S ribosomal protein L2P



- Molecule 2: 50S ribosomal protein L3P

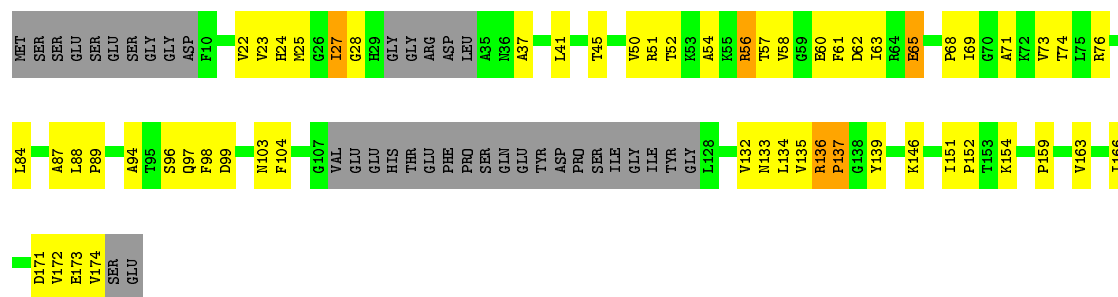


- Molecule 3: 50S ribosomal protein L4P



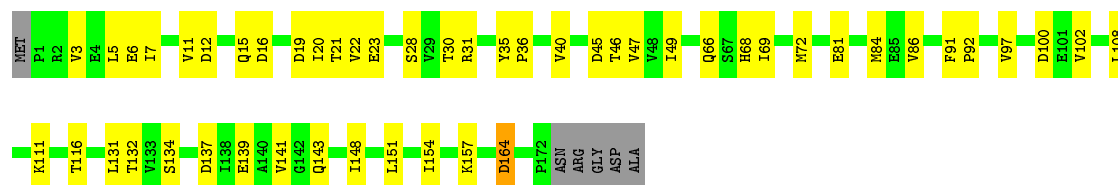
- Molecule 4: 50S ribosomal protein L5P





- Molecule 5: 50S ribosomal protein L6P

Chain E: 69% 28% ..



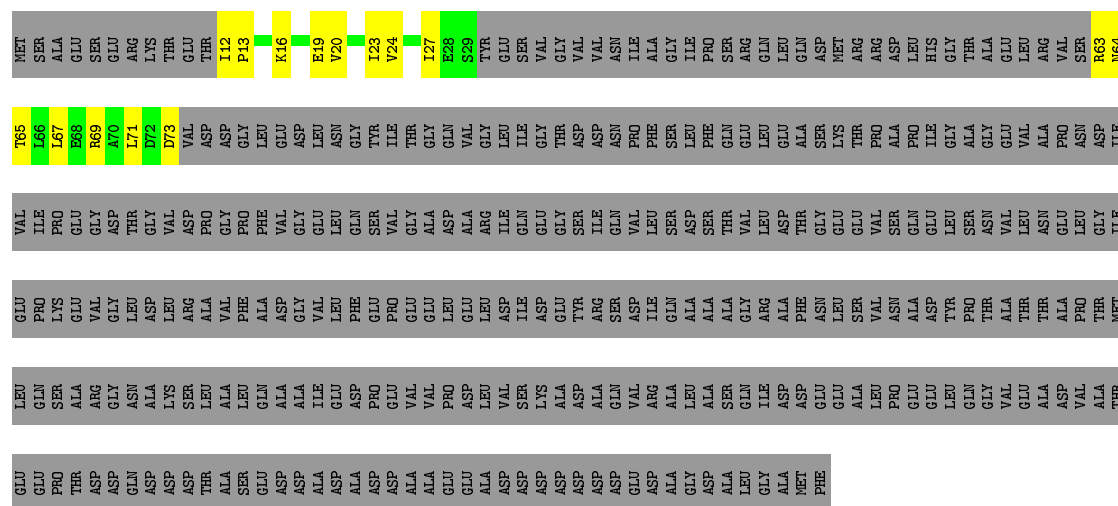
- Molecule 6: 50S ribosomal protein L7Ae

Chain F:  73% 26%



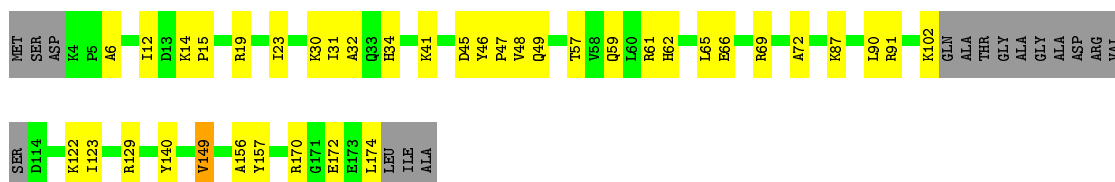
- Molecule 7: 50S ribosomal protein L10E

Chain G:  92%



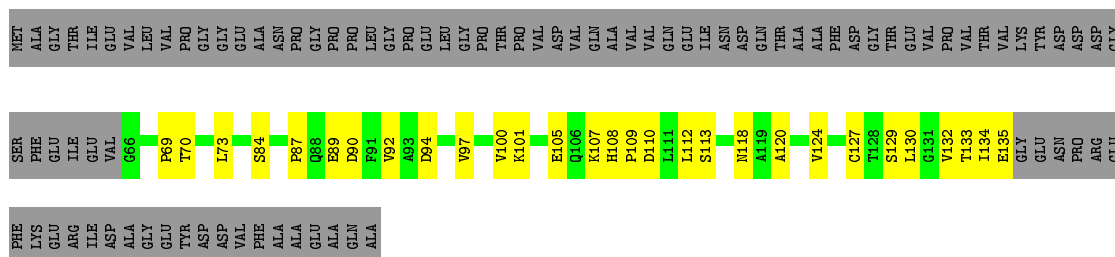
- Molecule 8: 50S ribosomal protein L10e

Chain H:  69% 21% • 10%



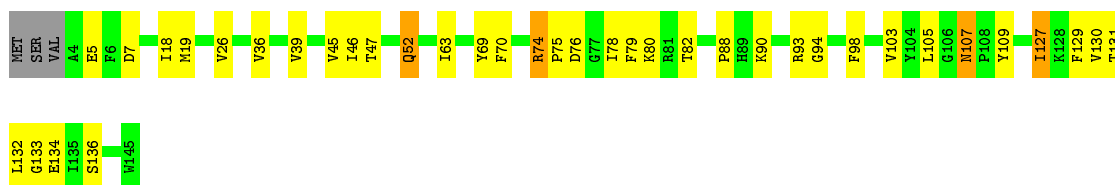
- Molecule 9: 50S ribosomal protein L11P

Chain I: 25% 18% 57%



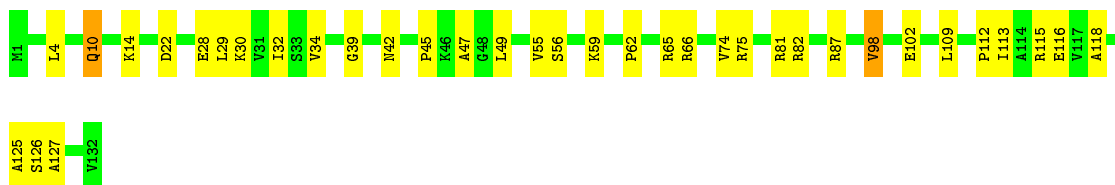
- Molecule 10: 50S ribosomal protein L13P

Chain J: 72% 23% . .



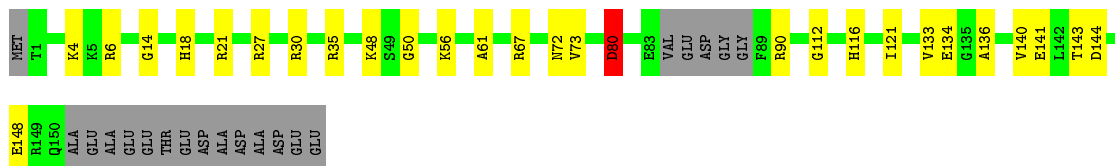
- Molecule 11: 50S ribosomal protein L14P

Chain K: 73% 26% .




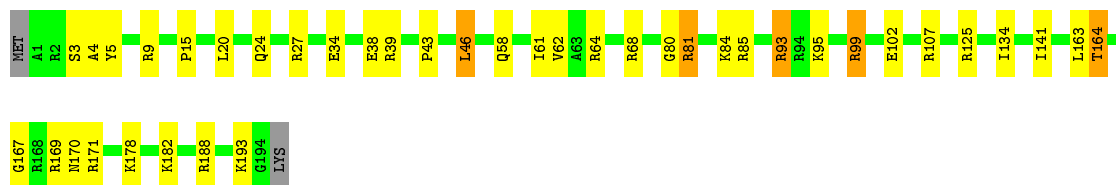
- Molecule 12: 50S ribosomal protein L15P

Chain L: 71% 16% . 12%



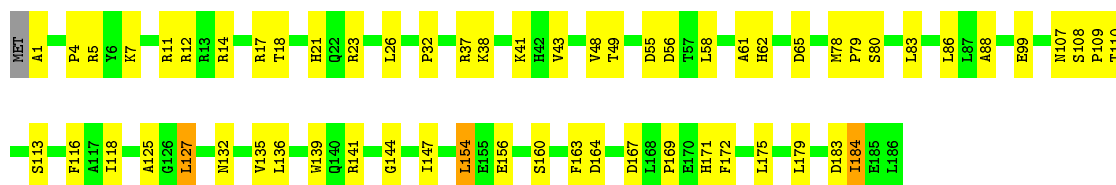
- Molecule 13: 50S ribosomal protein L15e

Chain M:  79% 18% ..




- Molecule 14: 50S ribosomal protein L18P

Chain N:  67% 31% ..




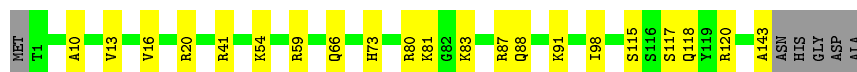
- Molecule 15: 50S ribosomal protein L18e

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% ..



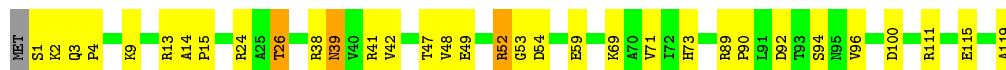
- Molecule 19: 50S ribosomal protein L23P

Chain S:  74% 21% 5%



- Molecule 20: 50S ribosomal protein L24P

Chain T: 72% 25% ..



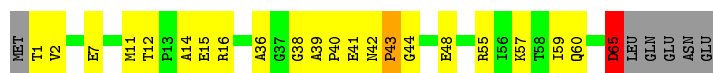
- Molecule 21: 50S ribosomal protein L24e

Chain U: 51% 28% 21%



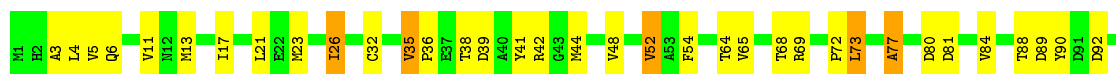
- Molecule 22: 50S ribosomal protein L29P

Chain V: 61% 28% 8%



- Molecule 23: 50S ribosomal protein L30P

Chain W: 62% 33% ..



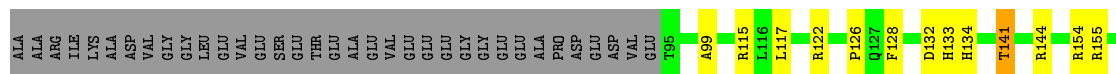
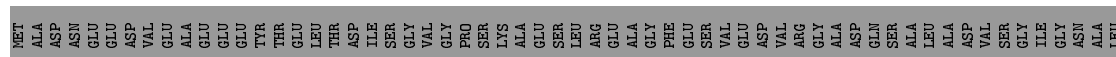
- Molecule 24: 50S ribosomal protein L31e

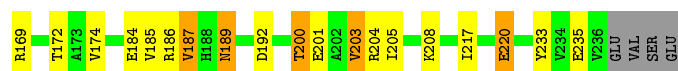
Chain X: 62% 25% 11%



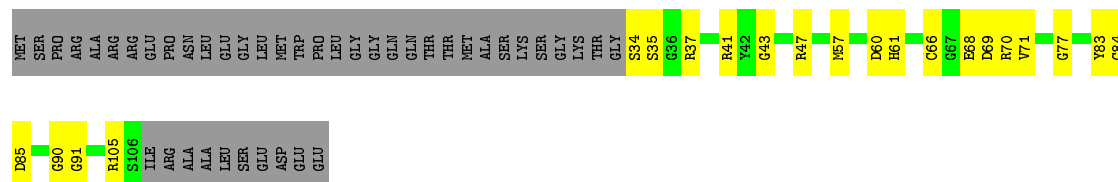
- Molecule 25: 50S ribosomal protein L32e

Chain Y: 46% 11% 41%





- Molecule 26: 50S ribosomal protein L37Ae



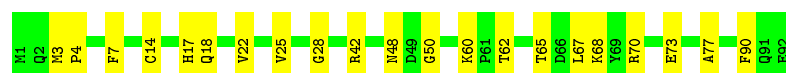
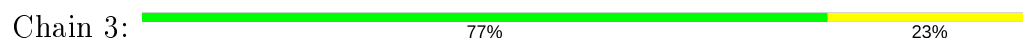
- Molecule 27: 50S ribosomal protein L37e



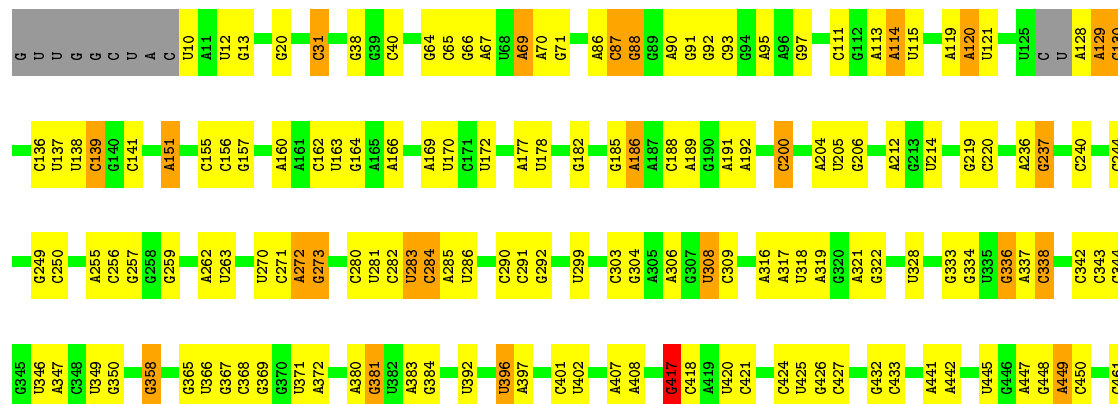
- Molecule 28: 50S ribosomal protein L39e



- Molecule 29: 50S ribosomal protein L44E



- Molecule 30: 23S RIBOSOMAL RNA



C2114	U1996	G1878	A1733	A1615	A1482	C1360	U1244	G1187	G1059	U	A867	G716	G604	G469
U2115	A1997	U1879	G1734	A1624	C1483	A1367	G1245	C1188	C1060	G	G868	G735	C605	U470
U2116		C1380	C1735	A1694	A1484	U1368	A1246	A1171	G1072	U	G869	A736	U619	G471
	G2001	A1881	A1736	U1625	A1485	A1369	U1249	A1172	G1076	C	A620	A737	A620	G482
G2128	G2002	C1882	U1741	A1626	A1493	G1370	C1250	A1173	G1077	G	G621	G738	G621	C483
G2134	U2004	G1884	A1742	G1627	G1497	U1371	C1251	A1174	A1078	C	G622		G622	A484
A2135	G2005	G1894		A1632	U1500	A1372	A1252	G1175	A1079	U	U623	C757	U623	A485
		A1909	G1752	C1633	U1501		C1253		A1078		U624	A758	U625	A486
A	U2008			G1634	U1504	C1377		U1180	A1079		A875	C759		G487
C	G2009	A1919	U1766	U1635	U1503	C1384	C1257	A1181	A1081	C	A876	G764	A629	A498
G	A2011	A1920	U1771	G1636	U1504		G1258	C1182	A1082	G	A630	G765	A630	A498
U	A2012	A1921	C1772	A1637	U1505	A1389	U1266	C1183	C1083	A	G631		G631	G499
G	U2013	A1922	G1773	A1641	U1506	C1394	C1267	C1184	C1084	G	A632	G775	A632	G500
U	G2014			A1642	U1524	A1406	G1268	U1185	C1085	A	G638	G776		G506
C	A2015	G1925	A1778	A1642	U1525	A1407	G1269	C1186	C1086	G	A639	U777		A507
G	U2016	A1927	A1779	U1654	U1526	U1408	A1278	A1188	A1087	C	A894	A790	G644	A508
C				G1655	A1527	U1409	U1279	G1189	A1097	U	G868	A791	U645	A509
C	A2019	C1940	A1783	U1656	A1528	G1409	A1291	A1191	A1098	C	G899	G792	U646	U510
G		A1941	U1784	A1657	A1529	A1413	C1289	A1192	G1099	G	G902	U794	U647	A511
A	C2031	A1942	C1787	A1658	G1535	A1414	G1290	A1193				G795		G514
U	U2032	C1943	U1788		G1536		A1291		C1103	C	C905	A796	U653	
G	G2033		G1789	C1666	C1536	G1417	A1291	A1200		A	G906	A797	A654	G518
U	U2034	C1946		A1667		U1418	A1294	C1201	U1109	C	A907		A655	A524
G		G1947		U1668	C1545	U1419	G1295	A1202	G1110	A		G809	G656	
C	G2044	G1948	C1798	C1675	G1546	C1420		G1203					G657	A532
A	G2050	G1949	G1799	G1676	G1556	C1423	G1299	C1204	U1116	C1000	A912	A812		
C	C2051	G1950	A1815	U1677	G1557	A1424	G1300	U1205	A1117		C920	C813	A660	A536
A	A2054	U	C1816	A1678	C1558		U1304	U1206	A1118	A1006	G921	G814	G661	G537
U		A		C1679	G1559	A1427	C1305	A1207	G1119	A1007	A922	U815	U664	C538
A	C2061	A	G1819	U1680	U1561	C1428	U1306	C1208	U1120	G	A923	G816	U665	G539
G	A2062	C	G1820	G1681	U1562	U1429	U1314	C1209	G1121	C1010		A818	A666	A540
G	U2063	U	U1825	A1682	C1562	G1430	A1313	G1211	C1127		U932	A819	C667	C541
U	U2064	A	C1826	G1683			U1314	G1212	U1128	A1014	G933	G820		A542
A		U		A1684	C1565	G1433	G1315	G1213	C1129	C1015		U821	A671	G543
G	G2070	G	A1829	A1685	G1571	A1434	G1316	G1214	U1130		G940	G827	G672	G544
G	C2071	A	C1834	C1692	G1571	U1435	G1325	A1215	G1131	C1023	G941	A827	G672	G545
A	G2072	C	U1835		G1588	C1436	G1325	G1216	A1132	C1025	U942	G828		
G	A2074	C	U1835	G1697	G1589	C1439	G1328	G1217			G681		G681	G553
C		U1964	A1840	U1698		U1440	A1328	U1218	G1135	U1026	U946	G834	A686	
G	A2081		C1841	A1701	G1592	G1441	G1329	U1219	U1136	G1027	U947	U835	A687	C558
U		G1971	A1842	U1702	A1603	A1462	A1330		G1137	U1028	G948	U836	C687	C559
U	A2089	U1972			U1593	U1463		C1229	G1138	U1029	U949	U840	A688	U560
A	G2090	A1973	A1845	C1714	C1594	A1470	U1333	A1230	G1139		G950	A841	U560	
C	G2091			C1715	U1595	C1450	C1334	A1231	C1140	G1039	G699			A563
A		G1976	G1848	A1716	A1597	G1453	G1339	A1232			A700	A844	A700	G563
G	A2096	U1977		A1717	A1598		G1340	U1234	G1151	U1042	G701		G701	G564
A		A1978				C1462	A1341	U1235		C1043	G702		G702	
G	A2101	G1979	C1856	U1722	A1603	U1463	A1342	G1236	G1158	C1044	G703		G703	U567
G	G2102	U1980	C1862	U1724	G1604		C1343	U1237	G1159	G1045	C704		C704	
U			G1863	C1725	G1605	A1470		A1238	G1160	G1046	G574		G574	G574
G	C2104	U1985					U1350	G1239	A1161	G1053	A961		G709	A575
A					G1611	C1474	G1351	G1240	G1162		C962		G710	
C		U1992	G1867	G1730	A1612		C1352	G1241	G1163		G969	U858	G711	G888
C	G2110	C1993	G1968		C1613		C1353	G1242	U1164	U1056	U970	U860	G711	
C	G2111	A1994		C1732		C1477		G1243	G1165	A1057	U714	A861	U714	A602
G	A2112		G1877	A1732	G1614				A1166	A1058	U		U	A603
C	G2113													

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	30:0:656:G:OP2	2.17	0.44
30:0:1477:C:H5'	30:0:1868:G:H5''	1.98	0.44
30:0:2090:G:H2'	30:0:2091:G:C8	2.51	0.44
30:0:2103:A:N7	30:0:2538:A:N6	2.65	0.44
30:0:212:A:O4'	30:0:214:U:C6	2.71	0.44
30:0:2135:A:O2'	30:0:2136:G:H5'	2.16	0.44
30:0:2642:G:H2'	30:0:2643:G:O4'	2.17	0.44
30:0:2712:G:P	37:0:4763:HOH:O	2.75	0.44
30:0:2791:U:H1'	30:0:2792:A:H5''	1.99	0.44
30:0:958:G:H2'	30:0:959: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	30:0:2054:A:H2	1.61	0.44
30:0:2812:A:N7	37:0:7067: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
30:0:2115:U:H2'	30:0:2116:U:C6	2.53	0.44
30:0:281:U:H3'	37:0:6755:HOH:O	2.17	0.44
2:B:244:PRO:HB3	30:0:1234: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
30:0:1014:A:H5''	31:9:101:G:O2'	2.18	0.44
30:0:1940:C:H4'	37:0:6896: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%)	17	25
2	B	335/338 (99%)	315 (94%)	17 (5%)	3 (1%)	17	25
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%)	4	3
5	E	170/178 (96%)	165 (97%)	5 (3%)	0	100	100
6	F	117/120 (98%)	106 (91%)	9 (8%)	2 (2%)	9	11
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%)	22	32
11	K	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	19	29
12	L	141/165 (86%)	126 (89%)	14 (10%)	1 (1%)	22	32
13	M	192/196 (98%)	187 (97%)	5 (3%)	0	100	100
14	N	184/187 (98%)	170 (92%)	11 (6%)	3 (2%)	9	13
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%)	7	9
22	V	63/71 (89%)	60 (95%)	2 (3%)	1 (2%)	9	13
23	W	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	22	32
24	X	80/92 (87%)	74 (92%)	5 (6%)	1 (1%)	12	17
25	Y	140/241 (58%)	140 (100%)	0	0	100	100
26	Z	71/116 (61%)	63 (89%)	6 (8%)	2 (3%)	5	4
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%)	25	36

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%)	27	44
2	B	282/283 (100%)	268 (95%)	14 (5%)	24	40
3	C	193/193 (100%)	179 (93%)	14 (7%)	14	22
4	D	117/148 (79%)	112 (96%)	5 (4%)	29	46
5	E	152/156 (97%)	148 (97%)	4 (3%)	46	66
6	F	93/94 (99%)	92 (99%)	1 (1%)	73	87
7	G	27/282 (10%)	26 (96%)	1 (4%)	34	53
8	H	134/145 (92%)	129 (96%)	5 (4%)	34	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	58/130 (45%)	57 (98%)	1 (2%)	60	78
10	J	118/121 (98%)	110 (93%)	8 (7%)	16	25
11	K	106/106 (100%)	103 (97%)	3 (3%)	43	63
12	L	113/127 (89%)	110 (97%)	3 (3%)	44	65
13	M	158/160 (99%)	152 (96%)	6 (4%)	33	51
14	N	149/150 (99%)	146 (98%)	3 (2%)	55	74
15	O	93/94 (99%)	90 (97%)	3 (3%)	39	59
16	P	113/117 (97%)	111 (98%)	2 (2%)	59	76
17	Q	79/80 (99%)	75 (95%)	4 (5%)	24	39
18	R	117/122 (96%)	115 (98%)	2 (2%)	60	78
19	S	71/74 (96%)	69 (97%)	2 (3%)	43	63
20	T	105/106 (99%)	98 (93%)	7 (7%)	16	26
21	U	44/53 (83%)	44 (100%)	0	100	100
22	V	51/57 (90%)	49 (96%)	2 (4%)	32	50
23	W	130/130 (100%)	123 (95%)	7 (5%)	22	36
24	X	66/74 (89%)	60 (91%)	6 (9%)	9	14
25	Y	120/196 (61%)	112 (93%)	8 (7%)	16	26
26	Z	60/94 (64%)	58 (97%)	2 (3%)	38	57
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	49	68
29	3	79/79 (100%)	78 (99%)	1 (1%)	69	84
All	All	3095/3646 (85%)	2972 (96%)	123 (4%)	31	49

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	1.01	1 (7%)	14,31,34	1.15	1 (7%)
30	UR3	0	2619	30	14,22,23	0.74	0	15,32,35	0.64	0
30	1MA	0	628	33,30	15,25,26	0.73	0	15,37,40	1.37	1 (6%)
30	PSU	0	2621	30	17,21,22	1.56	3 (17%)	20,30,33	5.46	4 (20%)
30	OMG	0	2588	30	18,26,27	1.08	2 (11%)	20,38,41	2.61	4 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	OMU	0	2587	30	-	0/7/27/28	0/2/2/2
30	UR3	0	2619	30	-	0/5/25/26	0/2/2/2
30	1MA	0	628	33,30	-	0/3/25/26	0/3/3/3
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-4.87	1.48	1.52
30	0	2588	OMG	C6-N1	3.50	1.39	1.33
30	0	2621	PSU	C4-N3	2.84	1.38	1.33
30	0	2587	OMU	C4-N3	2.78	1.37	1.33
30	0	2621	PSU	C2-N1	2.52	1.43	1.38
30	0	2588	OMG	C8-N7	-2.14	1.30	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-17.53	114.50	128.43
30	0	2621	PSU	C4-N3-C2	14.26	127.18	115.14
30	0	2588	OMG	C5-C6-N1	-8.67	111.57	123.43
30	0	2621	PSU	C5-C4-N3	-8.15	114.85	125.36
30	0	2588	OMG	C6-N1-C2	5.87	125.25	115.93
30	0	628	1MA	C2-N3-C4	-4.74	110.65	116.58
30	0	2587	OMU	C5-C4-N3	-3.93	114.66	123.31
30	0	2588	OMG	C2-N3-C4	-3.11	111.81	115.36
30	0	2621	PSU	C6-N1-C2	2.89	120.12	115.36
30	0	2588	OMG	N3-C2-N1	-2.46	123.94	127.22

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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