



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:56 am BST

PDB ID : 1VQN
Title : The structure of CC-HPMN AND CCA-PHE-CAP-BIO bound to the large ribosomal subunit of haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
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

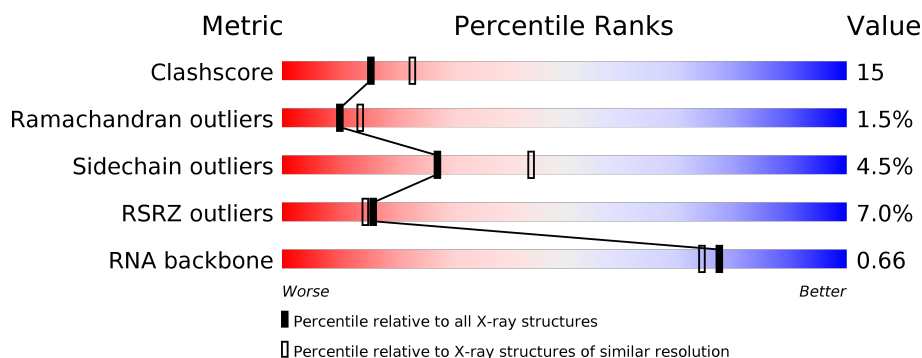
1 Overall quality at a glance i

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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>27%</div> <div>5%</div> <div>6%</div> </div> </div>
2	9	122	<div> <div>5%</div> <div> <div></div> <div>57%</div> <div>32%</div> <div>11%</div> </div> </div>
3	4	4	<div> <div></div> <div> <div></div> <div>50%</div> <div>50%</div> </div> </div>
4	5	6	<div> <div>17%</div> <div> <div></div> <div>17%</div> <div>67%</div> <div>17%</div> </div> </div>
5	A	240	<div> <div>5%</div> <div> <div></div> <div>61%</div> <div>33%</div> <div>5%</div> </div> </div>
6	B	338	<div> <div>3%</div> <div> <div></div> <div>57%</div> <div>39%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
7	C	246	
8	D	177	
9	E	178	
10	F	120	
11	G	348	
12	H	171	
13	J	145	
14	K	132	
15	L	165	
16	M	194	
17	N	187	
18	O	116	
19	P	149	
20	Q	96	
21	R	155	
22	S	85	
23	T	120	
24	U	66	
25	V	71	
26	W	154	
27	X	92	
28	Y	241	
29	Z	83	
30	1	57	
31	2	50	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	MG	0	8047	-	-	-	X
36	NA	0	9152	-	-	-	X
36	NA	0	9184	-	-	-	X
38	SR	B	9521	-	-	-	X

2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 99077 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal rna.

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

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

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

- Molecule 3 is a RNA chain called 5'-R(*CP*CP*(PPU)*(LOF))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	4	Total	C	N	O	P	0	0	0
			72	39	12	19	2			

- Molecule 4 is a RNA chain called 5'-R(*CP*CP*AP*(PHE)*(ACA)*(BTN))-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	5	6	Total	C	N	O	P	S	0	0	0
			93	53	15	22	2	1			

- Molecule 5 is a protein called 50S ribosomal protein L2P.

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

- Molecule 6 is a protein called 50S ribosomal protein L3P.

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

- Molecule 7 is a protein called 50S ribosomal protein L4E.

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

- Molecule 8 is a protein called 50S ribosomal protein L5P.

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

- Molecule 9 is a protein called 50S ribosomal protein L6P.

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

- Molecule 10 is a protein called 50S ribosomal protein L7AE.

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

- Molecule 11 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L10E.

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

- Molecule 13 is a protein called 50S ribosomal protein L13P.

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

- Molecule 14 is a protein called 50S ribosomal protein L14P.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 15 is a protein called 50S ribosomal protein L15P.

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

- Molecule 16 is a protein called 50S Ribosomal Protein L15E.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 17 is a protein called 50S ribosomal protein L18P.

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

- Molecule 18 is a protein called 50S ribosomal protein L18e.

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

- Molecule 19 is a protein called 50S ribosomal protein L19E.

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

- Molecule 20 is a protein called 50S ribosomal protein L21e.

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

- Molecule 21 is a protein called 50S ribosomal protein L22P.

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

- Molecule 22 is a protein called 50S ribosomal protein L23P.

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

- Molecule 23 is a protein called 50S ribosomal protein L24P.

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

- Molecule 24 is a protein called 50S ribosomal protein L24E.

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

- Molecule 25 is a protein called 50S ribosomal protein L29P.

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

- Molecule 26 is a protein called 50S ribosomal protein L30P.

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

- Molecule 27 is a protein called 50S ribosomal protein L31e.

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

- Molecule 28 is a protein called 50S ribosomal protein L32E.

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

- Molecule 29 is a protein called 50S ribosomal protein L37Ae.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 30 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 31 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 32 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	87	Total	Mg	0	0
			87	87		
34	Y	1	Total	Mg	0	0
			1	1		
34	K	1	Total	Mg	0	0
			1	1		
34	A	1	Total	Mg	0	0
			1	1		
34	T	1	Total	Mg	0	0
			1	1		
34	5	1	Total	Mg	0	0
			1	1		
34	2	1	Total	Mg	0	0
			1	1		
34	9	1	Total	Mg	0	0
			1	1		

- Molecule 35 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	2	Total	K	0	0
			2	2		

- Molecule 36 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	66	Total	Na	0	0
			66	66		
36	J	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	Q	1	Total 1	Na 1	0	0
36	D	1	Total 1	Na 1	0	0
36	C	1	Total 1	Na 1	0	0
36	R	2	Total 2	Na 2	0	0
36	9	1	Total 1	Na 1	0	0
36	S	1	Total 1	Na 1	0	0
36	M	1	Total 1	Na 1	0	0

- Molecule 37 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	10	Total 10	Cl 10	0	0
37	J	3	Total 3	Cl 3	0	0
37	B	1	Total 1	Cl 1	0	0
37	A	1	Total 1	Cl 1	0	0
37	N	1	Total 1	Cl 1	0	0
37	O	1	Total 1	Cl 1	0	0
37	R	1	Total 1	Cl 1	0	0
37	Y	1	Total 1	Cl 1	0	0
37	L	1	Total 1	Cl 1	0	0
37	3	1	Total 1	Cl 1	0	0
37	M	1	Total 1	Cl 1	0	0

- Molecule 38 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	98	Total 98	Sr 98	0	0
38	1	2	Total 2	Sr 2	0	0
38	H	1	Total 1	Sr 1	0	0
38	B	2	Total 2	Sr 2	0	0
38	3	1	Total 1	Sr 1	0	0
38	A	3	Total 3	Sr 3	0	0
38	R	1	Total 1	Sr 1	0	0
38	9	3	Total 3	Sr 3	0	0
38	L	1	Total 1	Sr 1	0	0
38	S	1	Total 1	Sr 1	0	0
38	F	1	Total 1	Sr 1	0	0

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

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

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	0	5727	Total 5727	O 5727	0	0
40	9	137	Total 137	O 137	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	4	1	Total O 1 1	0	0
40	5	2	Total O 2 2	0	0
40	A	120	Total O 120 120	0	0
40	B	138	Total O 138 138	0	0
40	C	180	Total O 180 180	0	0
40	D	48	Total O 48 48	0	0
40	E	44	Total O 44 44	0	0
40	F	24	Total O 24 24	0	0
40	G	14	Total O 14 14	0	0
40	H	72	Total O 72 72	0	0
40	J	54	Total O 54 54	0	0
40	K	61	Total O 61 61	0	0
40	L	83	Total O 83 83	0	0
40	M	128	Total O 128 128	0	0
40	N	58	Total O 58 58	0	0
40	O	39	Total O 39 39	0	0
40	P	61	Total O 61 61	0	0
40	Q	51	Total O 51 51	0	0
40	R	78	Total O 78 78	0	0
40	S	31	Total O 31 31	0	0
40	T	35	Total O 35 35	0	0

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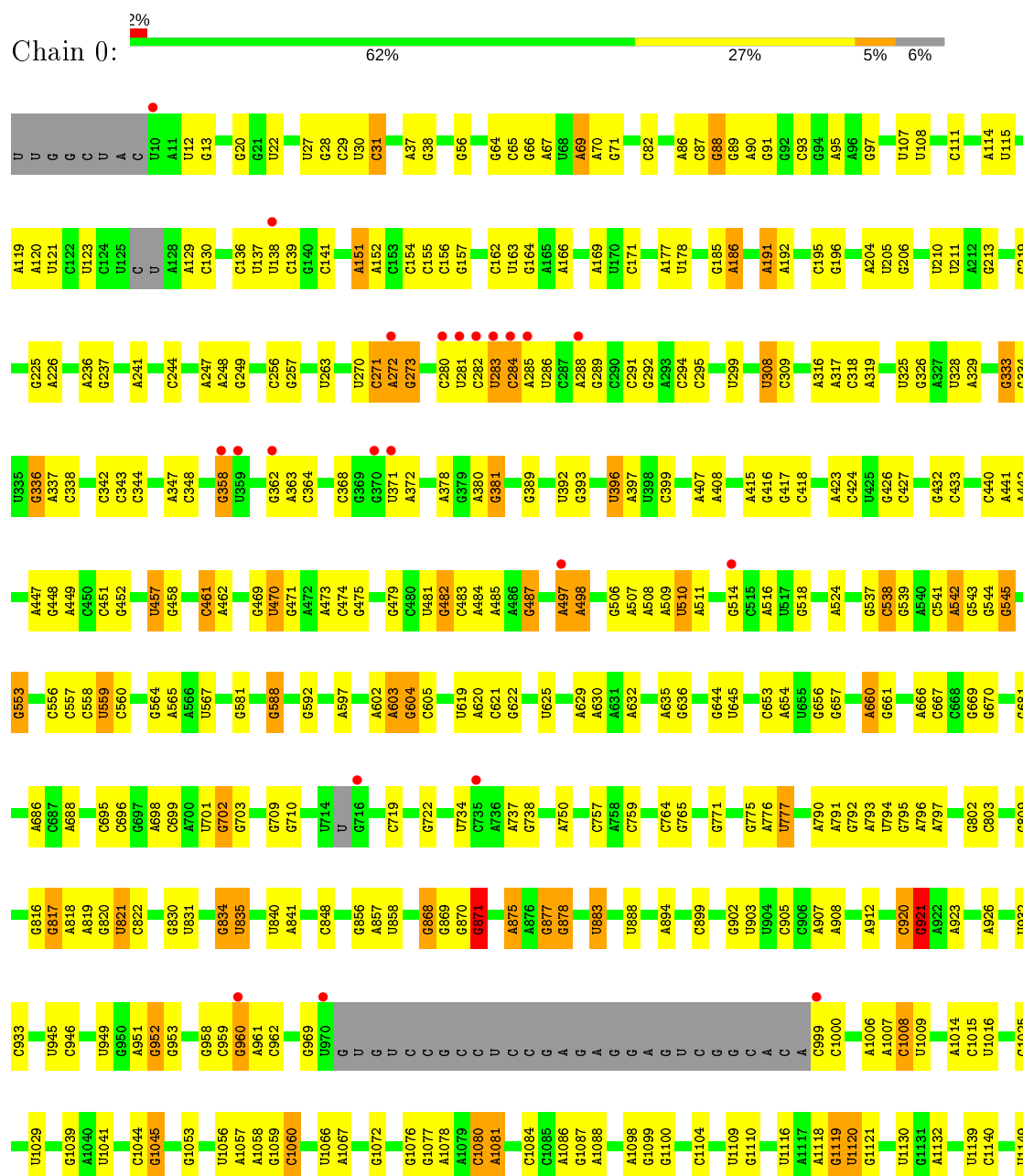
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	U	28	Total 28	O 28	0	0
40	V	12	Total 12	O 12	0	0
40	W	62	Total 62	O 62	0	0
40	X	21	Total 21	O 21	0	0
40	Y	93	Total 93	O 93	0	0
40	Z	34	Total 34	O 34	0	0
40	1	59	Total 59	O 59	0	0
40	2	40	Total 40	O 40	0	0
40	3	71	Total 71	O 71	0	0
40	I	10	Total 10	O 10	0	0

3 Residue-property plots

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

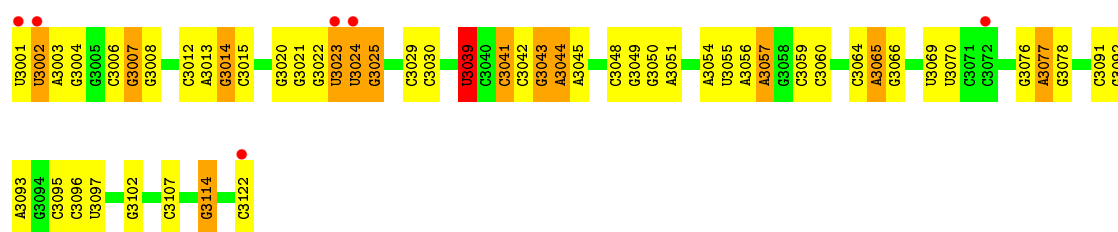
- Molecule 1: 23S ribosomal rna



G2564	A2467	C2476	C2351	C2243	G2091	C	U1845	U1741	C1633	A1482	C1343	A1232	A1150
C2565	A2468	C2477	G2352	C2248	A2096	U1964	A1847	G1744	C1634	A1483	U1350	A1233	G1151
A2568	A2469	C2478	C2353	C2249	C	U1965	G1948	G1745	U1635	G1484	G1351	U1234	G1158
A2569	C2472	C2479	A2354	G2249	A2100	U1966	G1949	U1748	G1636	A1352	A1352	G1235	G1159
G2578	C2473	C2480	G2355	G2250	A2101	U1967	C1853	U1749	A1637	G1491	C1353	U1237	G1160
U2586	C2476	G2481	A2356	G2251	G2102	G1970	C1856	U1750	A1641	U1503	C1360	C1238	A1161
U2478	C2477	G2482	G2357	A2252	A2103	U1971	U1856	G1751	A1642	A1504	U1361	G1239	G1162
U2587	C2478	G2483	A2358	G2253	G2110	U1972	G1863	U1752	U1654	U1505	G1363	U1242	G1163
G2480	C2479	A2484	A2359	A2254	G2111	A1973	U1863	U1753	U1655	U1506	U1364	C1243	U1164
U2588	C2480	G2485	G2360	A2255	U2115	G1974	G1867	U1754	G1656	U1507	A1365	C1244	A1165
G2481	G2481	G2486	G2361	G2256	U2116	U1975	G1868	U1755	A1657	U1508	U1366	C1245	A1166
U2589	G2482	A2486	G2362	G2257	U2117	U1976	G1869	U1756	A1658	U1509	U1367	U1246	G1167
G2482	A2483	C2487	G2363	A2258	U2118	U1977	G1870	U1757	U1659	U1510	U1368	C1247	C1168
C2591	C2487	C2488	G2364	A2259	U2119	U1978	G1871	U1758	U1660	U1511	U1369	C1248	U1169
G2592	C2488	C2489	G2365	A2260	U2120	U1979	G1872	U1759	U1661	U1512	U1370	C1249	U1170
A2599	C2489	C2490	G2366	A2261	U2121	U1980	G1873	U1760	U1662	U1513	U1371	C1250	G1171
A2600	C2490	C2491	G2367	A2262	U2122	U1981	G1874	U1761	U1663	U1514	U1372	C1251	A1172
A2601	C2491	C2492	G2368	A2263	U2123	U1982	G1875	U1762	U1664	U1515	U1373	C1252	U1173
G2602	U2492	C2493	G2369	A2264	U2124	U1983	G1876	U1763	U1665	U1516	U1374	C1253	A1174
U2607	C2493	C2494	G2370	A2265	U2125	U1984	G1877	U1764	U1666	U1517	U1375	C1254	G1175
C2608	C2502	C2503	G2371	A2266	U2126	U1985	G1878	U1765	U1667	U1518	U1376	C1255	A1176
G2613	A2503	A2504	G2372	A2267	U2127	U1986	G1879	U1766	U1668	U1519	U1377	C1256	U1177
A2504	A2504	C2505	U2373	A2268	U2128	U1987	G1880	U1767	U1669	U1520	U1378	C1257	G1178
A2505	C2505	C2506	G2374	A2269	U2129	U1988	G1881	U1768	U1670	U1521	U1379	C1258	A1179
A2506	C2506	C2507	G2375	A2270	U2130	U1989	G1882	U1769	U1671	U1522	U1380	C1259	U1180
C2508	C2507	C2508	G2376	A2271	U2131	U1990	G1883	U1770	U1672	U1523	U1381	C1260	A1181
A2511	C2508	C2509	G2377	A2272	U2132	U1991	G1884	U1771	U1673	U1524	U1382	C1261	G1182
U2512	C2509	C2510	G2378	A2273	U2133	U1992	G1885	U1772	U1674	U1525	U1383	C1262	C1183
C2515	C2510	C2511	G2379	A2274	U2134	U1993	G1886	U1773	U1675	U1526	U1384	C1263	U1184
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G2524	C2513	C2514	G2382	A2277	U2137	U1996	G1889	U1776	U1678	U1529	U1387	C1266	U1187
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U2534	C2519	C2520	G2388	A2283	U2143	U2002	G1895	U1782	U1684	U1535	U1393	C1272	A1193
C2535	C2520	C2521	G2389	A2284	U2144	U2003	G1896	U1783	U1685	U1536	U1394	C1273	U1198
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U2541	C2523	C2524	G2392	A2287	U2147	U2006	G1899	U1786	U1688	U1539	U1397	C1276	C1201
C2542	C2524	C2525	G2393	A2288	U2148	U2007	G1900	U1787	U1689	U1540	U1398	C1277	A1202
C2548	C2525	C2526	G2394	A2289	U2149	U2008	G1901	U1788	U1690	U1541	U1399	C1278	G1203
U2552	C2526	C2527	G2395	A2290	U2150	U2009	G1902	U1789	U1691	U1542	U1400	C1279	C1204
C2553	C2527	C2528	G2396	A2291	U2151	U2010	G1903	U1790	U1692	U1543	U1401	C1280	U1205
U2554	C2528	C2529	G2397	A2292	U2152	U2011	G1904	U1791	U1693	U1544	U1402	C1281	U1206
C2555	C2529	C2530	G2398	A2293	U2153	U2012	G1905	U1792	U1694	U1545	U1403	C1282	A1207
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C2563	C2537	C2538	G2406	A2301	U2161	U2020	G1913	U1800	U1702	U1553	U1411	C1290	G1215
U2564	C2538	C2539	G2407	A2302	U2162	U2021	G1914	U1801	U1703	U1554	U1412	C1291	U1216
C2565	C2539	C2540	G2408	A2303	U2163	U2022	G1915	U1802	U1704	U1555	U1413	C1292	G1217
U2566	C2540	C2541	G2409	A2304	U2164	U2023	G1916	U1803	U1705	U1556	U1414	C1293	U1218
C2567	C2541	C2542	G2410	A2305	U2165	U2024	G1917	U1804	U1706	U1557	U1415	C1294	C1219
U2568	C2542	C2543	G2411	A2306	U2166	U2025	G1918	U1805	U1707	U1558	U1416	C1295	U1220
C2569	C2543	C2544	G2412	A2307	U2167	U2026	G1919	U1806	U1708	U1559	U1417	C1296	G1221
U2570	C2544	C2545	G2413	A2308	U2168	U2027	G1920	U1807	U1709	U1560	U1418	C1297	C1222
C2571	C2545	C2546	G2414	A2309	U2169	U2028	G1921	U1808	U1710	U1561	U1419	C1298	U1223
U2572	C2546	C2547	G2415	A2310	U2170	U2029	G1922	U1809	U1711	U1562	U1420	C1299	G1224
C2573	C2547	C2548	G2416	A2311	U2171	U2030	G1923	U1810	U1712	U1563	U1421	C1300	U1225
U2574	C2548	C2549	G2417	A2312	U2172	U2031	G1924	U1811	U1713	U1564	U1422	C1301	C1226
C2575	C2549	C2550	G2418	A2313	U2173	U2032	G1925	U1812	U1714	U1565	U1423	C1302	G1227
U2576	C2550	C2551	G2419	A2314	U2174	U2033	G1926	U1813	U1715	U1566	U1424	C1303	U1228
C2577	C2551	C2552	G2420	A2315	U2175	U2034	G1927	U1814	U1716	U1567	U1425	C1304	C1229
U2578	C2552	C2553	G2421	A2316	U2176	U2035	G1928	U1815	U1717	U1568	U1426	C1305	U1230
C2579	C2553	C2554	G2422	A2317	U2177	U2036	G1929	U1816	U1718	U1569	U1427	C1306	G1231
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C2581	C2555	C2556	G2424	A2319	U2179	U2038	G1931	U1818	U1720	U1571	U1429	C1308	C1233
U2582	C2556	C2557	G2425	A2320	U2180	U2039	G1932	U1819	U1721	U1572	U1430	C1309	U1234
C2583	C2557	C2558	G2426	A2321	U2181	U2040	G1933	U1820	U1722	U1573	U1431	C1310	G1235
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C2585	C2559	C2560	G2428	A2323	U2183	U2042	G1935	U1822	U1724	U1575	U1433	C1312	G1237
U2586	C2560	C2561	G2429	A2324	U2184	U2043	G1936	U1823	U1725	U1576	U1434	C1313	U1238
C2587	C2561	C2562	G2430	A2325	U2185	U2044	G1937	U1824	U1726	U1577	U1435	C1314	C1239
U2588	C2562	C2563	G2431	A2326	U2186	U2045	G1938	U1825	U1727	U1578	U1436	C1315	U1240
C2589	C2563	C2564	G2432	A2327	U2187	U2046	G1939	U1826	U1728	U1579	U1437	C1316	G1241
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C2591	C2565	C2566	G2434	A2329	U2189	U2048	G1941	U1828	U1730	U1581	U1439	C1318	C1243
U2592	C2566	C2567	G2435	A2330	U2190	U2049	G1942	U1829	U1731	U1582	U1440	C1319	U1244
A2599	C2567	C2568	G2436	A2331	U2191	U2050	G1943	U1830	U1732	U1583	U1441	C1320	G1245
C2599	C2568	C2569	G2437	A2332	U2192	U2051	G1944	U1831	U1733	U1584	U1442	C1321	U1246
A2600	C2569	C2570	G2438	A2333	U2193	U2052	G1945	U1832	U1734	U1585	U1443	C1322	G1247
A2601	C2570	C2571	G2439	A2334	U2194	U2053	G1946	U183					



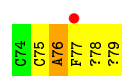
- Molecule 2: 5S ribosomal RNA



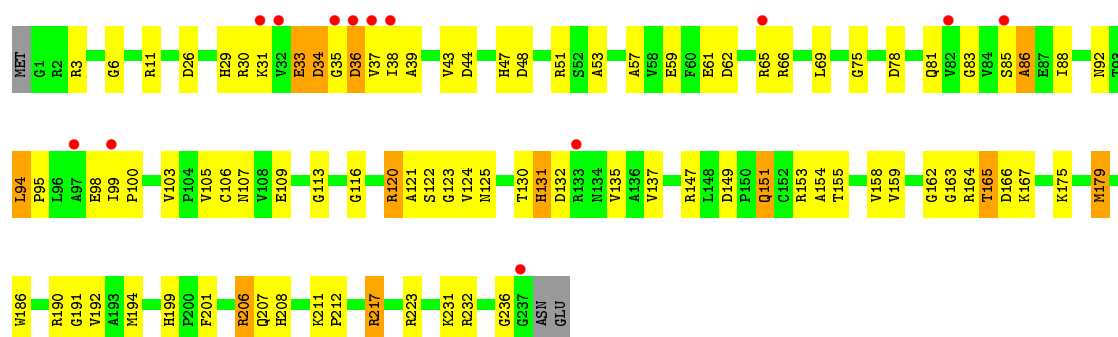
- Molecule 3: 5'-R(*CP*CP*(PPU)*(LOF))-3'



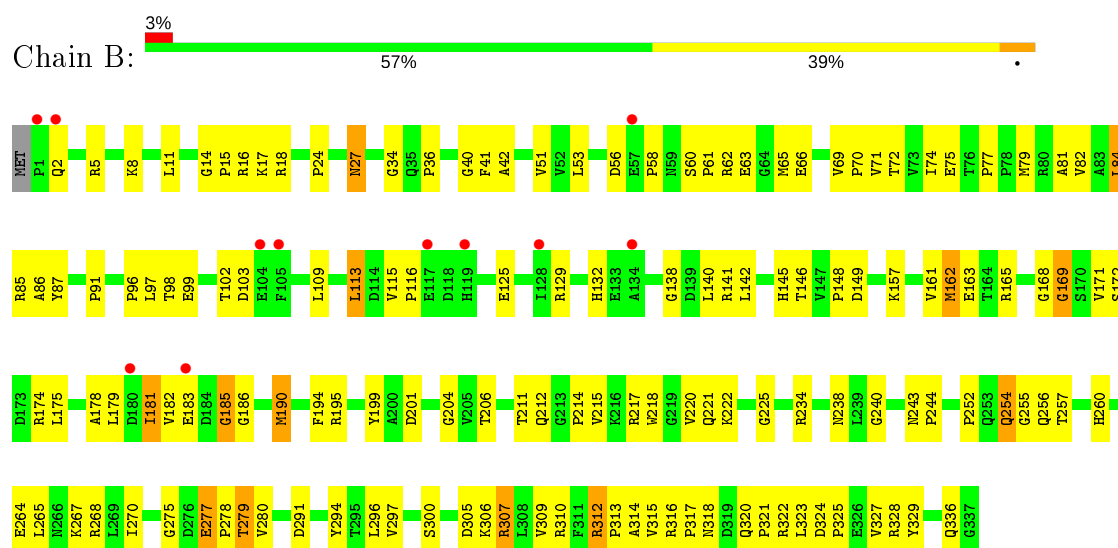
- Molecule 4: 5'-R(*CP*CP*AP*(PHE)*(ACA)*(BTN))-3'



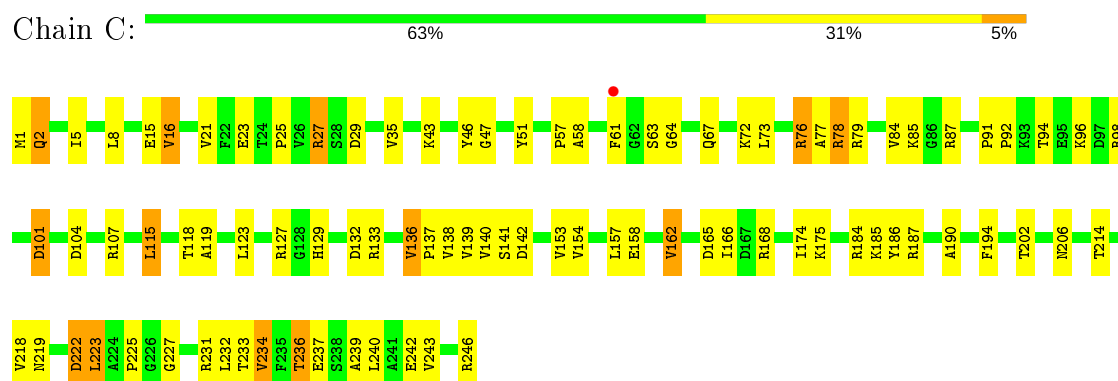
- Molecule 5: 50S ribosomal protein L2P



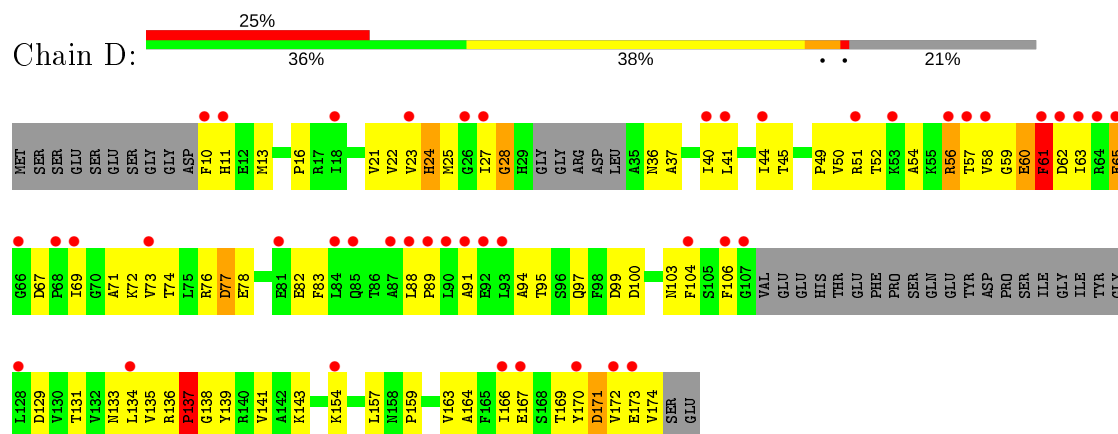
- Molecule 6: 50S ribosomal protein L3P



• Molecule 7: 50S ribosomal protein L4E

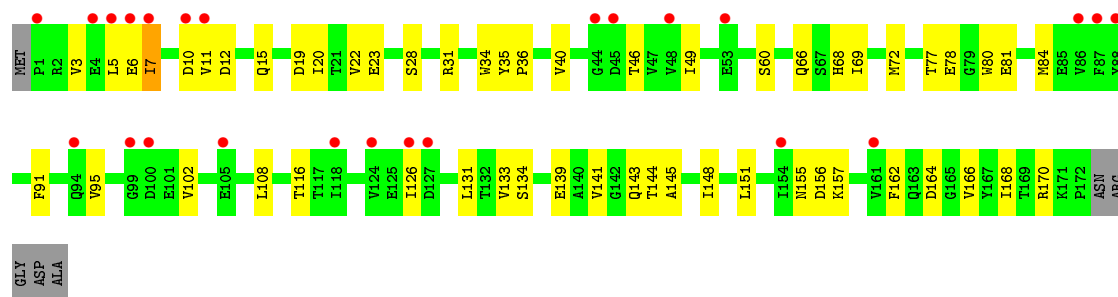


• Molecule 8: 50S ribosomal protein L5P

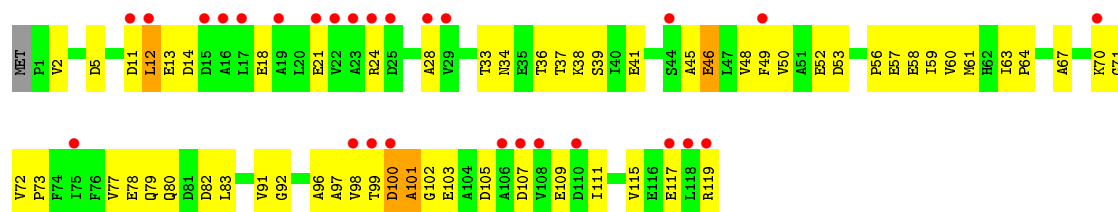


• Molecule 9: 50S ribosomal protein L6P

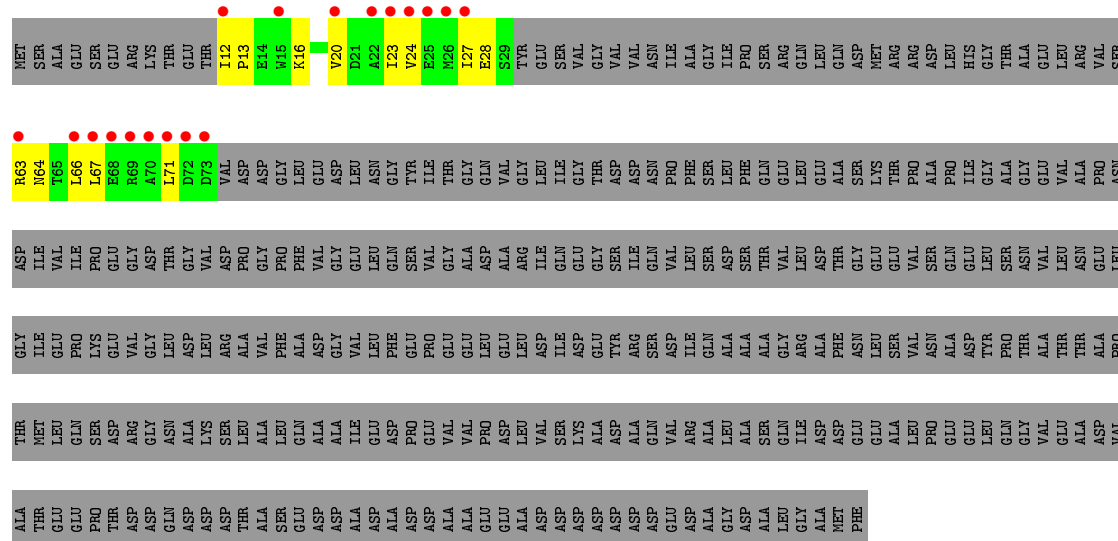




- Molecule 10: 50S ribosomal protein L7AE

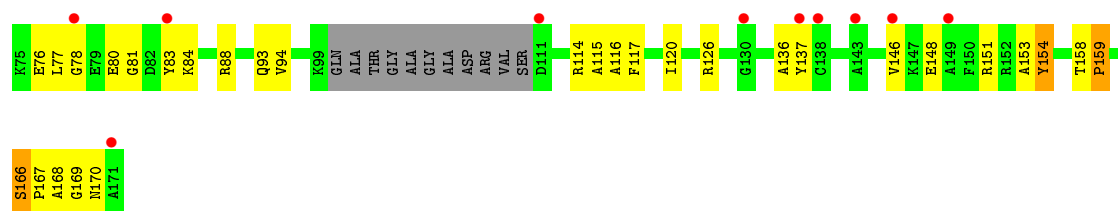


- Molecule 11: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

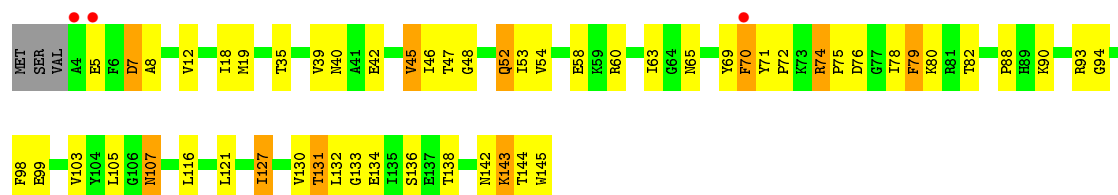


- Molecule 12: 50S RIBOSOMAL PROTEIN L10E

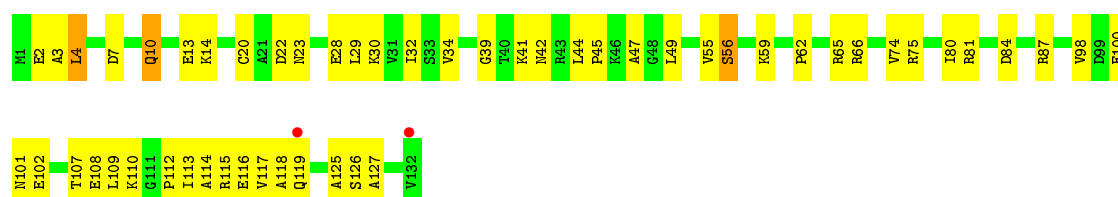




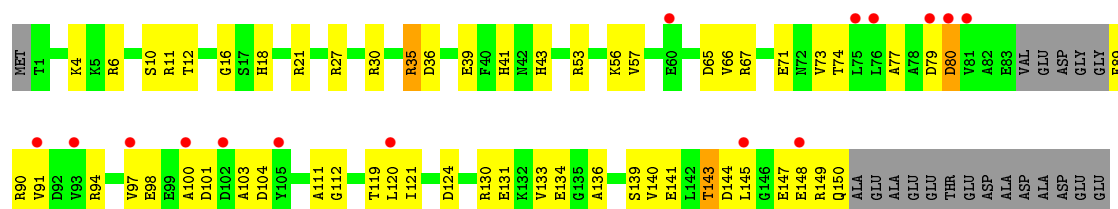
• Molecule 13: 50S ribosomal protein L13P



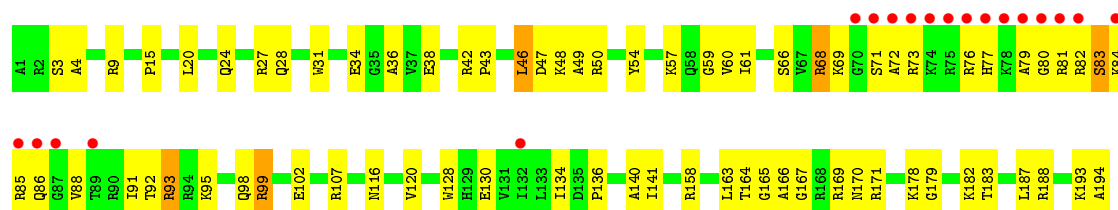
• Molecule 14: 50S ribosomal protein L14P



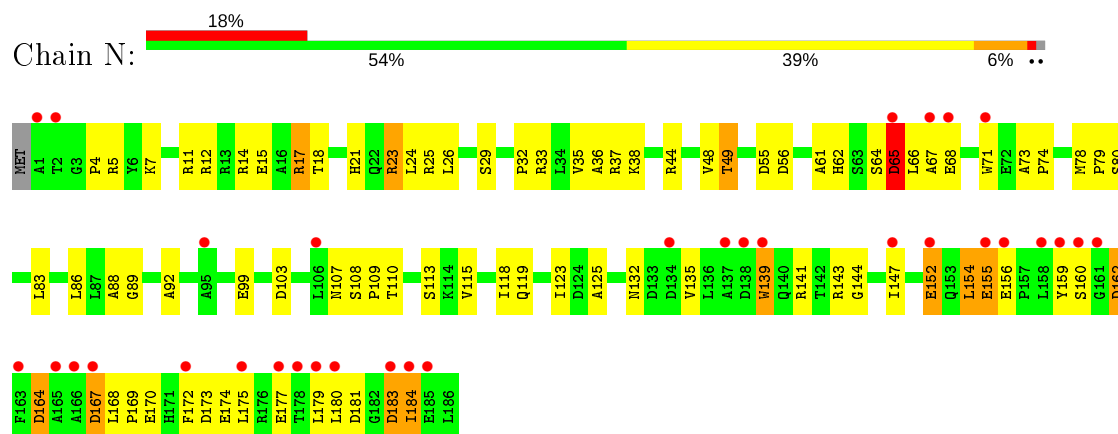
• Molecule 15: 50S ribosomal protein L15P



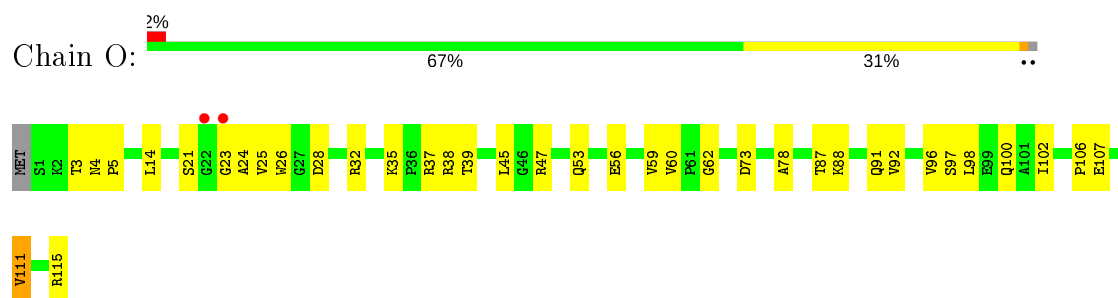
• Molecule 16: 50S Ribosomal Protein L15E



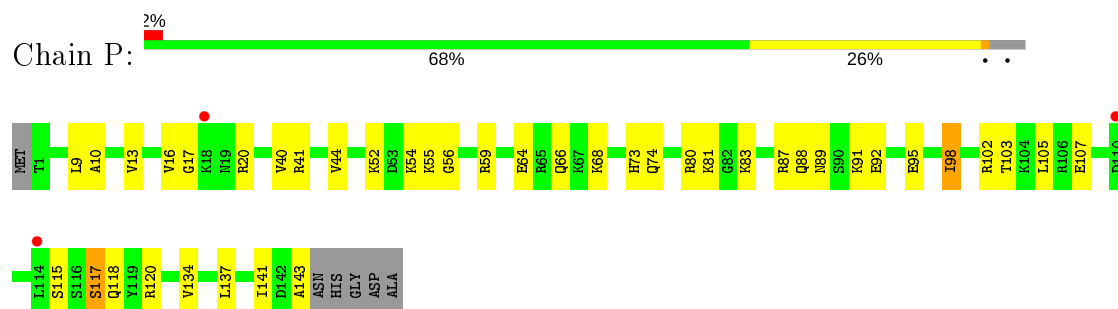
- Molecule 17: 50S ribosomal protein L18P



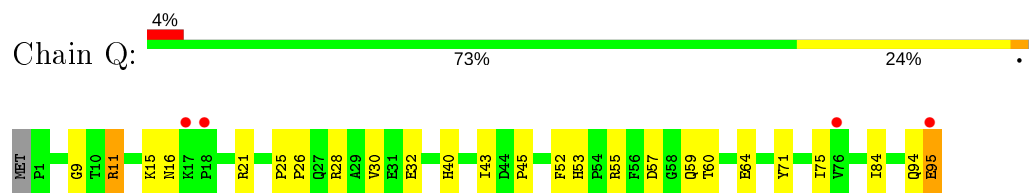
- Molecule 18: 50S ribosomal protein L18e



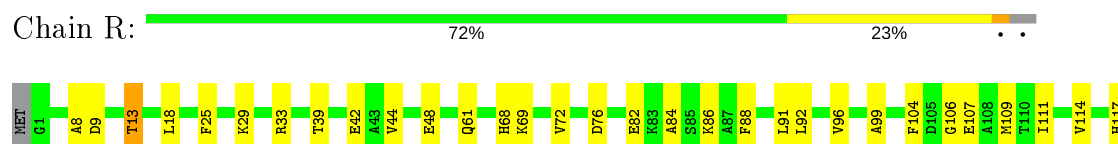
- Molecule 19: 50S ribosomal protein L19E



- Molecule 20: 50S ribosomal protein L21e

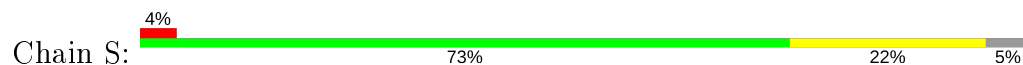


- Molecule 21: 50S ribosomal protein L22P

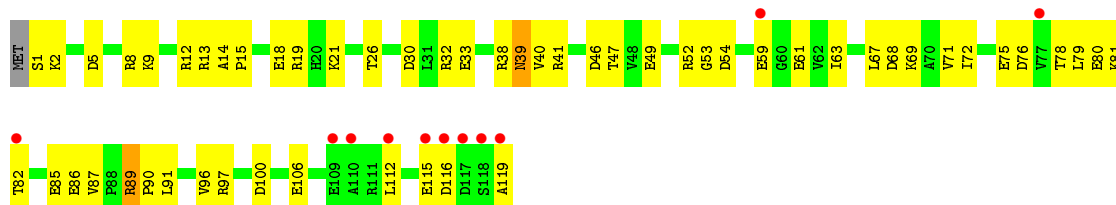




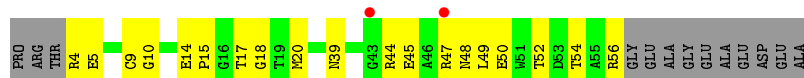
- Molecule 22: 50S ribosomal protein L23P



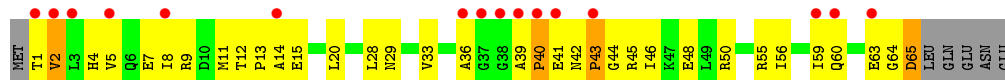
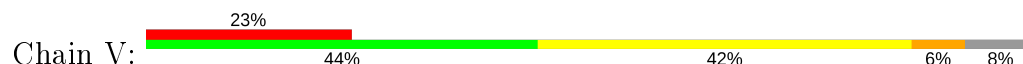
- Molecule 23: 50S ribosomal protein L24P



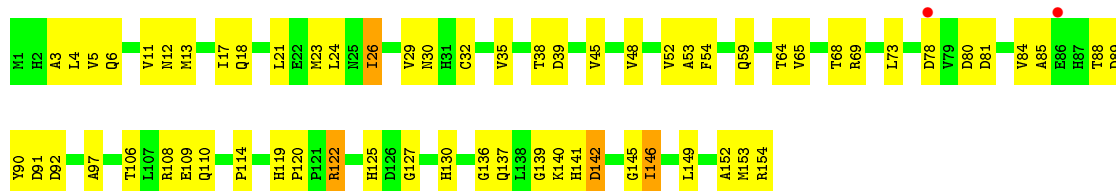
- Molecule 24: 50S ribosomal protein L24E



- Molecule 25: 50S ribosomal protein L29P

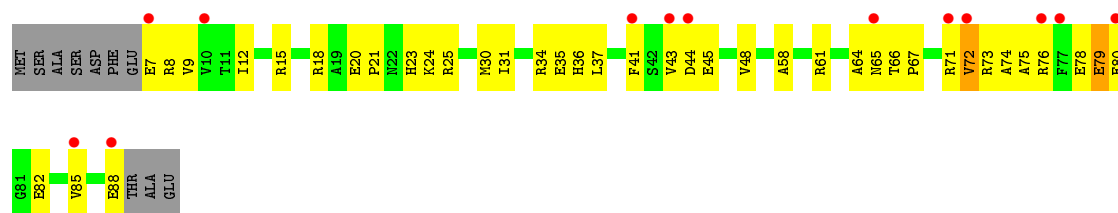


- Molecule 26: 50S ribosomal protein L30P

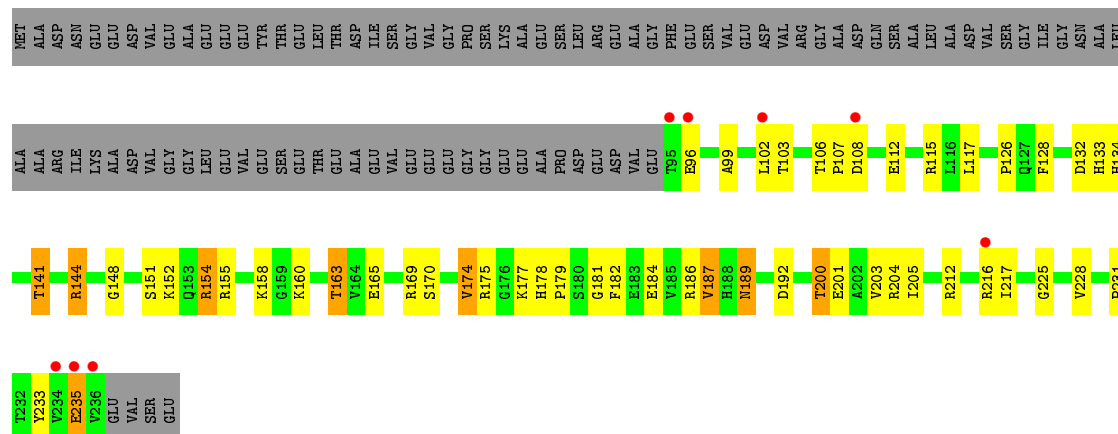
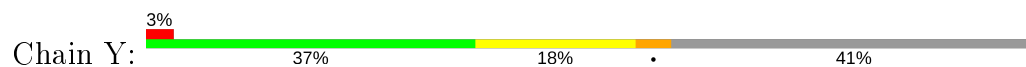


- Molecule 27: 50S ribosomal protein L31e

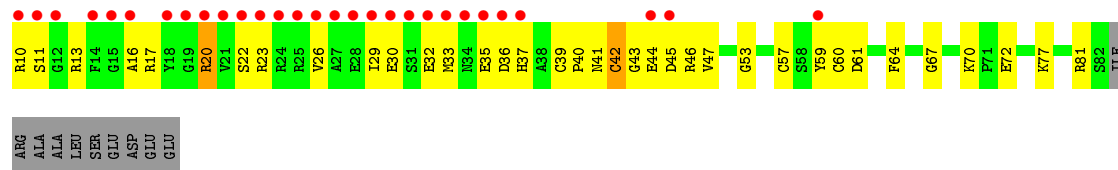
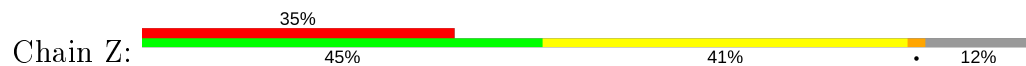




- Molecule 28: 50S ribosomal protein L32E



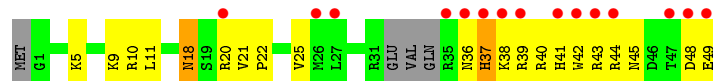
- Molecule 29: 50S ribosomal protein L37Ae



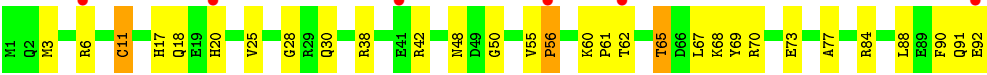
- Molecule 30: 50S ribosomal protein L37e



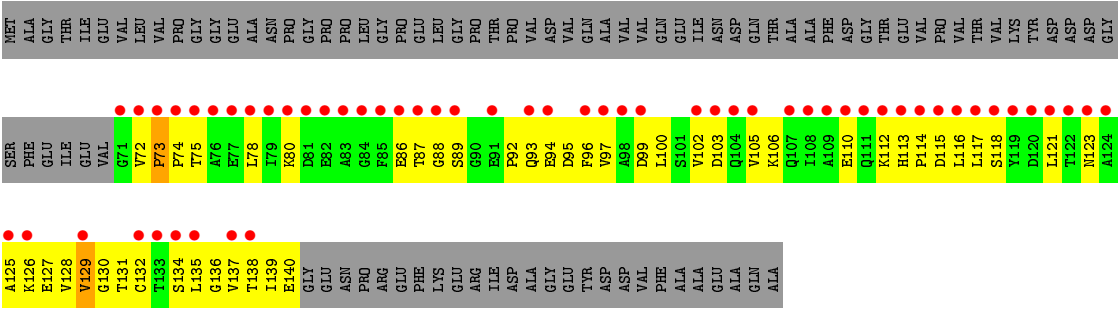
- Molecule 31: 50S ribosomal protein L39e



- Molecule 32: 50S ribosomal protein L44E



● Molecule 33: 50S RIBOSOMAL PROTEIN L11P



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.72Å 298.78Å 575.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 49.32 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.40) 89.2 (49.32-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.74 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.248 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99077	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% 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: ACA, OMG, PPU, CL, SR, NA, K, MG, CD, HFA, OMU, UR3, 1MA, BTN, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.38	0/65959	0.70	25/102870 (0.0%)
2	9	0.33	0/2905	0.70	1/4528 (0.0%)
3	4	0.47	0/40	0.68	0/60
4	5	0.51	0/76	0.79	0/112
5	A	0.33	0/1786	0.65	0/2408
6	B	0.34	0/2690	0.65	0/3652
7	C	0.38	0/1884	0.65	0/2551
8	D	0.29	0/1111	0.54	0/1498
9	E	0.32	0/1382	0.58	0/1880
10	F	0.33	0/901	0.54	0/1224
11	G	0.28	0/241	0.48	0/324
12	H	0.34	0/1287	0.64	0/1725
13	J	0.35	0/1136	0.62	0/1530
14	K	0.36	0/1001	0.68	0/1347
15	L	0.32	0/1130	0.64	0/1509
16	M	0.34	0/1584	0.59	0/2119
17	N	0.29	0/1474	0.61	0/1999
18	O	0.32	0/874	0.58	0/1181
19	P	0.35	0/1147	0.55	0/1528
20	Q	0.34	0/749	0.69	0/1005
21	R	0.37	0/1172	0.67	0/1578
22	S	0.32	0/648	0.56	0/875
23	T	0.31	0/958	0.63	0/1289
24	U	0.35	0/417	0.58	0/562
25	V	0.27	0/502	0.52	0/675
26	W	0.35	0/1219	0.60	0/1655
27	X	0.34	0/664	0.61	0/895
28	Y	0.37	0/1146	0.66	0/1536
29	Z	0.32	0/589	0.57	0/787
30	1	0.43	0/438	0.63	0/578
31	2	0.32	0/401	0.57	0/529
32	3	0.35	0/771	0.57	0/1024

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	I	0.29	0/526	0.51	0/716
All	All	0.37	0/98808	0.67	26/147749 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	55
2	9	0	1
All	All	0	56

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	871	G	C5'-C4'-O4'	-7.44	100.17	109.10
1	0	1942	A	C5'-C4'-C3'	7.11	127.37	116.00
1	0	1592	G	N9-C1'-C2'	6.67	122.67	114.00
1	0	1819	G	C5'-C4'-C3'	6.40	126.24	116.00
1	0	883	U	N1-C1'-C2'	6.20	122.06	114.00
1	0	2726	U	N1-C1'-C2'	6.13	121.97	114.00
1	0	1504	A	C1'-O4'-C4'	-6.08	105.03	109.90
1	0	777	U	O4'-C1'-N1	5.98	112.98	108.20
2	9	3039	U	N1-C1'-C2'	5.95	121.73	114.00
1	0	1120	U	C5'-C4'-C3'	-5.79	106.73	116.00
1	0	2467	A	C1'-O4'-C4'	-5.79	105.27	109.90
1	0	2541	U	C2'-C3'-O3'	5.76	122.91	113.70
1	0	1819	G	C1'-O4'-C4'	-5.69	105.35	109.90
1	0	1504	A	N9-C1'-C2'	5.65	121.34	114.00
1	0	1979	G	C2'-C3'-O3'	5.55	122.58	113.70
1	0	2291	A	N9-C1'-C2'	5.45	121.09	114.00
1	0	206	G	C5'-C4'-C3'	-5.26	107.58	116.00
1	0	2313	C	C5'-C4'-O4'	5.26	115.42	109.10
1	0	841	A	C1'-O4'-C4'	-5.24	105.70	109.90
1	0	1615	A	C5'-C4'-C3'	5.20	124.33	116.00
1	0	2301	A	N9-C1'-C2'	5.12	120.66	114.00
1	0	1352	A	OP1-P-O3'	5.07	116.36	105.20
1	0	921	G	N9-C1'-C2'	5.05	120.57	114.00
1	0	1261	A	N9-C1'-C2'	5.05	120.57	114.00
1	0	457	U	C1'-O4'-C4'	-5.04	105.86	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	389	G	C5'-C4'-C3'	-5.00	108.00	116.00

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1039	G	Sidechain
1	0	1078	A	Sidechain
1	0	1080	C	Sidechain
1	0	1132	A	Sidechain
1	0	1340	G	Sidechain
1	0	1458	A	Sidechain
1	0	1491	G	Sidechain
1	0	1592	G	Sidechain
1	0	1718	G	Sidechain
1	0	1744	G	Sidechain
1	0	1777	G	Sidechain
1	0	1819	G	Sidechain
1	0	1829	A	Sidechain
1	0	1845	A	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1885	A	Sidechain
1	0	191	A	Sidechain
1	0	1970	G	Sidechain
1	0	2115	U	Sidechain
1	0	22	U	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2552	C	Sidechain
1	0	2599	A	Sidechain
1	0	2607	U	Sidechain
1	0	2620	U	Sidechain
1	0	2630	G	Sidechain
1	0	2632	G	Sidechain
1	0	2645	U	Sidechain
1	0	2681	A	Sidechain
1	0	270	U	Sidechain

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Mol	Chain	Res	Type	Group
1	0	2726	U	Sidechain
1	0	2842	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	458	G	Sidechain
1	0	469	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	507	A	Sidechain
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	722	G	Sidechain
1	0	771	G	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	868	G	Sidechain
1	0	888	U	Sidechain
1	0	952	G	Sidechain
2	9	3039	U	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29812	769	0
2	9	2600	0	1326	58	0
3	4	72	0	47	1	0
4	5	93	0	68	4	0
5	A	1753	0	1765	111	0
6	B	2625	0	2532	151	0
7	C	1859	0	1816	97	0
8	D	1094	0	1085	92	0
9	E	1357	0	1266	50	0
10	F	890	0	843	55	0
11	G	240	0	231	12	0
12	H	1266	0	1268	63	0
13	J	1120	0	1098	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	K	992	0	1031	58	0
15	L	1118	0	1076	61	0
16	M	1560	0	1568	75	0
17	N	1445	0	1401	87	0
18	O	865	0	873	42	0
19	P	1136	0	1123	42	0
20	Q	735	0	728	22	0
21	R	1149	0	1122	39	0
22	S	641	0	605	17	0
23	T	950	0	923	52	0
24	U	410	0	364	22	0
25	V	499	0	511	43	0
26	W	1196	0	1137	83	0
27	X	654	0	653	41	0
28	Y	1130	0	1133	60	0
29	Z	578	0	539	39	0
30	1	431	0	426	29	0
31	2	396	0	413	30	0
32	3	755	0	728	30	0
33	I	519	0	500	60	0
34	0	87	0	0	0	0
34	2	1	0	0	0	0
34	5	1	0	0	0	0
34	9	1	0	0	0	0
34	A	1	0	0	0	0
34	K	1	0	0	0	0
34	T	1	0	0	0	0
34	Y	1	0	0	0	0
35	0	2	0	0	0	0
36	0	66	0	0	0	0
36	9	1	0	0	0	0
36	C	1	0	0	0	0
36	D	1	0	0	0	0
36	J	1	0	0	0	0
36	M	1	0	0	0	0
36	Q	1	0	0	0	0
36	R	2	0	0	0	0
36	S	1	0	0	0	0
37	0	10	0	0	0	0
37	3	1	0	0	0	0
37	A	1	0	0	0	0
37	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	J	3	0	0	1	0
37	L	1	0	0	0	0
37	M	1	0	0	0	0
37	N	1	0	0	0	0
37	O	1	0	0	0	0
37	R	1	0	0	0	0
37	Y	1	0	0	0	0
38	0	98	0	0	0	0
38	1	2	0	0	0	0
38	3	1	0	0	0	0
38	9	3	0	0	0	0
38	A	3	0	0	0	0
38	B	2	0	0	0	0
38	F	1	0	0	0	0
38	H	1	0	0	0	0
38	L	1	0	0	0	0
38	R	1	0	0	0	0
38	S	1	0	0	0	0
39	1	1	0	0	0	0
39	3	1	0	0	0	0
39	O	1	0	0	0	0
39	U	1	0	0	0	0
39	Z	1	0	0	0	0
40	0	5727	0	0	102	0
40	1	59	0	0	3	0
40	2	40	0	0	1	0
40	3	71	0	0	5	0
40	4	1	0	0	0	0
40	5	2	0	0	0	0
40	9	137	0	0	5	0
40	A	120	0	0	8	0
40	B	138	0	0	18	0
40	C	180	0	0	19	0
40	D	48	0	0	11	0
40	E	44	0	0	4	0
40	F	24	0	0	2	0
40	G	14	0	0	0	0
40	H	72	0	0	6	0
40	I	10	0	0	2	0
40	J	54	0	0	3	0
40	K	61	0	0	4	0
40	L	83	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	M	128	0	0	3	0
40	N	58	0	0	4	0
40	O	39	0	0	3	0
40	P	61	0	0	2	0
40	Q	51	0	0	5	0
40	R	78	0	0	4	0
40	S	31	0	0	1	0
40	T	35	0	0	4	0
40	U	28	0	0	3	0
40	V	12	0	0	2	0
40	W	62	0	0	6	0
40	X	21	0	0	5	0
40	Y	93	0	0	10	0
40	Z	34	0	0	2	0
All	All	99077	0	60011	2220	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 15.

All (2220) 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)
26:W:21:LEU:HD21	26:W:48:VAL:HG11	1.35	1.08
14:K:29:LEU:HB3	14:K:55:VAL:HG11	1.33	1.07
1:O:1160:G:H5'	1:O:1161:A:H5'	1.36	1.07
27:X:37:LEU:HD13	27:X:85:VAL:HG21	1.39	1.04
2:9:3076:G:H3'	2:9:3077:A:H5''	1.36	1.04
23:T:9:LYS:HE3	23:T:13:ARG:NH1	1.73	1.04
13:J:93:ARG:HH11	13:J:93:ARG:HB3	1.21	1.02
25:V:12:THR:HG22	25:V:15:GLU:HG3	1.38	1.02
8:D:25:MET:HE2	8:D:41:LEU:HG	1.41	1.00
6:B:162:MET:HE2	6:B:310:ARG:HD3	1.44	0.99
1:O:871:G:C8	1:O:871:G:H5'	1.96	0.99
22:S:51:GLN:HE21	22:S:53:ASN:HD21	1.05	0.99
9:E:20:ILE:HD11	9:E:40:VAL:HG11	1.46	0.98
7:C:236:THR:HG22	7:C:239:ALA:H	1.24	0.98
1:O:156:C:H5''	16:M:171:ARG:HD3	1.46	0.97
5:A:211:LYS:HG2	5:A:212:PRO:HD2	1.45	0.96
7:C:127:ARG:NH2	7:C:225:PRO:HG2	1.80	0.96
10:F:91:VAL:HG12	10:F:92:GLY:H	1.26	0.96
23:T:71:VAL:HG11	23:T:90:PRO:HB3	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:78:ARG:HG3	7:C:78:ARG:HH11	1.30	0.96
1:0:1771:U:H5'	29:Z:20:ARG:HH21	1.31	0.95
1:0:871:G:H8	1:0:871:G:H5'	1.28	0.95
1:0:870:G:H2'	1:0:871:G:H5''	1.48	0.95
1:0:542:A:H5'	1:0:542:A:H8	1.34	0.93
14:K:10:GLN:H	14:K:10:GLN:HE21	0.93	0.92
1:0:1242:A:H5'	13:J:82:THR:HG23	1.50	0.92
17:N:11:ARG:HG3	17:N:14:ARG:HH12	1.34	0.92
14:K:10:GLN:H	14:K:10:GLN:NE2	1.66	0.91
8:D:28:GLY:HA2	8:D:69:ILE:HG23	1.52	0.91
1:0:1372:A:H3'	40:0:7638:HOH:O	1.70	0.91
5:A:192:VAL:HG12	5:A:207:GLN:HB3	1.53	0.91
5:A:81:GLN:HB2	5:A:92:ASN:ND2	1.86	0.90
26:W:6:GLN:HB2	26:W:26:ILE:HD12	1.53	0.90
1:0:2812:A:H2	1:0:2814:A:H62	1.19	0.90
17:N:144:GLY:O	17:N:147:ILE:HG22	1.70	0.90
28:Y:235:GLU:H	28:Y:235:GLU:CD	1.75	0.90
6:B:238:ASN:HD22	6:B:240:GLY:H	1.18	0.90
31:2:18:ASN:HD21	31:2:40:ARG:H	1.17	0.89
14:K:74:VAL:HG13	14:K:113:ILE:HG23	1.54	0.89
6:B:307:ARG:HH11	6:B:307:ARG:HG3	1.36	0.89
12:H:29:ALA:HB3	12:H:66:ARG:HH12	1.37	0.89
7:C:1:MET:HG2	7:C:2:GLN:H	1.38	0.89
6:B:36:PRO:HA	6:B:168:GLY:HA3	1.55	0.89
8:D:58:VAL:HB	8:D:62:ASP:HB3	1.54	0.89
18:O:32:ARG:HE	18:O:35:LYS:HD2	1.36	0.88
14:K:81:ARG:HB2	14:K:87:ARG:HH11	1.37	0.88
1:0:2717:C:H2'	1:0:2718:C:H5''	1.53	0.88
14:K:74:VAL:HG11	14:K:113:ILE:HG12	1.54	0.88
1:0:289:G:H22	1:0:363:A:H2	1.21	0.87
16:M:102:GLU:OE1	16:M:164:THR:HG21	1.73	0.87
19:P:115:SER:H	19:P:118:GLN:HE21	1.20	0.87
21:R:25:PHE:CE2	21:R:29:LYS:HE2	2.09	0.87
1:0:541:C:H2'	1:0:542:A:H5''	1.57	0.86
17:N:49:THR:HG22	17:N:56:ASP:HB2	1.55	0.86
29:Z:11:SER:HB3	29:Z:23:ARG:HB2	1.55	0.86
17:N:113:SER:HB2	40:N:9354:HOH:O	1.75	0.86
17:N:83:LEU:HD13	17:N:175:LEU:HD23	1.56	0.85
7:C:5:ILE:HD11	7:C:16:VAL:HG22	1.57	0.85
5:A:192:VAL:CG1	5:A:207:GLN:HB3	2.07	0.85
1:0:1835:U:H5	1:0:1840:A:N7	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3056:A:H2'	2:9:3057:A:H5''	1.57	0.85
26:W:137:GLN:HE21	26:W:141:HIS:HE1	1.25	0.85
9:E:15:GLN:HG2	9:E:19:ASP:O	1.77	0.85
8:D:172:VAL:HG12	8:D:173:GLU:H	1.40	0.85
29:Z:37:HIS:HB2	29:Z:47:VAL:HB	1.59	0.84
16:M:99:ARG:HH21	16:M:170:ASN:HD22	1.25	0.84
21:R:8:ALA:HB1	21:R:13:THR:HG21	1.58	0.84
28:Y:200:THR:HG22	28:Y:201:GLU:HG3	1.58	0.84
14:K:10:GLN:N	14:K:10:GLN:HE21	1.74	0.84
15:L:80:ASP:HB2	15:L:90:ARG:O	1.78	0.83
2:9:3006:C:H5''	17:N:37:ARG:NH1	1.94	0.83
1:0:1116:U:HO2'	1:0:1118:A:H2	0.85	0.83
19:P:115:SER:OG	19:P:118:GLN:HG3	1.78	0.83
1:0:2506:A:O2'	1:0:2507:G:H8	1.62	0.83
5:A:192:VAL:HG22	40:A:9617:HOH:O	1.78	0.83
26:W:122:ARG:HH11	26:W:122:ARG:HG2	1.43	0.83
1:0:2717:C:C2'	1:0:2718:C:H5''	2.08	0.83
1:0:1474:C:H6	1:0:1474:C:H5'	1.43	0.82
1:0:2506:A:HO2'	1:0:2507:G:H8	0.87	0.82
1:0:2840:A:OP1	6:B:211:THR:HG23	1.77	0.82
29:Z:36:ASP:HB3	29:Z:45:ASP:HB3	1.62	0.82
12:H:56:GLN:HE22	12:H:93:GLN:HG2	1.45	0.82
14:K:39:GLY:HA2	40:K:4183:HOH:O	1.80	0.82
6:B:162:MET:CE	6:B:310:ARG:HD3	2.10	0.82
2:9:3006:C:H5''	17:N:37:ARG:HH12	1.45	0.81
21:R:99:ALA:HB1	21:R:109:MET:HE1	1.61	0.81
1:0:871:G:H8	1:0:871:G:C5'	1.94	0.81
16:M:134:ILE:HG23	16:M:141:ILE:HD13	1.63	0.81
31:2:41:HIS:H	31:2:45:ASN:HD22	1.26	0.81
1:0:288:A:H61	1:0:364:C:H42	1.29	0.80
5:A:191:GLY:HA2	5:A:194:MET:CE	2.11	0.80
8:D:134:LEU:HD11	8:D:166:ILE:HD11	1.63	0.80
14:K:107:THR:HG22	14:K:108:GLU:HG3	1.64	0.80
1:0:2851:G:C2'	1:0:2852:A:H5'	2.12	0.80
8:D:136:ARG:HH12	8:D:157:LEU:HA	1.46	0.79
6:B:179:LEU:O	6:B:183:GLU:HG2	1.81	0.79
26:W:6:GLN:HB2	26:W:26:ILE:CD1	2.13	0.79
26:W:88:THR:HB	40:W:6679:HOH:O	1.82	0.79
1:0:1160:G:C5'	1:0:1161:A:H5'	2.13	0.79
1:0:2716:G:H5''	6:B:206:THR:HG21	1.65	0.79
14:K:4:LEU:HD22	14:K:116:GLU:HB3	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:12:ILE:N	11:G:13:PRO:HD3	1.97	0.79
27:X:72:VAL:HG22	27:X:85:VAL:HG12	1.64	0.79
1:0:1603:A:H5'	1:0:1605:G:O4'	1.83	0.79
1:0:1119:G:H2'	13:J:52:GLN:NE2	1.98	0.79
14:K:98:VAL:HG13	14:K:102:GLU:HA	1.63	0.79
9:E:81:GLU:HG2	9:E:134:SER:HB3	1.64	0.79
17:N:11:ARG:HA	17:N:14:ARG:NH1	1.97	0.79
26:W:4:LEU:HD22	26:W:52:VAL:HG21	1.63	0.79
1:0:2534:C:H1'	40:0:4081:HOH:O	1.80	0.78
21:R:99:ALA:HB1	21:R:109:MET:CE	2.12	0.78
1:0:541:C:C2'	1:0:542:A:H5''	2.11	0.78
33:I:102:VAL:HG12	33:I:106:LYS:HE3	1.62	0.78
16:M:107:ARG:HH11	16:M:107:ARG:HG3	1.47	0.78
1:0:969:G:H1	1:0:999:C:H42	1.32	0.78
26:W:88:THR:HG23	26:W:110:GLN:NE2	1.99	0.78
1:0:2054:A:N3	21:R:128:ARG:NH2	2.31	0.78
1:0:1973:A:H5'	1:0:1973:A:H8	1.49	0.77
31:2:22:PRO:HG2	31:2:25:VAL:HG23	1.67	0.77
17:N:12:ARG:HD3	17:N:18:THR:OG1	1.85	0.77
1:0:2073:G:H5''	40:0:4400:HOH:O	1.83	0.77
12:H:27:LYS:H	12:H:59:HIS:HD2	1.30	0.77
1:0:1118:A:H3'	1:0:1118:A:H8	1.50	0.77
6:B:212:GLN:HB2	6:B:257:THR:HG21	1.66	0.77
5:A:199:HIS:HD2	5:A:201:PHE:H	1.32	0.76
21:R:18:LEU:HD12	21:R:143:VAL:HG11	1.68	0.76
13:J:93:ARG:NH1	13:J:93:ARG:HB3	1.99	0.76
10:F:91:VAL:HG12	10:F:92:GLY:N	2.01	0.76
40:0:5371:HOH:O	13:J:47:THR:HB	1.83	0.76
26:W:122:ARG:HH11	26:W:122:ARG:CG	1.97	0.76
26:W:125:HIS:HD2	26:W:127:GLY:H	1.30	0.76
1:0:559:U:H5'	1:0:559:U:H6	1.50	0.76
14:K:98:VAL:CG1	14:K:102:GLU:HA	2.15	0.76
1:0:560:C:H42	1:0:597:A:H61	1.33	0.76
17:N:11:ARG:HG3	17:N:14:ARG:NH1	2.01	0.76
1:0:1041:U:H5'	40:L:9491:HOH:O	1.85	0.76
8:D:57:THR:HG23	8:D:63:ILE:HA	1.67	0.76
16:M:79:ALA:HB3	16:M:81:ARG:NH1	2.00	0.76
1:0:1667:A:H8	1:0:1667:A:H5'	1.51	0.75
1:0:960:G:H4'	40:0:7866:HOH:O	1.84	0.75
2:9:3014:G:H8	2:9:3014:G:H5'	1.50	0.75
21:R:111:ILE:HG23	21:R:145:LEU:HD11	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:104:ASP:HA	7:C:107:ARG:HH12	1.50	0.75
13:J:93:ARG:HH11	13:J:93:ARG:CB	2.00	0.75
1:O:1119:G:N2	1:O:1246:A:C2	2.53	0.75
1:O:2533:C:H5'	1:O:2533:C:H6	1.51	0.75
6:B:195:ARG:HG2	6:B:323:LEU:HD22	1.68	0.75
1:O:506:G:H22	1:O:509:A:C5'	2.00	0.75
9:E:15:GLN:HG3	9:E:20:ILE:HG12	1.68	0.75
5:A:153:ARG:HH11	5:A:153:ARG:HB2	1.50	0.75
13:J:19:MET:HE1	13:J:132:LEU:HD21	1.69	0.75
25:V:39:ALA:N	25:V:40:PRO:HD2	2.02	0.75
26:W:13:MET:HE1	26:W:18:GLN:HA	1.67	0.75
1:O:1116:U:O2'	1:O:1118:A:H2	1.67	0.74
8:D:25:MET:HE1	8:D:37:ALA:HB1	1.67	0.74
13:J:19:MET:HE3	13:J:132:LEU:HD11	1.68	0.74
14:K:14:LYS:HB2	14:K:45:PRO:HG2	1.70	0.74
32:3:70:ARG:HG2	32:3:77:ALA:HB2	1.69	0.74
5:A:206:ARG:HD3	5:A:206:ARG:H	1.51	0.74
9:E:3:VAL:HG22	9:E:49:ILE:HB	1.69	0.74
1:O:1244:U:OP1	13:J:18:ILE:HD13	1.87	0.74
6:B:51:VAL:CG2	6:B:327:VAL:HG13	2.18	0.74
1:O:1118:A:C8	1:O:1118:A:H3'	2.22	0.74
29:Z:46:ARG:HD2	29:Z:59:TYR:HB2	1.68	0.74
1:O:281:U:H2'	1:O:282:C:O4'	1.86	0.74
9:E:84:MET:HE1	9:E:148:ILE:HD12	1.69	0.74
5:A:35:GLY:O	5:A:36:ASP:HB3	1.88	0.74
33:I:78:LEU:HD12	33:I:112:LYS:HZ2	1.53	0.74
17:N:80:SER:HB2	40:N:9333:HOH:O	1.85	0.74
8:D:54:ALA:HB2	8:D:69:ILE:HD12	1.70	0.74
21:R:39:THR:HB	21:R:42:GLU:HG3	1.69	0.74
1:O:1377:C:H6	1:O:1377:C:H5'	1.52	0.73
28:Y:154:ARG:HH12	28:Y:155:ARG:HG3	1.53	0.73
1:O:1751:G:H2'	1:O:1752:G:H5''	1.70	0.73
9:E:36:PRO:HD3	13:J:127:ILE:HD12	1.68	0.73
13:J:74:ARG:HB3	13:J:74:ARG:HH11	1.51	0.73
15:L:143:THR:HG22	15:L:144:ASP:H	1.52	0.73
26:W:88:THR:HG22	26:W:89:ASP:N	2.03	0.73
1:O:1206:U:H6	1:O:1206:U:H5'	1.52	0.73
33:I:99:ASP:OD1	33:I:138:THR:HB	1.89	0.73
22:S:57:THR:HG22	22:S:59:ASP:H	1.54	0.73
32:3:65:THR:HG22	32:3:67:LEU:HG	1.69	0.73
7:C:236:THR:HG22	7:C:239:ALA:N	2.00	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:567:U:H5''	40:W:5817:HOH:O	1.88	0.73
1:0:111:C:O2'	30:1:20:ARG:HG2	1.88	0.73
25:V:1:THR:HG23	25:V:2:VAL:H	1.54	0.73
26:W:137:GLN:HE21	26:W:141:HIS:CE1	2.07	0.73
1:0:1165:G:H4'	1:0:1174:A:O2'	1.89	0.73
23:T:49:GLU:HB3	23:T:59:GLU:HG2	1.71	0.73
16:M:69:LYS:O	16:M:73:ARG:NH2	2.22	0.72
18:O:32:ARG:HD3	18:O:32:ARG:O	1.87	0.72
1:0:506:G:H22	1:0:509:A:H5''	1.53	0.72
1:0:1118:A:H62	1:0:1244:U:H3	1.35	0.72
1:0:870:G:C2'	1:0:871:G:H5''	2.18	0.72
1:0:656:G:H5'	18:O:3:THR:HB	1.71	0.72
1:0:2890:A:H1'	24:U:56:ARG:NH2	2.04	0.72
15:L:143:THR:HG22	15:L:144:ASP:N	2.05	0.72
2:9:3039:U:H1'	2:9:3044:A:H61	1.55	0.72
7:C:104:ASP:HA	7:C:107:ARG:NH1	2.05	0.72
1:0:545:G:H8	1:0:545:G:H5'	1.55	0.71
19:P:115:SER:H	19:P:118:GLN:NE2	1.88	0.71
1:0:1700:C:H5''	1:0:1701:A:OP2	1.90	0.71
14:K:74:VAL:CG1	14:K:113:ILE:HG12	2.19	0.71
14:K:81:ARG:HB2	14:K:87:ARG:NH1	2.04	0.71
1:0:2851:G:H2'	1:0:2852:A:H5'	1.72	0.71
5:A:88:ILE:HD13	5:A:100:PRO:HD3	1.71	0.71
1:0:2005:G:H3'	1:0:2005:G:OP2	1.91	0.71
8:D:58:VAL:HG12	8:D:60:GLU:HG2	1.72	0.71
33:I:110:GLU:HA	33:I:113:HIS:NE2	2.06	0.71
10:F:58:GLU:OE1	16:M:27:ARG:NH2	2.23	0.71
10:F:50:VAL:HG13	10:F:60:VAL:HG11	1.71	0.71
13:J:74:ARG:NH1	13:J:76:ASP:HB2	2.06	0.71
14:K:29:LEU:HB3	14:K:55:VAL:CG1	2.19	0.71
1:0:544:G:H2'	1:0:545:G:H5''	1.72	0.71
5:A:191:GLY:HA2	5:A:194:MET:HE2	1.72	0.71
1:0:1299:G:O6	15:L:6:ARG:HD3	1.91	0.71
28:Y:165:GLU:HB3	40:Y:9390:HOH:O	1.90	0.71
1:0:1701:A:H4'	1:0:1702:U:H5''	1.73	0.70
40:0:7889:HOH:O	6:B:211:THR:HG21	1.91	0.70
8:D:135:VAL:HG21	8:D:139:TYR:CD1	2.26	0.70
16:M:31:TRP:HA	16:M:34:GLU:HG3	1.72	0.70
7:C:236:THR:CG2	7:C:239:ALA:H	2.04	0.70
1:0:2364:A:H5''	20:Q:15:LYS:HD3	1.73	0.70
1:0:962:C:H1'	17:N:5:ARG:NH1	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:77:VAL:HG21	10:F:83:LEU:HD13	1.74	0.70
26:W:80:ASP:O	26:W:84:VAL:HG23	1.90	0.70
10:F:96:ALA:HA	40:F:3111:HOH:O	1.91	0.70
12:H:21:THR:O	12:H:120:ILE:HD12	1.92	0.70
19:P:115:SER:N	19:P:118:GLN:HE21	1.89	0.70
27:X:74:ALA:HB2	27:X:85:VAL:HG13	1.72	0.70
16:M:79:ALA:HB3	16:M:81:ARG:HH12	1.57	0.70
7:C:132:ASP:HB3	40:C:9172:HOH:O	1.91	0.70
33:I:132:CYS:HB3	33:I:137:VAL:HB	1.74	0.70
5:A:33:GLU:CD	5:A:33:GLU:H	1.93	0.70
7:C:78:ARG:HG3	7:C:78:ARG:NH1	2.04	0.70
17:N:17:ARG:HB3	17:N:17:ARG:HH11	1.57	0.70
19:P:59:ARG:NH2	19:P:66:GLN:HE22	1.89	0.70
30:1:25:LYS:HD2	31:2:48:ASP:HA	1.72	0.70
6:B:275:GLY:O	6:B:291:ASP:HA	1.91	0.70
23:T:71:VAL:HG11	23:T:90:PRO:CB	2.21	0.70
33:I:78:LEU:HD12	33:I:112:LYS:NZ	2.07	0.69
26:W:52:VAL:HG22	26:W:53:ALA:H	1.57	0.69
1:0:1160:G:H5'	1:0:1161:A:C5'	2.18	0.69
31:2:18:ASN:HD21	31:2:40:ARG:N	1.89	0.69
30:1:28:HIS:CD2	30:1:31:LYS:HG3	2.27	0.69
10:F:37:THR:O	10:F:41:GLU:HG3	1.93	0.69
1:0:1771:U:H5'	29:Z:20:ARG:NH2	2.07	0.69
1:0:542:A:C8	1:0:542:A:H5'	2.22	0.69
1:0:481:U:H5''	40:0:6167:HOH:O	1.92	0.69
6:B:125:GLU:O	6:B:129:ARG:HG3	1.93	0.69
1:0:2491:G:H1'	40:0:7335:HOH:O	1.93	0.69
22:S:77:VAL:O	22:S:80:ARG:HG2	1.92	0.69
28:Y:212:ARG:HD2	40:Y:9398:HOH:O	1.92	0.69
5:A:51:ARG:HB2	40:A:9591:HOH:O	1.93	0.69
7:C:47:GLY:HA2	7:C:92:PRO:HB2	1.74	0.69
12:H:56:GLN:NE2	12:H:126:ARG:HE	1.90	0.69
26:W:13:MET:HE3	26:W:17:ILE:HG22	1.74	0.69
26:W:88:THR:HG22	26:W:89:ASP:H	1.57	0.69
1:0:380:A:OP2	16:M:9:ARG:HD2	1.93	0.69
8:D:172:VAL:HG12	8:D:173:GLU:N	2.07	0.69
1:0:1474:C:C6	1:0:1474:C:H5'	2.26	0.69
1:0:1641:A:H2'	1:0:1642:A:H5'	1.74	0.69
18:O:32:ARG:NE	18:O:35:LYS:HD2	2.08	0.69
1:0:2749:U:H5'	40:0:8429:HOH:O	1.92	0.68
26:W:122:ARG:NH2	26:W:154:ARG:HG2	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:76:ARG:HH11	27:X:76:ARG:HG3	1.57	0.68
1:0:871:G:C8	1:0:871:G:C5'	2.70	0.68
26:W:130:HIS:O	26:W:136:GLY:HA3	1.93	0.68
16:M:107:ARG:NH1	16:M:107:ARG:HG3	2.05	0.68
6:B:238:ASN:HD22	6:B:240:GLY:N	1.92	0.68
14:K:23:ASN:HD21	14:K:107:THR:HB	1.58	0.68
15:L:67:ARG:O	15:L:71:GLU:HG3	1.93	0.68
33:I:134:SER:O	33:I:135:LEU:HD23	1.93	0.68
21:R:18:LEU:HD12	21:R:143:VAL:CG1	2.23	0.68
26:W:137:GLN:NE2	26:W:141:HIS:HE1	1.90	0.68
26:W:81:ASP:OD1	26:W:92:ASP:HB2	1.94	0.68
7:C:2:GLN:HB3	40:C:9195:HOH:O	1.94	0.68
9:E:6:GLU:HA	9:E:46:THR:HG22	1.74	0.68
13:J:131:THR:HG22	13:J:134:GLU:H	1.56	0.68
1:0:1201:C:H2'	1:0:1202:A:H5'	1.74	0.68
12:H:56:GLN:NE2	12:H:93:GLN:HG2	2.08	0.68
14:K:81:ARG:HD3	14:K:87:ARG:NH1	2.08	0.68
19:P:91:LYS:O	19:P:95:GLU:HG3	1.93	0.68
1:0:1116:U:O2'	1:0:1118:A:C2	2.46	0.67
13:J:74:ARG:HH12	13:J:76:ASP:HB2	1.60	0.67
17:N:62:HIS:HB3	17:N:65:ASP:OD1	1.95	0.67
1:0:1182:C:H1'	1:0:1192:A:H8	1.58	0.67
6:B:62:ARG:HA	6:B:65:MET:CE	2.24	0.67
12:H:30:GLN:H	12:H:66:ARG:NH1	1.93	0.67
12:H:59:HIS:HA	12:H:62:LEU:HD23	1.76	0.67
21:R:18:LEU:HB2	21:R:143:VAL:CG1	2.24	0.67
18:O:96:VAL:HG13	18:O:100:GLN:HB2	1.75	0.67
1:0:2908:A:H2'	1:0:2909:G:O4'	1.95	0.67
1:0:1166:A:H1'	1:0:1192:A:C2	2.29	0.67
8:D:159:PRO:O	8:D:163:VAL:HG23	1.94	0.67
27:X:71:ARG:HD3	40:X:2171:HOH:O	1.95	0.67
1:0:1184:C:H1'	40:0:7899:HOH:O	1.93	0.67
1:0:2676:C:H4'	13:J:70:PHE:CE1	2.30	0.67
1:0:2676:C:H4'	13:J:70:PHE:CD1	2.30	0.67
23:T:115:GLU:HG3	23:T:116:ASP:N	2.09	0.67
24:U:5:GLU:HG2	24:U:10:GLY:O	1.95	0.67
1:0:2468:A:H61	32:3:48:ASN:HD21	1.43	0.67
1:0:883:U:H2'	1:0:883:U:O2	1.95	0.67
5:A:199:HIS:CD2	5:A:201:PHE:H	2.11	0.67
5:A:100:PRO:HG2	5:A:103:VAL:HG21	1.75	0.67
12:H:27:LYS:N	12:H:59:HIS:HD2	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:797:A:C4'	29:Z:10:ARG:N	2.57	0.67
1:0:2420:G:O2'	1:0:2421:G:H5'	1.96	0.66
26:W:21:LEU:CD2	26:W:48:VAL:HG11	2.19	0.66
1:0:1183:C:H2'	40:0:6739:HOH:O	1.94	0.66
1:0:877:G:H5'	1:0:878:G:OP1	1.95	0.66
10:F:13:GLU:OE2	10:F:78:GLU:HG2	1.95	0.66
27:X:71:ARG:HB3	27:X:88:GLU:OE1	1.95	0.66
1:0:1838:U:O2'	1:0:2644:C:H5'	1.95	0.66
1:0:2073:G:OP2	1:0:2490:A:H5'	1.94	0.66
5:A:153:ARG:NH1	5:A:153:ARG:HB2	2.10	0.66
19:P:59:ARG:HH22	19:P:66:GLN:HE22	1.42	0.66
1:0:2578:G:H5'	1:0:2578:G:H8	1.59	0.66
1:0:541:C:H2'	1:0:542:A:C5'	2.26	0.66
8:D:41:LEU:HA	8:D:44:ILE:HG22	1.76	0.66
28:Y:189:ASN:HA	28:Y:217:ILE:HD11	1.78	0.66
1:0:1666:C:H2'	1:0:1667:A:H5'	1.77	0.66
6:B:140:LEU:HA	40:B:9575:HOH:O	1.95	0.66
28:Y:144:ARG:HH11	28:Y:144:ARG:CG	2.09	0.66
1:0:2505:G:O2'	1:0:2506:A:H5'	1.96	0.66
29:Z:22:SER:O	29:Z:26:VAL:HG23	1.94	0.66
6:B:51:VAL:HG23	6:B:329:TYR:O	1.96	0.66
26:W:68:THR:HG23	26:W:69:ARG:HG2	1.78	0.66
10:F:58:GLU:CD	16:M:27:ARG:HH22	1.97	0.66
1:0:1116:U:H3	1:0:1246:A:H62	1.44	0.65
1:0:1159:G:H21	1:0:1189:A:H8	1.44	0.65
6:B:254:GLN:HG2	6:B:255:GLY:N	2.10	0.65
22:S:10:VAL:HG11	25:V:36:ALA:HA	1.78	0.65
6:B:53:LEU:HD11	6:B:327:VAL:HG22	1.77	0.65
13:J:45:VAL:HG11	13:J:121:LEU:HD22	1.79	0.65
18:O:32:ARG:HH21	18:O:35:LYS:NZ	1.94	0.65
19:P:9:LEU:O	19:P:13:VAL:HG12	1.97	0.65
23:T:41:ARG:HG2	23:T:41:ARG:HH11	1.59	0.65
1:0:1687:C:O2	30:I:9:GLY:HA2	1.97	0.65
6:B:16:ARG:NH1	40:B:9612:HOH:O	2.28	0.65
7:C:162:VAL:HG22	7:C:232:LEU:HD21	1.77	0.65
15:L:73:VAL:HG23	15:L:74:THR:H	1.62	0.65
23:T:49:GLU:OE2	23:T:97:ARG:HD2	1.95	0.65
28:Y:144:ARG:CZ	40:Y:9409:HOH:O	2.44	0.65
18:O:32:ARG:HH21	18:O:35:LYS:HZ2	1.44	0.65
23:T:32:ARG:NH1	23:T:38:ARG:HH12	1.94	0.65
1:0:1162:G:H1'	33:I:117:LEU:HD11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:48:ASP:HB3	40:A:9591:HOH:O	1.95	0.65
12:H:166:SER:HB3	12:H:167:PRO:HD3	1.78	0.65
1:O:2661:U:H3	1:O:2812:A:H62	1.43	0.65
6:B:201:ASP:HB2	6:B:312:ARG:HD2	1.79	0.65
1:O:2521:A:OP2	12:H:3:ALA:HB3	1.96	0.65
17:N:48:VAL:CG1	17:N:55:ASP:HB3	2.27	0.65
28:Y:144:ARG:HG3	28:Y:144:ARG:HH11	1.60	0.65
1:O:1175:G:H1'	1:O:1193:A:H2'	1.78	0.65
6:B:307:ARG:NH1	6:B:307:ARG:HG3	2.05	0.65
1:O:1119:G:H22	1:O:1246:A:H2	1.41	0.64
1:O:1730:G:H5'	1:O:1731:C:C5	2.31	0.64
1:O:282:C:O2'	1:O:283:U:H5'	1.96	0.64
16:M:134:ILE:CG2	16:M:141:ILE:HD13	2.26	0.64
1:O:2896:A:H5''	40:O:6599:HOH:O	1.96	0.64
6:B:74:ILE:HD13	6:B:309:VAL:HG21	1.78	0.64
10:F:2:VAL:HG22	10:F:57:GLU:OE1	1.97	0.64
10:F:53:ASP:OD1	10:F:80:GLN:HB2	1.96	0.64
17:N:139:TRP:HA	17:N:139:TRP:CE3	2.33	0.64
26:W:88:THR:HG23	26:W:110:GLN:HE21	1.61	0.64
26:W:48:VAL:HG12	26:W:48:VAL:O	1.97	0.64
1:O:1209:C:H2'	1:O:1210:G:H8	1.61	0.64
1:O:272:A:H5'	1:O:273:G:OP2	1.97	0.64
16:M:68:ARG:NH2	16:M:73:ARG:HD3	2.13	0.64
18:O:21:SER:OG	18:O:106:PRO:HB2	1.98	0.64
23:T:112:LEU:HD23	23:T:119:ALA:HB3	1.79	0.64
29:Z:42:CYS:SG	29:Z:43:GLY:N	2.70	0.64
1:O:544:G:C2'	1:O:545:G:H5''	2.27	0.64
6:B:18:ARG:HG3	6:B:256:GLN:HG3	1.78	0.64
6:B:41:PHE:CD2	6:B:190:MET:HE3	2.32	0.64
1:O:1878:G:H1'	40:O:6620:HOH:O	1.97	0.64
1:O:381:G:H5''	40:M:9373:HOH:O	1.97	0.64
10:F:63:ILE:HB	10:F:64:PRO:HD3	1.80	0.64
12:H:46:GLN:HB3	12:H:167:PRO:HD2	1.78	0.64
13:J:75:PRO:HG2	13:J:105:LEU:HD21	1.79	0.64
24:U:45:GLU:HB2	24:U:48:ASN:ND2	2.12	0.64
31:2:18:ASN:ND2	31:2:40:ARG:H	1.93	0.64
6:B:190:MET:HE2	6:B:194:PHE:HD1	1.61	0.64
14:K:49:LEU:HD12	14:K:80:ILE:HG21	1.80	0.64
16:M:187:LEU:CD2	16:M:194:ALA:HB3	2.28	0.64
20:Q:75:ILE:HD13	20:Q:84:ILE:HD11	1.78	0.64
1:O:709:G:O2'	18:O:25:VAL:HG12	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:9:LYS:HE3	23:T:13:ARG:HH12	1.58	0.64
26:W:108:ARG:HG3	26:W:114:PRO:HG3	1.80	0.64
33:I:125:ALA:O	33:I:129:VAL:HG23	1.97	0.64
1:O:2064:U:H5'	1:O:2652:U:H4'	1.80	0.64
9:E:20:ILE:CD1	9:E:40:VAL:HG11	2.26	0.64
14:K:75:ARG:HD3	14:K:112:PRO:O	1.98	0.64
21:R:111:ILE:HG23	21:R:145:LEU:CD1	2.28	0.64
7:C:157:LEU:HD13	7:C:166:ILE:HD11	1.81	0.63
12:H:166:SER:CB	12:H:167:PRO:CD	2.75	0.63
33:I:110:GLU:HA	33:I:113:HIS:CE1	2.33	0.63
2:9:3039:U:HO2'	2:9:3042:C:H5	1.44	0.63
2:9:3056:A:C2'	2:9:3057:A:H5''	2.26	0.63
7:C:77:ALA:O	7:C:78:ARG:HG3	1.97	0.63
28:Y:126:PRO:HG2	28:Y:128:PHE:CE1	2.33	0.63
1:O:1427:A:H61	1:O:1440:U:H1'	1.62	0.63
1:O:263:U:O4'	10:F:59:ILE:HD13	1.99	0.63
5:A:36:ASP:OD2	5:A:85:SER:HB2	1.98	0.63
17:N:164:ASP:CG	17:N:167:ASP:HA	2.18	0.63
33:I:113:HIS:N	33:I:114:PRO:HD2	2.14	0.63
16:M:80:GLY:O	16:M:81:ARG:HD2	1.99	0.63
1:O:447:A:P	23:T:1:SER:HB2	2.38	0.63
1:O:2587:OMU:H5	40:O:7918:HOH:O	1.97	0.63
1:O:88:G:H2'	1:O:89:G:C8	2.34	0.63
25:V:20:LEU:HD22	25:V:60:GLN:HE22	1.63	0.63
1:O:2541:U:H4'	1:O:2542:C:OP1	1.97	0.63
14:K:55:VAL:HG12	14:K:56:SER:N	2.13	0.63
40:O:9739:HOH:O	16:M:82:ARG:HD2	1.98	0.63
2:9:3014:G:C8	2:9:3014:G:H5'	2.33	0.63
5:A:94:LEU:HG	5:A:99:ILE:HD11	1.80	0.63
1:O:2533:C:C6	1:O:2533:C:H5'	2.32	0.62
13:J:90:LYS:HB2	37:J:9302:CL:CL	2.35	0.62
30:1:25:LYS:HD2	31:2:49:GLU:H	1.64	0.62
32:3:38:ARG:HB3	32:3:42:ARG:HH12	1.64	0.62
1:O:2896:A:N3	1:O:2896:A:H2'	2.15	0.62
30:1:45:ARG:NH2	40:1:9488:HOH:O	2.31	0.62
1:O:1206:U:H2'	1:O:1207:A:O4'	2.00	0.62
1:O:1528:A:H2'	1:O:1529:G:O4'	1.98	0.62
12:H:27:LYS:H	12:H:59:HIS:CD2	2.17	0.62
12:H:40:ALA:HB1	12:H:137:TYR:CE2	2.34	0.62
31:2:22:PRO:HG2	31:2:25:VAL:CG2	2.29	0.62
16:M:164:THR:HG22	16:M:166:ALA:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:W:4:LEU:HD11	26:W:45:VAL:HG12	1.81	0.62
1:0:2780:C:H1'	9:E:143:GLN:HE21	1.64	0.62
1:0:524:A:H5"	21:R:29:LYS:HD3	1.82	0.62
30:1:10:LYS:HG3	40:1:9492:HOH:O	1.98	0.62
2:9:3029:C:O3'	8:D:138:GLY:HA2	2.00	0.62
9:E:23:GLU:HG2	9:E:28:SER:HB3	1.80	0.62
17:N:139:TRP:HA	17:N:139:TRP:HE3	1.65	0.62
17:N:154:LEU:HG	17:N:155:GLU:H	1.63	0.62
21:R:18:LEU:HB2	21:R:143:VAL:HG13	1.82	0.62
21:R:44:VAL:O	21:R:48:GLU:HG3	2.00	0.62
23:T:71:VAL:HG12	23:T:72:ILE:N	2.15	0.62
26:W:141:HIS:HB2	26:W:146:ILE:HG12	1.80	0.62
27:X:25:ARG:HD3	27:X:64:ALA:O	1.99	0.62
1:0:1183:C:N4	1:0:1184:C:H41	1.98	0.62
2:9:3020:G:O2'	2:9:3021:G:H5'	1.99	0.62
2:9:3051:A:H5'	17:N:160:SER:HB3	1.82	0.62
40:9:4707:HOH:O	17:N:147:ILE:HD12	1.99	0.62
19:P:80:ARG:HG2	19:P:87:ARG:CZ	2.30	0.62
1:0:1118:A:H8	1:0:1119:G:H5"	1.64	0.62
1:0:1328:A:OP1	28:Y:169:ARG:HD2	2.00	0.62
5:A:135:VAL:HG21	5:A:147:ARG:NH1	2.15	0.62
12:H:20:ILE:HG23	12:H:120:ILE:HD11	1.81	0.62
16:M:164:THR:HG22	16:M:167:GLY:H	1.65	0.62
1:0:470:U:O2'	30:1:16:HIS:HD2	1.83	0.62
2:9:3029:C:H2'	2:9:3030:C:H5'	1.81	0.62
11:G:12:ILE:N	11:G:13:PRO:CD	2.63	0.62
19:P:64:GLU:HG2	40:P:165:HOH:O	2.00	0.62
29:Z:72:GLU:OE1	29:Z:77:LYS:HE2	1.99	0.62
30:1:8:GLN:HE22	30:1:11:LYS:NZ	1.97	0.61
6:B:141:ARG:HD2	6:B:163:GLU:OE2	1.99	0.61
7:C:118:THR:HG22	7:C:137:PRO:HB3	1.81	0.61
13:J:19:MET:CE	13:J:132:LEU:HD11	2.29	0.61
14:K:109:LEU:HD13	14:K:113:ILE:HD11	1.81	0.61
1:0:2586:U:H3	1:0:2592:G:H22	1.47	0.61
6:B:225:GLY:HA3	40:B:9562:HOH:O	2.00	0.61
24:U:14:GLU:O	24:U:17:THR:HB	2.01	0.61
28:Y:112:GLU:OE1	28:Y:112:GLU:HA	2.00	0.61
28:Y:187:VAL:HG12	28:Y:205:ILE:HA	1.81	0.61
1:0:2807:U:P	6:B:27:ASN:HD21	2.24	0.61
1:0:485:A:N3	1:0:487:G:H5"	2.14	0.61
30:1:25:LYS:HD2	31:2:49:GLU:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:11:ARG:CG	17:N:14:ARG:HH12	2.09	0.61
24:U:52:THR:HG22	24:U:54:THR:N	2.16	0.61
1:O:289:G:N2	1:O:363:A:H2	1.94	0.61
2:9:3039:U:H1'	2:9:3044:A:N6	2.15	0.61
5:A:107:ASN:OD1	5:A:120:ARG:HD2	2.00	0.61
5:A:105:VAL:CG1	5:A:154:ALA:HB1	2.31	0.61
6:B:175:LEU:O	6:B:175:LEU:HD23	2.00	0.61
8:D:59:GLY:O	8:D:61:PHE:N	2.33	0.61
25:V:56:ILE:HG22	25:V:60:GLN:HE21	1.66	0.61
6:B:217:ARG:HG3	6:B:257:THR:HG22	1.80	0.61
27:X:43:VAL:HG12	27:X:44:ASP:N	2.16	0.61
1:O:282:C:H1'	1:O:368:C:N4	2.15	0.61
8:D:136:ARG:NH1	8:D:157:LEU:HA	2.15	0.61
9:E:35:TYR:HA	13:J:127:ILE:HD12	1.82	0.61
18:O:25:VAL:HG23	18:O:26:TRP:N	2.16	0.61
1:O:553:G:P	28:Y:204:ARG:HH22	2.23	0.61
1:O:280:C:H2'	1:O:281:U:O4'	2.01	0.61
5:A:191:GLY:HA2	5:A:194:MET:HE3	1.81	0.61
17:N:164:ASP:OD1	17:N:167:ASP:HA	2.01	0.61
20:Q:25:PRO:HB2	40:Q:4350:HOH:O	2.00	0.61
6:B:329:TYR:CE2	24:U:15:PRO:HG2	2.35	0.61
27:X:66:THR:HG23	27:X:67:PRO:HD2	1.83	0.61
5:A:69:LEU:HD23	5:A:107:ASN:HB2	1.81	0.61
1:O:263:U:O2	16:M:42:ARG:HD2	2.01	0.61
1:O:2563:U:H2'	1:O:2565:C:O5'	2.00	0.61
32:3:65:THR:HG23	32:3:88:LEU:HD22	1.83	0.61
6:B:102:THR:CG2	6:B:182:VAL:HG12	2.31	0.61
8:D:13:MET:HA	8:D:137:PRO:HG2	1.83	0.61
17:N:132:ASN:O	17:N:135:VAL:HG12	2.00	0.61
1:O:475:G:OP1	7:C:73:LEU:HD22	2.01	0.60
5:A:81:GLN:HB2	5:A:92:ASN:HD21	1.62	0.60
7:C:129:HIS:CE1	7:C:231:ARG:HA	2.36	0.60
8:D:58:VAL:CG1	8:D:60:GLU:HG2	2.30	0.60
17:N:61:ALA:HB3	17:N:88:ALA:HB2	1.83	0.60
1:O:2769:C:C2'	1:O:2770:G:H5'	2.32	0.60
5:A:123:GLY:HA3	5:A:162:GLY:HA2	1.83	0.60
7:C:136:VAL:HG22	7:C:137:PRO:HA	1.83	0.60
9:E:68:HIS:O	9:E:72:MET:HG3	2.00	0.60
1:O:902:G:N7	15:L:18:HIS:HD2	1.99	0.60
26:W:21:LEU:HD22	26:W:26:ILE:CD1	2.31	0.60
7:C:139:VAL:HG13	40:C:9254:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:I:129:VAL:O	33:I:129:VAL:HG12	2.01	0.60
33:I:92:PRO:C	33:I:94:GLU:H	2.05	0.60
16:M:71:SER:HB2	16:M:92:THR:HG22	1.83	0.60
1:0:2291:A:C8	1:0:2309:C:H5'	2.36	0.60
1:0:2426:G:H1'	40:0:6592:HOH:O	2.00	0.60
1:0:338:C:H4'	7:C:174:ILE:CD1	2.32	0.60
16:M:183:THR:HG22	16:M:194:ALA:HB1	1.82	0.60
25:V:39:ALA:N	25:V:40:PRO:CD	2.64	0.60
28:Y:187:VAL:HB	28:Y:203:VAL:HG22	1.83	0.60
1:0:2365:G:H5''	40:Q:6597:HOH:O	2.01	0.60
1:0:848:C:H5'	40:0:7714:HOH:O	2.02	0.60
5:A:105:VAL:HG11	5:A:154:ALA:HB1	1.83	0.60
7:C:27:ARG:HG3	7:C:29:ASP:OD1	2.02	0.60
8:D:94:ALA:HA	8:D:174:VAL:HA	1.83	0.60
1:0:1201:C:H5''	40:0:6728:HOH:O	2.01	0.60
1:0:156:C:H5''	16:M:171:ARG:CD	2.28	0.60
2:9:3013:A:O2'	2:9:3014:G:H5''	2.01	0.60
1:0:1943:C:H4'	5:A:211:LYS:O	2.02	0.60
10:F:58:GLU:HA	10:F:61:MET:HE2	1.82	0.60
1:0:2346:C:O2'	8:D:52:THR:HG21	2.00	0.60
2:9:3076:G:C3'	2:9:3077:A:H5''	2.24	0.60
22:S:57:THR:HG22	22:S:59:ASP:N	2.16	0.60
1:0:796:A:HO2'	29:Z:10:ARG:N	1.98	0.60
1:0:2427:C:OP2	32:3:84:ARG:HD2	2.00	0.60
2:9:3004:G:H21	17:N:44:ARG:NH1	2.00	0.60
26:W:21:LEU:HB3	26:W:26:ILE:HG12	1.83	0.60
1:0:2507:G:H2'	1:0:2510:C:H42	1.66	0.60
8:D:135:VAL:HG22	8:D:136:ARG:N	2.17	0.60
8:D:23:VAL:HG21	8:D:45:THR:HG21	1.83	0.60
10:F:46:GLU:O	10:F:73:PRO:HD2	2.02	0.60
26:W:125:HIS:CD2	26:W:127:GLY:H	2.16	0.60
1:0:236:A:H8	1:0:236:A:OP1	1.84	0.60
33:I:113:HIS:CE1	33:I:121:LEU:HD22	2.36	0.60
1:0:1164:U:OP1	33:I:74:PRO:HA	2.01	0.60
14:K:113:ILE:HG22	14:K:114:ALA:N	2.16	0.60
8:D:23:VAL:HG22	8:D:73:VAL:HB	1.82	0.59
13:J:75:PRO:HD3	13:J:136:SER:OG	2.01	0.59
19:P:16:VAL:HG12	19:P:17:GLY:N	2.17	0.59
6:B:264:GLU:HG2	6:B:267:LYS:HE2	1.84	0.59
6:B:71:VAL:HG11	6:B:296:LEU:HD22	1.83	0.59
12:H:170:ASN:N	12:H:170:ASN:HD22	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:V:39:ALA:C	25:V:41:GLU:H	2.06	0.59
25:V:56:ILE:O	25:V:60:GLN:HG3	2.02	0.59
1:0:396:U:O2'	1:0:418:C:H4'	2.02	0.59
10:F:50:VAL:HG21	10:F:63:ILE:HG21	1.83	0.59
40:0:4936:HOH:O	16:M:83:SER:HB3	2.01	0.59
25:V:11:MET:HB3	25:V:15:GLU:HB2	1.84	0.59
28:Y:154:ARG:NH1	28:Y:155:ARG:HG3	2.16	0.59
5:A:153:ARG:CB	5:A:153:ARG:HH11	2.15	0.59
17:N:162:ASP:HA	40:N:9328:HOH:O	2.03	0.59
26:W:119:HIS:HD2	26:W:120:PRO:O	1.86	0.59
6:B:62:ARG:HA	6:B:65:MET:HE3	1.83	0.59
33:I:106:LYS:O	33:I:110:GLU:HG3	2.02	0.59
1:0:1555:G:H4'	1:0:1630:A:H2	1.68	0.59
1:0:1878:G:O2'	1:0:1879:U:C6	2.55	0.59
1:0:462:A:N3	31:2:37:HIS:HB3	2.18	0.59
10:F:91:VAL:CG1	10:F:92:GLY:H	2.10	0.59
33:I:105:VAL:HG11	33:I:129:VAL:HG22	1.84	0.59
23:T:38:ARG:NH1	40:T:6217:HOH:O	2.35	0.59
31:2:36:ASN:HB3	31:2:39:ARG:NE	2.17	0.59
7:C:236:THR:H	7:C:239:ALA:HB3	1.68	0.59
1:0:1946:C:H2'	1:0:1971:G:C8	2.37	0.59
5:A:33:GLU:O	5:A:34:ASP:HB2	2.02	0.59
7:C:233:THR:HG22	7:C:234:VAL:N	2.17	0.59
17:N:23:ARG:HH11	17:N:23:ARG:HG2	1.67	0.59
1:0:1187:U:HO2'	1:0:1189:A:H2	1.51	0.58
1:0:1418:U:OP1	31:2:42:TRP:HB3	2.02	0.58
1:0:1819:G:H2'	1:0:1820:G:H4'	1.85	0.58
1:0:2649:A:H5'	1:0:2649:A:H8	1.67	0.58
1:0:316:A:H5'	23:T:54:ASP:OD2	2.02	0.58
5:A:36:ASP:C	5:A:38:ILE:H	2.06	0.58
1:0:558:C:C2'	1:0:559:U:H5''	2.33	0.58
1:0:797:A:H4'	29:Z:10:ARG:N	2.18	0.58
6:B:265:LEU:HD21	6:B:316:ARG:HD3	1.85	0.58
12:H:46:GLN:HE21	12:H:137:TYR:HE2	1.51	0.58
14:K:62:PRO:HG3	14:K:65:ARG:HH21	1.66	0.58
25:V:12:THR:HG22	25:V:15:GLU:CG	2.21	0.58
1:0:343:C:O2'	1:0:344:C:H5'	2.02	0.58
6:B:254:GLN:HG2	6:B:255:GLY:H	1.68	0.58
32:3:55:VAL:HG22	40:3:9444:HOH:O	2.02	0.58
16:M:24:GLN:NE2	16:M:27:ARG:HH11	2.02	0.58
29:Z:11:SER:CB	29:Z:23:ARG:HB2	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1973:A:H5'	1:0:1973:A:C8	2.37	0.58
6:B:145:HIS:HD2	6:B:146:THR:O	1.85	0.58
9:E:116:THR:HG22	9:E:151:LEU:HD22	1.85	0.58
1:0:1163:G:H5'	33:I:115:ASP:O	2.04	0.58
14:K:109:LEU:CD1	14:K:113:ILE:HD11	2.32	0.58
15:L:148:GLU:HB2	40:L:9486:HOH:O	2.03	0.58
16:M:164:THR:HG22	16:M:166:ALA:H	1.68	0.58
17:N:143:ARG:HH21	17:N:169:PRO:HB2	1.68	0.58
17:N:78:MET:HB2	17:N:79:PRO:HD3	1.85	0.58
1:0:2769:C:O2'	1:0:2770:G:H5'	2.04	0.58
1:0:316:A:N3	1:0:336:G:O2'	2.35	0.58
6:B:87:TYR:O	6:B:138:GLY:N	2.27	0.58
8:D:54:ALA:CB	8:D:69:ILE:HD12	2.32	0.58
14:K:32:ILE:HD11	14:K:56:SER:HB3	1.86	0.58
8:D:50:VAL:O	8:D:71:ALA:HA	2.04	0.58
1:0:2081:A:H4'	13:J:69:TYR:CE1	2.39	0.58
15:L:133:VAL:HA	40:L:9470:HOH:O	2.04	0.58
24:U:47:ARG:HG3	40:U:4381:HOH:O	2.03	0.58
1:0:1187:U:O2'	1:0:1189:A:H2	1.86	0.58
1:0:1701:A:H4'	1:0:1702:U:C5'	2.32	0.58
1:0:558:C:O2'	1:0:559:U:H5''	2.04	0.58
7:C:168:ARG:NH2	7:C:190:ALA:O	2.36	0.58
12:H:58:ARG:HG3	12:H:58:ARG:HH11	1.68	0.58
1:0:119:A:H2'	1:0:120:A:H5''	1.86	0.58
1:0:69:A:H5'	1:0:69:A:C8	2.39	0.58
1:0:969:G:H1	1:0:999:C:N4	2.01	0.58
6:B:85:ARG:NH1	40:B:9629:HOH:O	2.37	0.58
13:J:47:THR:HG22	13:J:48:GLY:N	2.17	0.58
26:W:38:THR:HG22	26:W:39:ASP:N	2.19	0.58
7:C:242:GLU:HB2	40:C:9192:HOH:O	2.04	0.58
17:N:115:VAL:HG22	40:N:9354:HOH:O	2.04	0.58
1:0:681:G:N3	1:0:681:G:H5'	2.19	0.57
7:C:115:LEU:HD13	7:C:223:LEU:HD21	1.86	0.57
1:0:474:C:O3'	7:C:73:LEU:HD21	2.03	0.57
8:D:25:MET:CE	8:D:37:ALA:HB1	2.33	0.57
9:E:81:GLU:HG2	9:E:134:SER:CB	2.33	0.57
10:F:60:VAL:HG12	10:F:60:VAL:O	2.04	0.57
12:H:30:GLN:H	12:H:66:ARG:HH11	1.51	0.57
1:0:2443:C:O3'	15:L:56:LYS:HE3	2.04	0.57
32:3:60:LYS:HG3	32:3:61:PRO:HD2	1.85	0.57
6:B:5:ARG:HH11	6:B:8:LYS:HE2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:54:VAL:HG11	13:J:138:THR:HG21	1.86	0.57
1:0:558:C:H2'	1:0:559:U:C5'	2.33	0.57
17:N:110:THR:HB	17:N:113:SER:OG	2.04	0.57
1:0:1835:U:C5	1:0:1840:A:N7	2.65	0.57
11:G:24:VAL:O	11:G:28:GLU:HB2	2.04	0.57
18:O:25:VAL:HG23	18:O:26:TRP:H	1.69	0.57
25:V:64:GLY:O	25:V:65:ASP:HB2	2.03	0.57
5:A:179:MET:HG2	5:A:186:TRP:CB	2.35	0.57
5:A:88:ILE:HG22	5:A:88:ILE:O	2.03	0.57
8:D:138:GLY:N	40:D:7597:HOH:O	2.36	0.57
1:0:1205:U:H2'	1:0:1206:U:C5'	2.35	0.57
1:0:1878:G:HO2'	1:0:1879:U:H6	1.49	0.57
1:0:2541:U:H3'	1:0:2541:U:H6	1.70	0.57
6:B:321:PRO:HA	40:B:9650:HOH:O	2.03	0.57
13:J:74:ARG:O	13:J:78:ILE:HG12	2.03	0.57
1:0:1666:C:O2'	1:0:1667:A:H5''	2.04	0.57
9:E:126:ILE:HB	9:E:131:LEU:HD23	1.86	0.57
25:V:55:ARG:O	25:V:59:ILE:HG12	2.04	0.57
27:X:37:LEU:CD1	27:X:85:VAL:HG21	2.25	0.57
6:B:17:LYS:O	6:B:260:HIS:HD2	1.87	0.57
8:D:170:TYR:O	8:D:171:ASP:HB3	2.03	0.57
26:W:139:GLY:O	26:W:141:HIS:HD2	1.87	0.57
29:Z:30:GLU:HA	29:Z:33:MET:HE3	1.87	0.57
1:0:1352:A:O2'	1:0:1353:C:OP1	2.22	0.57
5:A:165:THR:HG22	40:A:9604:HOH:O	2.05	0.57
1:0:1351:G:OP1	7:C:96:LYS:NZ	2.36	0.57
1:0:1625:U:H4'	40:0:5209:HOH:O	2.05	0.57
1:0:1919:A:H4'	40:0:5385:HOH:O	2.05	0.57
1:0:2795:C:O2'	1:0:2796:U:H5'	2.05	0.57
1:0:462:A:C2	31:2:37:HIS:HB3	2.39	0.57
2:9:3008:G:O6	17:N:11:ARG:NH1	2.33	0.57
16:M:77:HIS:HD2	16:M:79:ALA:O	1.88	0.57
9:E:126:ILE:HB	9:E:131:LEU:CD2	2.35	0.56
10:F:21:GLU:O	10:F:24:ARG:HG3	2.05	0.56
11:G:23:ILE:HD13	11:G:67:LEU:HD23	1.86	0.56
33:I:128:VAL:C	33:I:130:GLY:H	2.08	0.56
1:0:20:G:H21	21:R:117:HIS:HD2	1.53	0.56
26:W:88:THR:CG2	26:W:89:ASP:H	2.18	0.56
1:0:1684:A:H1'	31:2:43:ARG:HH22	1.70	0.56
1:0:2718:C:H6	1:0:2718:C:H5'	1.69	0.56
1:0:2824:C:H5''	1:0:2825:C:H5'	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:820:G:O2'	1:0:856:G:H4'	2.05	0.56
6:B:190:MET:HE2	6:B:194:PHE:CD1	2.39	0.56
6:B:195:ARG:HD2	6:B:324:ASP:OD1	2.04	0.56
1:0:2815:G:N7	13:J:80:LYS:NZ	2.53	0.56
16:M:60:VAL:C	16:M:61:ILE:HD12	2.25	0.56
24:U:17:THR:CG2	24:U:18:GLY:N	2.67	0.56
26:W:84:VAL:HG12	40:W:6679:HOH:O	2.04	0.56
1:0:1189:A:H1'	1:0:1209:C:O4'	2.05	0.56
1:0:2878:U:H2'	1:0:2879:A:O4'	2.04	0.56
13:J:99:GLU:HA	40:J:7377:HOH:O	2.05	0.56
14:K:114:ALA:HB3	14:K:117:VAL:HG23	1.86	0.56
21:R:9:ASP:O	21:R:13:THR:HB	2.05	0.56
28:Y:235:GLU:CD	28:Y:235:GLU:N	2.52	0.56
1:0:1426:C:H2'	40:0:3203:HOH:O	2.05	0.56
1:0:2032:U:H2'	1:0:2033:G:C5'	2.35	0.56
8:D:49:PRO:HA	8:D:73:VAL:HG22	1.87	0.56
24:U:17:THR:HG22	24:U:18:GLY:N	2.19	0.56
26:W:4:LEU:O	26:W:32:CYS:HA	2.05	0.56
28:Y:187:VAL:HB	28:Y:203:VAL:CG2	2.35	0.56
1:0:2090:G:H2'	1:0:2091:G:C8	2.41	0.56
1:0:757:C:OP1	15:L:27:ARG:HD2	2.05	0.56
8:D:22:VAL:HG22	8:D:74:THR:HG22	1.87	0.56
17:N:169:PRO:O	17:N:172:PHE:HB3	2.06	0.56
19:P:10:ALA:HA	19:P:13:VAL:CG1	2.35	0.56
26:W:122:ARG:CG	26:W:122:ARG:NH1	2.64	0.56
29:Z:29:ILE:O	29:Z:33:MET:HB2	2.06	0.56
1:0:2346:C:O5'	1:0:2346:C:H6	1.87	0.56
1:0:93:C:H5''	25:V:1:THR:HB	1.88	0.56
40:0:9699:HOH:O	6:B:214:PRO:HD2	2.04	0.56
15:L:121:ILE:HG12	15:L:141:GLU:HB2	1.87	0.56
19:P:40:VAL:O	19:P:44:VAL:HG23	2.05	0.56
1:0:1118:A:C8	1:0:1119:G:H5''	2.40	0.56
1:0:1441:G:O2'	1:0:1442:A:H5'	2.05	0.56
1:0:2649:A:H5'	1:0:2649:A:C8	2.41	0.56
1:0:506:G:H22	1:0:509:A:H5'	1.71	0.56
1:0:538:C:OP2	28:Y:134:HIS:HE1	1.89	0.56
5:A:105:VAL:HG11	5:A:154:ALA:CB	2.35	0.56
1:0:2721:U:H4'	14:K:87:ARG:HG3	1.87	0.56
40:0:3149:HOH:O	19:P:81:LYS:HG2	2.06	0.56
1:0:2866:U:H4'	1:0:2867:G:H5'	1.88	0.56
1:0:920:C:H4'	1:0:921:G:C2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:57:ALA:HB1	5:A:65:ARG:HE	1.69	0.56
8:D:103:ASN:ND2	8:D:134:LEU:H	2.03	0.56
1:0:244:C:OP2	10:F:38:LYS:HE3	2.05	0.56
40:0:8433:HOH:O	12:H:154:TYR:HB2	2.06	0.56
15:L:136:ALA:HB3	40:L:9470:HOH:O	2.06	0.56
1:0:2421:G:H1'	40:0:4280:HOH:O	2.06	0.56
1:0:1594:C:OP2	19:P:120:ARG:HD2	2.06	0.56
21:R:18:LEU:HG	21:R:91:LEU:HD13	1.88	0.56
26:W:149:LEU:HG	26:W:153:MET:CE	2.36	0.56
27:X:30:MET:HE1	27:X:58:ALA:HB3	1.88	0.56
1:0:90:A:H2'	1:0:91:G:O4'	2.05	0.56
1:0:949:U:H4'	20:Q:95:GLU:HA	1.86	0.56
8:D:135:VAL:HG21	8:D:139:TYR:CG	2.41	0.56
8:D:76:ARG:O	8:D:77:ASP:HB2	2.06	0.56
1:0:2032:U:H2'	1:0:2033:G:H5''	1.88	0.55
1:0:120:A:H5'	30:1:20:ARG:HH21	1.71	0.55
6:B:297:VAL:HB	40:B:9600:HOH:O	2.05	0.55
14:K:34:VAL:HG22	14:K:47:ALA:HB2	1.86	0.55
1:0:625:U:H5''	1:0:1044:C:N4	2.21	0.55
1:0:558:C:H2'	1:0:559:U:H5'	1.88	0.55
8:D:135:VAL:HG22	8:D:136:ARG:H	1.71	0.55
1:0:1060:C:H6	1:0:1060:C:H5'	1.72	0.55
1:0:138:U:H5''	1:0:139:C:OP2	2.06	0.55
1:0:621:C:H5'	28:Y:132:ASP:OD2	2.07	0.55
2:9:3024:U:H3'	2:9:3025:G:H5'	1.88	0.55
8:D:24:HIS:HB2	8:D:72:LYS:CB	2.35	0.55
1:0:1748:U:H4'	40:0:7953:HOH:O	2.04	0.55
1:0:2481:G:H5''	40:0:5094:HOH:O	2.05	0.55
5:A:125:ASN:HB3	5:A:158:VAL:HG12	1.88	0.55
6:B:305:ASP:O	6:B:306:LYS:HB2	2.07	0.55
25:V:1:THR:HG23	25:V:2:VAL:N	2.20	0.55
1:0:2416:G:O2'	17:N:25:ARG:HG2	2.05	0.55
1:0:2502:C:C2'	1:0:2503:A:H5'	2.37	0.55
1:0:1180:U:O2'	33:I:92:PRO:HD2	2.05	0.55
1:0:164:G:H4'	15:L:30:ARG:HD3	1.89	0.55
17:N:86:LEU:HD12	17:N:125:ALA:HB2	1.88	0.55
1:0:1205:U:H2'	1:0:1206:U:H5'	1.89	0.55
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.88	0.55
1:0:407:A:H2'	1:0:408:A:C8	2.41	0.55
12:H:166:SER:HB3	12:H:167:PRO:CD	2.35	0.55
1:0:834:G:H4'	1:0:835:U:OP2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:57:LYS:HE2	16:M:140:ALA:O	2.06	0.55
1:0:2851:G:O2'	1:0:2852:A:H5'	2.05	0.55
6:B:132:HIS:CE1	6:B:171:VAL:HG21	2.42	0.55
16:M:34:GLU:HB3	16:M:38:GLU:HG3	1.89	0.55
1:0:121:U:OP2	31:2:10:ARG:NH2	2.35	0.55
1:0:137:U:H2'	1:0:139:C:C5	2.42	0.55
9:E:31:ARG:NH1	9:E:68:HIS:CG	2.75	0.55
10:F:50:VAL:CG2	10:F:63:ILE:HG21	2.37	0.55
1:0:1168:C:H5''	33:I:87:THR:CG2	2.37	0.55
16:M:120:VAL:HG11	16:M:130:GLU:HG3	1.88	0.55
29:Z:37:HIS:O	29:Z:45:ASP:HA	2.07	0.55
1:0:2591:C:H2'	1:0:2592:G:O4'	2.06	0.55
6:B:5:ARG:NH1	6:B:8:LYS:HE2	2.22	0.55
10:F:46:GLU:OE1	10:F:100:ASP:HA	2.07	0.55
13:J:130:VAL:HG12	13:J:131:THR:N	2.22	0.55
13:J:76:ASP:HA	40:J:5907:HOH:O	2.06	0.55
15:L:10:SER:O	15:L:11:ARG:HB3	2.06	0.55
23:T:63:ILE:HD11	23:T:75:GLU:HB2	1.89	0.55
27:X:78:GLU:HG2	27:X:79:GLU:OE2	2.07	0.55
27:X:9:VAL:HG22	27:X:88:GLU:OE2	2.07	0.55
1:0:1595:G:O2'	1:0:1596:U:H5'	2.06	0.54
1:0:2270:G:H4'	5:A:223:ARG:HH12	1.72	0.54
6:B:40:GLY:HA3	40:B:9641:HOH:O	2.06	0.54
14:K:30:LYS:O	14:K:55:VAL:HG13	2.06	0.54
17:N:32:PRO:HD2	17:N:99:GLU:O	2.06	0.54
28:Y:108:ASP:N	28:Y:108:ASP:OD1	2.36	0.54
28:Y:154:ARG:HH12	28:Y:155:ARG:CG	2.20	0.54
6:B:221:GLN:HE22	14:K:42:ASN:HD22	1.55	0.54
29:Z:53:GLY:HA2	29:Z:67:GLY:O	2.06	0.54
1:0:2670:G:O2'	1:0:2671:U:H5'	2.07	0.54
8:D:24:HIS:HB2	8:D:72:LYS:HB3	1.89	0.54
14:K:4:LEU:CD2	14:K:116:GLU:HB3	2.36	0.54
28:Y:133:HIS:HD2	40:Y:9381:HOH:O	1.90	0.54
1:0:1202:A:H2'	1:0:1203:G:O4'	2.08	0.54
5:A:65:ARG:C	5:A:66:ARG:HG3	2.26	0.54
1:0:1451:C:H5'	1:0:1505:U:C5	2.43	0.54
1:0:2414:A:H2'	1:0:2415:A:C8	2.43	0.54
5:A:192:VAL:HB	40:A:9580:HOH:O	2.06	0.54
5:A:66:ARG:HH11	5:A:66:ARG:HB2	1.72	0.54
6:B:321:PRO:HG3	40:B:9595:HOH:O	2.06	0.54
7:C:1:MET:HG2	7:C:2:GLN:N	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:87:THR:O	18:O:91:GLN:HG3	2.07	0.54
1:O:1189:A:O2'	1:O:1208:C:H2'	2.07	0.54
2:9:3107:C:H5	40:9:3167:HOH:O	1.90	0.54
1:O:1853:C:OP1	5:A:231:LYS:HG3	2.08	0.54
9:E:144:THR:O	9:E:148:ILE:HG13	2.08	0.54
10:F:50:VAL:CG1	10:F:60:VAL:HG11	2.36	0.54
15:L:53:ARG:NH2	15:L:57:VAL:HG12	2.22	0.54
16:M:164:THR:CG2	16:M:165:GLY:N	2.70	0.54
1:O:291:C:H2'	1:O:292:G:O4'	2.08	0.54
9:E:145:ALA:HB1	9:E:168:ILE:HD11	1.88	0.54
1:O:2748:G:H2'	40:0:7972:HOH:O	2.07	0.54
1:O:95:A:H5''	1:O:97:G:O4'	2.08	0.54
40:0:7978:HOH:O	16:M:91:ILE:HG12	2.07	0.54
18:O:47:ARG:HG3	18:O:47:ARG:HH11	1.73	0.54
1:O:1773:G:C8	29:Z:16:ALA:HA	2.43	0.54
29:Z:57:CYS:SG	29:Z:59:TYR:HB3	2.48	0.54
1:O:441:A:H1'	1:O:442:A:N7	2.22	0.54
1:O:482:G:H4'	1:O:508:A:N1	2.23	0.54
8:D:44:ILE:HG12	8:D:83:PHE:HE1	1.73	0.54
18:O:97:SER:H	18:O:100:GLN:NE2	2.05	0.54
28:Y:189:ASN:HD22	28:Y:189:ASN:C	2.11	0.54
1:O:1377:C:H5'	1:O:1377:C:C6	2.38	0.54
1:O:328:U:O4'	7:C:202:THR:HG22	2.08	0.54
1:O:603:A:H5''	1:O:604:G:OP1	2.08	0.54
1:O:69:A:H5'	1:O:69:A:H8	1.73	0.54
8:D:154:LYS:HD2	8:D:154:LYS:H	1.73	0.54
33:I:113:HIS:HE1	33:I:121:LEU:HD22	1.70	0.54
16:M:187:LEU:HD23	16:M:194:ALA:HB3	1.89	0.54
23:T:32:ARG:NH1	23:T:38:ARG:NH1	2.54	0.54
1:O:1847:A:OP1	5:A:175:LYS:HG3	2.08	0.53
1:O:2837:U:H2'	40:0:7305:HOH:O	2.09	0.53
5:A:105:VAL:HG12	5:A:106:CYS:N	2.24	0.53
16:M:61:ILE:N	16:M:61:ILE:HD12	2.23	0.53
28:Y:170:SER:OG	28:Y:175:ARG:HG3	2.08	0.53
1:O:1477:C:O2'	1:O:1478:U:H5'	2.08	0.53
1:O:1730:G:C5'	1:O:1731:C:C6	2.91	0.53
5:A:217:ARG:HH11	5:A:217:ARG:CG	2.20	0.53
16:M:182:LYS:O	16:M:194:ALA:HB2	2.07	0.53
1:O:1172:G:H1'	40:0:5505:HOH:O	2.09	0.53
1:O:1766:U:O2	1:O:1778:A:H5'	2.08	0.53
1:O:475:G:H5'	7:C:73:LEU:HD23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1184:C:H4'	33:I:126:LYS:HB3	1.89	0.53
33:I:93:GLN:HA	33:I:96:PHE:HE2	1.73	0.53
19:P:103:THR:O	19:P:107:GLU:HG3	2.08	0.53
1:0:12:U:H2'	1:0:13:G:H5'	1.91	0.53
1:0:1626:A:H2'	1:0:1627:G:O4'	2.08	0.53
1:0:653:C:H2'	1:0:654:A:C8	2.43	0.53
31:2:36:ASN:HB3	31:2:39:ARG:HG3	1.90	0.53
32:3:56:PRO:HA	40:3:9486:HOH:O	2.09	0.53
6:B:102:THR:HG21	6:B:182:VAL:O	2.07	0.53
6:B:320:GLN:HE21	6:B:321:PRO:HD2	1.73	0.53
8:D:36:ASN:HA	40:D:7500:HOH:O	2.07	0.53
8:D:95:THR:OG1	8:D:174:VAL:HG22	2.08	0.53
18:O:14:LEU:CD2	18:O:102:ILE:HD11	2.38	0.53
18:O:53:GLN:HG2	18:O:56:GLU:OE1	2.08	0.53
1:0:1066:U:H2'	1:0:1067:A:C8	2.44	0.53
1:0:1838:U:H1'	1:0:2644:C:H5'	1.91	0.53
1:0:2769:C:H2'	1:0:2770:G:C5'	2.39	0.53
30:1:25:LYS:HD2	31:2:48:ASP:CA	2.38	0.53
6:B:312:ARG:HD3	6:B:315:VAL:HG13	1.89	0.53
7:C:25:PRO:HG2	40:C:9126:HOH:O	2.09	0.53
15:L:119:THR:HG23	15:L:139:SER:OG	2.08	0.53
23:T:47:THR:HB	23:T:100:ASP:HB3	1.90	0.53
1:0:1077:G:H2'	1:0:1080:C:H42	1.73	0.53
1:0:1972:U:H2'	1:0:1973:A:H5'	1.91	0.53
1:0:2883:A:H2'	1:0:2884:G:O4'	2.09	0.53
9:E:3:VAL:CG2	9:E:49:ILE:HB	2.38	0.53
1:0:2694:A:H4'	9:E:91:PHE:CE1	2.44	0.53
1:0:151:A:H2'	1:0:152:A:O4'	2.08	0.53
1:0:2812:A:C2	1:0:2814:A:N6	2.70	0.53
1:0:516:A:H5'	40:0:6167:HOH:O	2.09	0.53
1:0:775:G:OP1	30:1:16:HIS:HE1	1.91	0.53
1:0:447:A:OP2	23:T:1:SER:HB2	2.08	0.53
7:C:233:THR:HG22	7:C:234:VAL:H	1.73	0.53
26:W:88:THR:HG22	26:W:90:TYR:HD1	1.72	0.53
28:Y:112:GLU:CD	28:Y:115:ARG:NH1	2.63	0.53
1:0:1786:C:OP1	19:P:74:GLN:HG2	2.09	0.53
1:0:545:G:C8	1:0:545:G:H5'	2.42	0.53
5:A:121:ALA:O	5:A:124:VAL:HG22	2.09	0.53
6:B:41:PHE:CD1	6:B:79:MET:HE2	2.44	0.53
14:K:49:LEU:HD12	14:K:80:ILE:HD13	1.90	0.53
18:O:97:SER:OG	18:O:100:GLN:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1552:G:N2	1:0:1634:G:H1'	2.24	0.53
1:0:1667:A:H2'	1:0:1668:U:C6	2.44	0.53
1:0:1741:U:H3'	40:0:3363:HOH:O	2.09	0.53
30:1:1:THR:HA	40:1:9468:HOH:O	2.08	0.53
40:0:4793:HOH:O	31:2:38:LYS:HE3	2.08	0.53
19:P:16:VAL:HG13	19:P:20:ARG:NH1	2.24	0.53
1:0:1252:A:H2'	1:0:1253:C:O4'	2.09	0.52
1:0:204:A:C2'	1:0:205:U:H5'	2.39	0.52
1:0:362:G:H2'	1:0:363:A:C8	2.44	0.52
1:0:1836:A:H1'	30:1:1:THR:O	2.09	0.52
32:3:30:GLN:HG3	40:3:9452:HOH:O	2.09	0.52
5:A:95:PRO:HG2	5:A:98:GLU:HG2	1.91	0.52
8:D:62:ASP:HA	40:D:4233:HOH:O	2.08	0.52
10:F:48:VAL:HG12	10:F:97:ALA:CB	2.39	0.52
33:I:113:HIS:N	33:I:114:PRO:CD	2.72	0.52
1:0:1730:G:H5''	1:0:1731:C:H6	1.74	0.52
1:0:2361:A:H2'	1:0:2362:A:C8	2.44	0.52
1:0:2817:G:P	40:0:8435:HOH:O	2.67	0.52
7:C:107:ARG:NH1	7:C:107:ARG:HB3	2.24	0.52
7:C:194:PHE:CD2	7:C:234:VAL:HG11	2.43	0.52
33:I:138:THR:HG22	33:I:139:ILE:N	2.24	0.52
22:S:73:ASP:OD1	22:S:76:GLU:HG3	2.09	0.52
27:X:12:ILE:HD12	27:X:36:HIS:ND1	2.24	0.52
6:B:36:PRO:HB3	6:B:174:ARG:CB	2.40	0.52
9:E:10:ASP:HA	40:E:3707:HOH:O	2.08	0.52
17:N:86:LEU:HD21	17:N:180:LEU:CD1	2.40	0.52
21:R:114:VAL:HA	21:R:144:GLU:O	2.09	0.52
26:W:88:THR:CG2	26:W:89:ASP:N	2.69	0.52
40:0:5237:HOH:O	29:Z:13:ARG:HD3	2.09	0.52
4:5:77:PHE:CE1	4:5:79:BTN:H62	2.43	0.52
7:C:236:THR:HG22	7:C:239:ALA:CB	2.40	0.52
15:L:134:GLU:HG3	40:L:9452:HOH:O	2.09	0.52
26:W:13:MET:CE	26:W:17:ILE:HG22	2.39	0.52
26:W:29:VAL:O	26:W:30:ASN:HB2	2.10	0.52
5:A:43:VAL:HG21	5:A:59:GLU:HG3	1.90	0.52
7:C:246:ARG:NH1	40:C:9180:HOH:O	2.43	0.52
12:H:63:GLU:HA	40:H:9546:HOH:O	2.08	0.52
19:P:98:ILE:HD12	19:P:102:ARG:NE	2.25	0.52
1:0:2326:U:H4'	1:0:2412:G:C4'	2.40	0.52
1:0:2644:C:O2'	1:0:2645:U:H5'	2.08	0.52
1:0:1562:C:H42	1:0:2738:G:H1	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1:28:HIS:HD2	30:1:31:LYS:H	1.57	0.52
6:B:141:ARG:HG2	6:B:165:ARG:HA	1.90	0.52
6:B:41:PHE:CG	6:B:79:MET:HE2	2.45	0.52
18:O:78:ALA:C	18:O:98:LEU:HD13	2.30	0.52
25:V:12:THR:HG23	25:V:14:ALA:H	1.73	0.52
26:W:52:VAL:HG22	26:W:53:ALA:N	2.23	0.52
1:O:2502:C:H2'	1:O:2503:A:H5'	1.91	0.52
32:3:70:ARG:HB3	40:3:9508:HOH:O	2.09	0.52
17:N:24:LEU:HD22	40:Q:2847:HOH:O	2.10	0.52
1:O:1462:C:H2'	1:O:1463:A:C8	2.45	0.52
5:A:109:GLU:HG2	5:A:116:GLY:N	2.25	0.52
23:T:40:VAL:HG22	23:T:41:ARG:N	2.25	0.52
1:O:497:A:H2'	1:O:498:A:C5'	2.40	0.52
8:D:136:ARG:HB3	8:D:137:PRO:HD2	1.91	0.52
12:H:38:LYS:HE2	12:H:42:ASP:HB2	1.92	0.52
14:K:34:VAL:CG2	14:K:47:ALA:HB2	2.39	0.52
16:M:31:TRP:CA	16:M:34:GLU:HG3	2.40	0.52
1:O:2419:U:H5''	1:O:2420:G:H5'	1.91	0.52
2:9:3069:U:OP1	17:N:4:PRO:HG3	2.10	0.52
12:H:76:GLU:O	12:H:77:LEU:HD23	2.09	0.52
16:M:107:ARG:NH1	40:M:9378:HOH:O	2.43	0.52
23:T:19:ARG:HD3	23:T:67:LEU:O	2.10	0.52
40:K:7438:HOH:O	24:U:20:MET:HE1	2.09	0.52
28:Y:184:GLU:OE1	28:Y:204:ARG:NH1	2.43	0.52
1:O:1119:G:H2'	13:J:52:GLN:HE22	1.73	0.51
6:B:41:PHE:HB3	6:B:190:MET:CE	2.40	0.51
6:B:254:GLN:HG3	40:B:9531:HOH:O	2.10	0.51
8:D:65:GLU:HA	40:D:6752:HOH:O	2.08	0.51
13:J:130:VAL:HG12	13:J:131:THR:H	1.74	0.51
15:L:36:ASP:HB2	40:L:9431:HOH:O	2.09	0.51
28:Y:187:VAL:HG23	40:Y:9369:HOH:O	2.10	0.51
1:O:2320:U:H4'	1:O:2321:A:O4'	2.10	0.51
1:O:2645:U:OP2	1:O:2645:U:C6	2.63	0.51
1:O:497:A:H2'	1:O:498:A:H5'	1.91	0.51
1:O:899:C:H5'	40:O:3792:HOH:O	2.09	0.51
6:B:58:PRO:HA	6:B:63:GLU:OE2	2.11	0.51
11:G:64:ASN:N	11:G:64:ASN:HD22	2.07	0.51
12:H:63:GLU:O	12:H:67:LEU:HB2	2.09	0.51
13:J:71:TYR:CD1	13:J:72:PRO:HD2	2.45	0.51
2:9:3051:A:H5'	17:N:160:SER:CB	2.40	0.51
23:T:49:GLU:CB	23:T:59:GLU:HG2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1118:A:C8	1:0:1118:A:C3'	2.86	0.51
1:0:2415:A:H2'	1:0:2416:G:H5'	1.91	0.51
30:1:21:ARG:HD2	30:1:37:CYS:SG	2.51	0.51
5:A:149:ASP:OD1	5:A:151:GLN:HB2	2.10	0.51
7:C:118:THR:CG2	7:C:137:PRO:HB3	2.40	0.51
7:C:127:ARG:CZ	7:C:225:PRO:HG2	2.40	0.51
7:C:236:THR:HA	40:C:9257:HOH:O	2.10	0.51
1:0:1159:G:H1	1:0:1208:C:H42	1.57	0.51
5:A:36:ASP:O	5:A:38:ILE:N	2.44	0.51
5:A:94:LEU:HD12	5:A:98:GLU:HB2	1.91	0.51
33:I:89:SER:HB3	33:I:97:VAL:CG2	2.40	0.51
24:U:9:CYS:O	24:U:52:THR:HG23	2.10	0.51
27:X:76:ARG:NH1	27:X:76:ARG:HG3	2.24	0.51
1:0:1234:U:N3	6:B:244:PRO:HB3	2.25	0.51
7:C:129:HIS:HD2	7:C:165:ASP:OD2	1.94	0.51
8:D:49:PRO:HB3	40:D:5828:HOH:O	2.10	0.51
9:E:34:TRP:O	13:J:127:ILE:HD11	2.11	0.51
16:M:99:ARG:NH2	16:M:170:ASN:HD22	2.00	0.51
17:N:67:ALA:HA	17:N:71:TRP:HB3	1.93	0.51
1:0:1384:C:H5'	27:X:30:MET:HG2	1.92	0.51
6:B:41:PHE:HB3	6:B:190:MET:HE3	1.93	0.51
6:B:199:TYR:CE2	6:B:268:ARG:HB2	2.46	0.51
1:0:926:A:H5'	15:L:39:GLU:OE2	2.09	0.51
1:0:1189:A:H3'	40:0:8193:HOH:O	2.10	0.51
1:0:1211:G:O2'	1:0:1212:C:H5'	2.10	0.51
1:0:317:A:H5''	23:T:52:ARG:HD2	1.92	0.51
40:0:5933:HOH:O	5:A:164:ARG:CZ	2.59	0.51
18:O:106:PRO:HG2	18:O:107:GLU:OE1	2.10	0.51
23:T:112:LEU:CD2	23:T:119:ALA:HB3	2.39	0.51
1:0:1209:C:H2'	1:0:1210:G:C8	2.45	0.51
1:0:2619:UR3:H6	1:0:2619:UR3:O5'	2.11	0.51
5:A:211:LYS:CG	5:A:212:PRO:HD2	2.30	0.51
10:F:36:THR:HG23	10:F:97:ALA:HB2	1.93	0.51
33:I:78:LEU:CD1	33:I:112:LYS:HZ2	2.24	0.51
18:O:73:ASP:HA	18:O:92:VAL:O	2.11	0.51
21:R:106:GLY:HA2	21:R:109:MET:HE3	1.92	0.51
21:R:39:THR:HG22	21:R:107:GLU:O	2.10	0.51
1:0:1484:G:H2'	40:0:9725:HOH:O	2.11	0.51
1:0:1669:A:H2'	1:0:1670:G:C8	2.46	0.51
1:0:248:A:H5'	1:0:249:G:OP2	2.11	0.51
11:G:67:LEU:O	11:G:71:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:35:ARG:HB2	15:L:35:ARG:NH1	2.25	0.51
1:0:1886:A:O2'	29:Z:20:ARG:HB2	2.11	0.51
1:0:1160:G:HO2'	1:0:1190:G:H8	1.59	0.51
1:0:475:G:C5'	7:C:73:LEU:HD23	2.40	0.51
1:0:2694:A:H4'	9:E:91:PHE:HE1	1.76	0.51
12:H:56:GLN:HE21	12:H:126:ARG:HE	1.56	0.51
40:0:7340:HOH:O	16:M:178:LYS:HB2	2.11	0.51
17:N:66:LEU:HD11	17:N:175:LEU:HD21	1.92	0.51
1:0:308:U:H5'	23:T:97:ARG:NH2	2.26	0.51
1:0:1077:G:H2'	1:0:1080:C:N4	2.25	0.50
1:0:1218:U:H2'	1:0:1219:U:C6	2.46	0.50
1:0:1306:U:OP1	7:C:184:ARG:HD2	2.11	0.50
1:0:1717:A:H5''	19:P:54:LYS:HB2	1.92	0.50
1:0:2421:G:H2'	40:0:4646:HOH:O	2.10	0.50
1:0:2894:C:O2'	1:0:2895:C:H5'	2.10	0.50
2:9:3054:A:H2	40:9:3535:HOH:O	1.93	0.50
2:9:3054:A:O2'	2:9:3055:U:H5'	2.11	0.50
6:B:53:LEU:HD21	6:B:270:ILE:HD12	1.92	0.50
6:B:72:THR:HB	40:B:9600:HOH:O	2.11	0.50
13:J:45:VAL:HG11	13:J:121:LEU:CD2	2.40	0.50
14:K:115:ARG:HG3	14:K:116:GLU:N	2.27	0.50
15:L:145:LEU:O	15:L:145:LEU:HD23	2.11	0.50
22:S:29:ASP:OD1	22:S:31:ARG:NH1	2.44	0.50
29:Z:30:GLU:HG2	29:Z:33:MET:HE3	1.94	0.50
1:0:2016:U:H2'	1:0:2017:U:O4'	2.10	0.50
1:0:2825:C:H4'	1:0:2826:G:O5'	2.12	0.50
1:0:299:U:H5'	40:0:7775:HOH:O	2.11	0.50
1:0:432:G:O2'	1:0:433:C:H5'	2.11	0.50
6:B:265:LEU:CD2	6:B:316:ARG:HD3	2.41	0.50
7:C:236:THR:HG21	40:C:9184:HOH:O	2.10	0.50
8:D:104:PHE:CE2	8:D:166:ILE:HD13	2.46	0.50
33:I:87:THR:HG22	33:I:88:GLY:N	2.25	0.50
20:Q:75:ILE:HD13	20:Q:84:ILE:CD1	2.41	0.50
26:W:21:LEU:HD22	26:W:26:ILE:HD13	1.92	0.50
1:0:2296:C:H2'	1:0:2297:U:H6	1.77	0.50
1:0:285:A:H2'	1:0:286:U:O4'	2.11	0.50
31:2:20:ARG:HG3	31:2:39:ARG:HH21	1.76	0.50
40:0:7989:HOH:O	32:3:61:PRO:HG2	2.10	0.50
17:N:179:LEU:HD23	17:N:184:ILE:HD12	1.94	0.50
19:P:115:SER:HG	19:P:118:GLN:HG3	1.76	0.50
40:0:6777:HOH:O	28:Y:158:LYS:HD3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1198:U:H2'	1:0:1200:A:OP2	2.11	0.50
1:0:1333:U:H2'	1:0:1334:C:C6	2.47	0.50
1:0:2906:A:H5'	1:0:2907:C:O4'	2.12	0.50
8:D:25:MET:HE1	8:D:37:ALA:O	2.11	0.50
9:E:133:VAL:HG12	9:E:141:VAL:HG13	1.94	0.50
21:R:92:LEU:HD23	21:R:145:LEU:HD21	1.94	0.50
1:0:177:A:H2'	1:0:178:U:O4'	2.11	0.50
1:0:1972:U:H2'	1:0:1973:A:C5'	2.42	0.50
1:0:2326:U:H4'	1:0:2412:G:H4'	1.94	0.50
1:0:2816:A:H2'	40:0:8435:HOH:O	2.12	0.50
5:A:163:GLY:HA2	5:A:166:ASP:OD2	2.12	0.50
6:B:268:ARG:NH2	6:B:325:PRO:HG3	2.25	0.50
13:J:75:PRO:HG2	13:J:105:LEU:CD2	2.41	0.50
26:W:122:ARG:CZ	40:W:5817:HOH:O	2.58	0.50
2:9:3059:C:H2'	2:9:3060:C:C6	2.46	0.50
6:B:314:ALA:HB3	6:B:317:PRO:HG3	1.92	0.50
9:E:145:ALA:HB1	9:E:168:ILE:CD1	2.42	0.50
12:H:158:THR:HB	12:H:159:PRO:HD3	1.94	0.50
13:J:74:ARG:NH1	13:J:105:LEU:HD11	2.27	0.50
1:0:1992:U:OP2	14:K:66:ARG:HD2	2.11	0.50
16:M:82:ARG:O	16:M:84:LYS:N	2.44	0.50
21:R:69:LYS:HB2	21:R:72:VAL:HG23	1.92	0.50
1:0:1714:C:O2'	1:0:1715:C:H5'	2.11	0.50
1:0:2338:G:OP1	8:D:97:GLN:HG2	2.11	0.50
10:F:48:VAL:HG12	10:F:97:ALA:HB2	1.94	0.50
1:0:155:C:OP2	16:M:188:ARG:HD3	2.11	0.50
26:W:110:GLN:NE2	26:W:110:GLN:HA	2.27	0.50
26:W:5:VAL:HG22	26:W:32:CYS:HB2	1.93	0.50
28:Y:107:PRO:HD3	28:Y:182:PHE:CE1	2.46	0.50
1:0:123:U:H5'	40:0:7132:HOH:O	2.12	0.50
1:0:2769:C:H2'	1:0:2770:G:H5'	1.92	0.50
7:C:154:VAL:O	7:C:158:GLU:HG3	2.12	0.50
29:Z:10:ARG:HA	40:Z:9215:HOH:O	2.11	0.50
1:0:1751:G:C2'	1:0:1752:G:H5''	2.40	0.50
1:0:247:A:H2'	40:0:4495:HOH:O	2.11	0.50
1:0:2827:A:H2'	1:0:2828:G:O4'	2.12	0.50
2:9:3007:G:H4'	17:N:55:ASP:OD2	2.12	0.50
2:9:3042:C:O2	8:D:76:ARG:NH1	2.45	0.50
6:B:58:PRO:HA	6:B:63:GLU:CD	2.32	0.50
8:D:28:GLY:CA	8:D:69:ILE:HG23	2.35	0.50
1:0:962:C:H1'	17:N:5:ARG:HH12	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:126:PRO:HG2	28:Y:128:PHE:CZ	2.47	0.50
1:0:1745:G:H22	1:0:2033:G:H5'	1.77	0.49
2:9:3049:G:O2'	2:9:3050:G:H5'	2.11	0.49
7:C:57:PRO:HG2	7:C:73:LEU:HD13	1.93	0.49
8:D:25:MET:SD	8:D:40:ILE:HD11	2.51	0.49
10:F:13:GLU:OE1	10:F:77:VAL:HG13	2.12	0.49
18:O:96:VAL:CG1	18:O:100:GLN:HB2	2.40	0.49
19:P:13:VAL:HG11	19:P:40:VAL:CG1	2.42	0.49
1:0:204:A:H2'	1:0:205:U:H5'	1.93	0.49
1:0:2748:G:H1'	40:0:8408:HOH:O	2.11	0.49
1:0:926:A:O2'	15:L:41:HIS:HD2	1.95	0.49
1:0:951:A:C2'	1:0:952:G:H5'	2.41	0.49
6:B:310:ARG:HD2	40:B:9586:HOH:O	2.10	0.49
6:B:51:VAL:HG23	6:B:327:VAL:HG13	1.94	0.49
7:C:185:LYS:HD3	7:C:186:TYR:CE1	2.47	0.49
33:I:131:THR:O	33:I:135:LEU:HG	2.12	0.49
13:J:19:MET:HE2	13:J:79:PHE:HA	1.92	0.49
25:V:59:ILE:O	25:V:63:GLU:HG2	2.11	0.49
1:0:820:G:H5'	1:0:821:U:H5'	1.94	0.49
1:0:920:C:H5''	1:0:921:G:O5'	2.13	0.49
7:C:127:ARG:HD3	7:C:129:HIS:HE1	1.76	0.49
13:J:88:PRO:O	13:J:94:GLY:HA3	2.12	0.49
15:L:143:THR:CG2	15:L:144:ASP:N	2.75	0.49
17:N:119:GLN:O	17:N:123:ILE:HG13	2.12	0.49
17:N:89:GLY:O	17:N:92:ALA:HB3	2.12	0.49
28:Y:177:LYS:HD3	28:Y:181:GLY:O	2.12	0.49
1:0:1506:U:H5'	1:0:1506:U:H6	1.78	0.49
30:1:21:ARG:HD2	30:1:39:PHE:HB2	1.95	0.49
32:3:3:MET:O	32:3:90:PHE:HA	2.12	0.49
2:9:3095:C:O2'	2:9:3096:C:H5'	2.12	0.49
11:G:20:VAL:O	11:G:24:VAL:HG23	2.13	0.49
13:J:12:VAL:HG21	13:J:116:LEU:HD11	1.94	0.49
14:K:22:ASP:O	14:K:110:LYS:HE3	2.12	0.49
14:K:55:VAL:CG1	14:K:56:SER:N	2.74	0.49
23:T:106:GLU:HG3	40:T:4913:HOH:O	2.11	0.49
23:T:38:ARG:HG3	23:T:38:ARG:HH11	1.77	0.49
27:X:61:ARG:HH11	27:X:61:ARG:HG3	1.77	0.49
1:0:1056:U:H2'	1:0:1057:A:O4'	2.11	0.49
1:0:1503:U:H2'	1:0:1504:A:O4'	2.12	0.49
1:0:734:U:H1'	1:0:737:A:N6	2.27	0.49
32:3:25:VAL:HG22	32:3:68:LYS:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:84:LEU:HD13	6:B:84:LEU:O	2.13	0.49
8:D:10:PHE:CE1	8:D:11:HIS:HB3	2.47	0.49
1:0:2333:G:P	8:D:56:ARG:HH22	2.36	0.49
8:D:56:ARG:N	40:D:6752:HOH:O	2.46	0.49
9:E:81:GLU:HA	9:E:133:VAL:O	2.12	0.49
14:K:125:ALA:C	14:K:127:ALA:H	2.14	0.49
10:F:38:LYS:NZ	16:M:3:SER:HA	2.27	0.49
1:0:1755:A:H2'	1:0:1756:G:O4'	2.12	0.49
1:0:288:A:H2'	1:0:289:G:C8	2.47	0.49
1:0:333:G:O2'	1:0:334:G:H5'	2.13	0.49
5:A:125:ASN:CB	5:A:158:VAL:HG12	2.42	0.49
24:U:39:ASN:ND2	24:U:44:ARG:HH11	2.10	0.49
25:V:1:THR:CG2	25:V:2:VAL:H	2.19	0.49
1:0:1119:G:H8	13:J:52:GLN:NE2	2.10	0.49
1:0:1878:G:O2'	1:0:1879:U:OP2	2.30	0.49
1:0:2453:G:H5''	40:L:9438:HOH:O	2.12	0.49
1:0:2531:U:O2'	1:0:2532:A:H5'	2.12	0.49
1:0:2735:U:H2'	1:0:2736:U:C6	2.47	0.49
1:0:830:G:O2'	1:0:831:U:H5'	2.13	0.49
1:0:960:G:H2'	1:0:960:G:N3	2.28	0.49
3:4:75:C:N4	3:4:76:PPU:H102	2.28	0.49
2:9:3078:G:N2	2:9:3102:G:H2'	2.28	0.49
5:A:94:LEU:HG	5:A:99:ILE:CD1	2.43	0.49
8:D:41:LEU:HA	8:D:44:ILE:CG2	2.43	0.49
10:F:34:ASN:HA	16:M:4:ALA:HB2	1.93	0.49
17:N:152:GLU:C	17:N:154:LEU:H	2.16	0.49
19:P:16:VAL:HG13	19:P:20:ARG:CZ	2.43	0.49
1:0:793:A:H5''	19:P:83:LYS:HG2	1.95	0.49
21:R:18:LEU:HB2	21:R:143:VAL:HG12	1.94	0.49
25:V:12:THR:HG23	25:V:14:ALA:N	2.27	0.49
25:V:1:THR:HG22	25:V:48:GLU:OE1	2.13	0.49
1:0:1666:C:H2'	1:0:1667:A:C5'	2.42	0.49
1:0:2032:U:C2'	1:0:2033:G:H5''	2.42	0.49
1:0:2781:U:H1'	9:E:139:GLU:OE2	2.12	0.49
1:0:669:G:O2'	1:0:670:G:H5'	2.12	0.49
5:A:94:LEU:N	5:A:94:LEU:HD23	2.28	0.49
12:H:148:GLU:HA	12:H:148:GLU:OE1	2.11	0.49
21:R:99:ALA:HB1	21:R:109:MET:HE3	1.92	0.49
23:T:41:ARG:NH1	23:T:41:ARG:HG2	2.27	0.49
23:T:69:LYS:O	23:T:71:VAL:HG23	2.13	0.49
1:0:2252:A:H2'	1:0:2253:G:O4'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:190:ARG:NH2	5:A:207:GLN:OE1	2.46	0.49
6:B:41:PHE:CG	6:B:190:MET:HE3	2.47	0.49
8:D:172:VAL:CG1	8:D:173:GLU:H	2.18	0.49
8:D:37:ALA:O	8:D:40:ILE:HG12	2.12	0.49
9:E:11:VAL:HG12	9:E:12:ASP:N	2.26	0.49
9:E:80:TRP:O	9:E:134:SER:HA	2.13	0.49
20:Q:32:GLU:HA	20:Q:71:TYR:OH	2.13	0.49
21:R:84:ALA:O	21:R:88:PHE:HD1	1.96	0.49
26:W:122:ARG:HG3	26:W:152:ALA:O	2.13	0.49
1:0:2445:U:H2'	1:0:2446:G:C8	2.47	0.49
1:0:65:C:O2'	1:0:66:G:H5'	2.12	0.49
6:B:62:ARG:HA	6:B:65:MET:HE2	1.93	0.49
8:D:51:ARG:HD3	40:D:7636:HOH:O	2.13	0.49
12:H:69:ALA:HB2	12:H:153:ALA:HB2	1.94	0.49
17:N:155:GLU:O	17:N:156:GLU:HG3	2.12	0.49
17:N:164:ASP:OD2	17:N:167:ASP:HA	2.12	0.49
18:O:97:SER:H	18:O:100:GLN:HE21	1.59	0.49
28:Y:186:ARG:HH11	28:Y:186:ARG:HG2	1.76	0.49
1:0:1730:G:H5'	1:0:1731:C:H5	1.77	0.48
1:0:2265:U:H2'	1:0:2266:A:C8	2.48	0.48
30:1:25:LYS:HG3	31:2:49:GLU:H	1.77	0.48
12:H:170:ASN:N	12:H:170:ASN:ND2	2.61	0.48
1:0:2784:A:H1'	9:E:60:SER:OG	2.13	0.48
1:0:750:A:O3'	7:C:101:ASP:HB2	2.12	0.48
31:2:41:HIS:HD2	31:2:44:ARG:H	1.61	0.48
33:I:138:THR:HG22	33:I:139:ILE:H	1.78	0.48
14:K:28:GLU:HB3	14:K:59:LYS:HB2	1.94	0.48
16:M:99:ARG:HH21	16:M:170:ASN:ND2	2.02	0.48
5:A:167:LYS:HB2	29:Z:29:ILE:HD13	1.95	0.48
1:0:2809:G:H2'	1:0:2810:G:O4'	2.13	0.48
2:9:3024:U:H3'	2:9:3025:G:C5'	2.43	0.48
7:C:142:ASP:OD1	7:C:236:THR:HG23	2.14	0.48
8:D:99:ASP:HB3	8:D:103:ASN:H	1.77	0.48
15:L:97:VAL:HG12	15:L:98:GLU:O	2.13	0.48
1:0:2064:U:H5'	1:0:2652:U:O3'	2.13	0.48
1:0:399:C:H5'	16:M:179:GLY:O	2.13	0.48
1:0:426:G:H2'	1:0:427:C:O4'	2.13	0.48
1:0:1654:U:H2'	5:A:47:HIS:HD2	1.77	0.48
8:D:103:ASN:HD21	8:D:134:LEU:H	1.60	0.48
1:0:1242:A:C5'	13:J:82:THR:HG23	2.34	0.48
40:0:6232:HOH:O	14:K:87:ARG:CZ	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:36:ALA:HB1	40:M:9352:HOH:O	2.13	0.48
40:O:5270:HOH:O	17:N:21:HIS:HD2	1.94	0.48
20:Q:40:HIS:CD2	20:Q:60:THR:HG23	2.49	0.48
20:Q:75:ILE:CD1	20:Q:84:ILE:HD11	2.42	0.48
22:S:44:GLN:HE21	25:V:28:LEU:CD2	2.27	0.48
26:W:65:VAL:HA	26:W:68:THR:HG22	1.95	0.48
28:Y:144:ARG:NH1	40:Y:9374:HOH:O	2.46	0.48
1:O:2541:U:H3'	1:O:2541:U:C6	2.47	0.48
6:B:146:THR:C	6:B:148:PRO:HD3	2.34	0.48
8:D:134:LEU:CD1	8:D:166:ILE:HD11	2.41	0.48
10:F:117:GLU:C	10:F:119:ARG:H	2.17	0.48
21:R:96:VAL:HG13	21:R:106:GLY:HA3	1.96	0.48
1:O:1171:A:H2'	1:O:1172:G:H5'	1.94	0.48
1:O:2456:A:H2'	1:O:2457:U:C6	2.48	0.48
1:O:2779:G:H21	9:E:143:GLN:NE2	2.12	0.48
10:F:39:SER:HB3	10:F:45:ALA:HB2	1.96	0.48
12:H:3:ALA:HA	12:H:58:ARG:NH1	2.28	0.48
25:V:7:GLU:O	25:V:11:MET:HG3	2.13	0.48
27:X:61:ARG:HB2	27:X:65:ASN:O	2.14	0.48
1:O:1736:A:H1'	40:O:8069:HOH:O	2.13	0.48
30:1:28:HIS:CE1	30:1:31:LYS:HE2	2.49	0.48
32:3:42:ARG:HH11	32:3:42:ARG:HG3	1.79	0.48
13:J:39:VAL:HG11	13:J:107:ASN:CG	2.34	0.48
17:N:154:LEU:O	17:N:155:GLU:HB3	2.14	0.48
1:O:31:C:OP2	23:T:8:ARG:NH1	2.44	0.48
27:X:61:ARG:HD2	27:X:65:ASN:O	2.14	0.48
2:9:3064:C:C2'	2:9:3065:A:H5'	2.42	0.48
6:B:212:GLN:HB2	6:B:257:THR:CG2	2.38	0.48
12:H:116:ALA:O	12:H:117:PHE:C	2.52	0.48
12:H:58:ARG:O	12:H:62:LEU:HD22	2.14	0.48
23:T:61:GLU:HG3	40:T:3851:HOH:O	2.14	0.48
25:V:39:ALA:O	25:V:41:GLU:N	2.47	0.48
1:O:1044:C:H3'	1:O:1045:G:H5''	1.96	0.48
1:O:1730:G:C5'	1:O:1731:C:H6	2.26	0.48
1:O:2480:G:H3'	40:O:4750:HOH:O	2.14	0.48
1:O:241:A:C2	1:O:378:A:H4'	2.49	0.48
1:O:602:A:O2'	1:O:605:C:H4'	2.12	0.48
1:O:656:G:OP2	18:O:37:ARG:HD2	2.13	0.48
1:O:776:A:OP1	30:1:28:HIS:HE1	1.97	0.48
6:B:277:GLU:N	6:B:278:PRO:HD2	2.29	0.48
9:E:166:VAL:HG12	40:E:3134:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:47:THR:CG2	13:J:48:GLY:N	2.77	0.48
16:M:134:ILE:O	16:M:136:PRO:HD3	2.13	0.48
40:O:7242:HOH:O	17:N:4:PRO:HD2	2.12	0.48
26:W:88:THR:HG22	26:W:90:TYR:CD1	2.49	0.48
1:O:1236:A:C8	13:J:63:ILE:HD11	2.49	0.48
1:O:666:A:H2'	1:O:667:C:O4'	2.14	0.48
4:5:75:C:H2'	4:5:76:A:O4'	2.14	0.48
16:M:59:GLY:HA3	16:M:141:ILE:HD12	1.96	0.48
21:R:29:LYS:NZ	40:R:9449:HOH:O	2.47	0.48
22:S:57:THR:HG22	22:S:58:MET:N	2.28	0.48
27:X:9:VAL:HG13	27:X:88:GLU:OE1	2.14	0.48
1:O:1098:A:H2'	1:O:1099:G:O4'	2.14	0.47
1:O:1189:A:H1'	1:O:1209:C:C1'	2.44	0.47
1:O:2862:G:H4'	6:B:336:GLN:O	2.14	0.47
1:O:558:C:C2'	1:O:559:U:C5'	2.92	0.47
10:F:49:PHE:HE1	10:F:98:VAL:HG23	1.79	0.47
1:O:2504:A:H4'	12:H:71:ARG:HH11	1.80	0.47
6:B:91:PRO:O	13:J:144:THR:HG21	2.14	0.47
14:K:10:GLN:N	14:K:10:GLN:NE2	2.48	0.47
15:L:145:LEU:O	15:L:148:GLU:HG3	2.13	0.47
24:U:4:ARG:HH11	24:U:4:ARG:HG2	1.79	0.47
1:O:2253:G:O2'	1:O:2254:G:H5'	2.15	0.47
1:O:2719:A:C2	6:B:70:PRO:HG3	2.49	0.47
12:H:46:GLN:NE2	12:H:137:TYR:HE2	2.11	0.47
23:T:26:THR:HA	23:T:39:ASN:HB3	1.96	0.47
23:T:96:VAL:CG1	23:T:97:ARG:N	2.78	0.47
1:O:308:U:C4	1:O:342:C:H1'	2.49	0.47
30:I:25:LYS:CD	31:2:49:GLU:H	2.27	0.47
7:C:133:ARG:NH1	40:C:9220:HOH:O	2.47	0.47
12:H:38:LYS:HE2	12:H:42:ASP:CB	2.45	0.47
33:I:139:ILE:C	33:I:140:GLU:HG3	2.34	0.47
13:J:54:VAL:O	13:J:58:GLU:HG3	2.14	0.47
1:O:392:U:C5'	16:M:193:LYS:HB3	2.45	0.47
21:R:82:GLU:O	21:R:86:LYS:HG3	2.14	0.47
25:V:5:VAL:CG1	25:V:9:ARG:NH1	2.77	0.47
1:O:1058:A:H2'	1:O:1060:C:H5''	1.96	0.47
1:O:1149:U:H5''	1:O:1151:G:O4'	2.14	0.47
1:O:210:U:H2'	1:O:211:U:C6	2.49	0.47
1:O:2626:C:H2'	1:O:2627:G:C8	2.50	0.47
1:O:347:A:H2'	1:O:348:C:O4'	2.14	0.47
32:3:11:CYS:HB2	32:3:20:HIS:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3076:G:H3'	2:9:3077:A:C5'	2.26	0.47
6:B:254:GLN:NE2	40:B:9587:HOH:O	2.44	0.47
9:E:31:ARG:HH12	9:E:68:HIS:CG	2.31	0.47
9:E:49:ILE:HD11	9:E:69:ILE:HD12	1.96	0.47
12:H:77:LEU:HD12	12:H:83:TYR:CD2	2.49	0.47
18:O:39:THR:O	18:O:115:ARG:NH2	2.47	0.47
21:R:119:VAL:HG12	21:R:119:VAL:O	2.13	0.47
22:S:57:THR:CG2	22:S:58:MET:N	2.77	0.47
1:0:912:A:C4	1:0:1294:A:C2	3.02	0.47
1:0:1878:G:O2'	1:0:1879:U:P	2.72	0.47
32:3:17:HIS:O	32:3:18:GLN:HG3	2.15	0.47
5:A:123:GLY:HA3	5:A:162:GLY:CA	2.44	0.47
6:B:178:ALA:O	6:B:182:VAL:HG23	2.15	0.47
7:C:157:LEU:CD1	7:C:166:ILE:HD11	2.44	0.47
17:N:15:GLU:HB3	17:N:17:ARG:HD2	1.97	0.47
26:W:64:THR:O	26:W:68:THR:HG22	2.15	0.47
1:0:29:C:C2'	1:0:30:U:H5'	2.44	0.47
1:0:329:A:OP2	7:C:206:ASN:HB2	2.15	0.47
2:9:3003:A:H2'	40:9:2430:HOH:O	2.15	0.47
6:B:87:TYR:OH	6:B:163:GLU:OE2	2.30	0.47
1:0:1167:G:H4'	33:I:135:LEU:HD22	1.96	0.47
17:N:154:LEU:O	17:N:155:GLU:CB	2.63	0.47
19:P:141:ILE:C	19:P:143:ALA:H	2.17	0.47
29:Z:32:GLU:CD	29:Z:70:LYS:HZ2	2.18	0.47
1:0:834:G:H3'	1:0:835:U:H4'	1.97	0.47
1:0:2434:A:O3'	32:3:28:GLY:HA3	2.15	0.47
32:3:20:HIS:HA	32:3:70:ARG:O	2.15	0.47
7:C:140:VAL:HB	40:C:9257:HOH:O	2.14	0.47
8:D:173:GLU:HG3	8:D:174:VAL:N	2.30	0.47
16:M:165:GLY:O	16:M:169:ARG:HG3	2.15	0.47
17:N:7:LYS:HE3	20:Q:21:ARG:O	2.13	0.47
1:0:1667:A:C8	1:0:1667:A:H5'	2.40	0.47
1:0:2133:U:H4'	1:0:2134:G:H5'	1.97	0.47
1:0:2379:G:N3	1:0:2418:G:H2'	2.30	0.47
1:0:635:A:H2'	1:0:636:G:H5''	1.96	0.47
1:0:999:C:H2'	1:0:1000:C:O4'	2.15	0.47
32:3:91:GLN:O	32:3:92:GLU:HB2	2.15	0.47
2:9:3048:C:H4'	17:N:141:ARG:HH21	1.79	0.47
6:B:75:GLU:C	6:B:77:PRO:HD3	2.35	0.47
10:F:14:ASP:O	10:F:18:GLU:HG3	2.14	0.47
10:F:60:VAL:O	10:F:60:VAL:CG1	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:142:ASN:O	13:J:144:THR:N	2.48	0.47
14:K:113:ILE:CG2	14:K:114:ALA:N	2.77	0.47
15:L:53:ARG:HH22	15:L:57:VAL:HG12	1.80	0.47
16:M:86:GLN:O	16:M:88:VAL:HG23	2.15	0.47
21:R:132:ARG:NH2	40:R:9489:HOH:O	2.46	0.47
22:S:38:ALA:O	22:S:42:GLU:HG3	2.15	0.47
24:U:49:LEU:HG	40:U:3805:HOH:O	2.14	0.47
25:V:64:GLY:O	25:V:65:ASP:CB	2.62	0.47
27:X:7:GLU:HA	27:X:74:ALA:O	2.15	0.47
1:0:1158:G:O2'	1:0:1159:G:H5'	2.15	0.47
1:0:1787:C:OP1	19:P:68:LYS:HE2	2.14	0.47
1:0:1921:A:O2'	1:0:1922:A:H5'	2.15	0.47
1:0:764:C:H2'	1:0:765:G:O4'	2.15	0.47
2:9:3029:C:C2'	2:9:3030:C:H5'	2.44	0.47
6:B:215:VAL:HA	6:B:220:VAL:HG22	1.97	0.47
6:B:294:TYR:HE2	40:B:9643:HOH:O	1.97	0.47
33:I:102:VAL:O	33:I:106:LYS:HG3	2.14	0.47
33:I:75:THR:HA	33:I:112:LYS:NZ	2.29	0.47
13:J:19:MET:CE	13:J:132:LEU:HD21	2.44	0.47
1:0:171:C:OP2	16:M:84:LYS:HG3	2.14	0.47
17:N:167:ASP:C	17:N:168:LEU:HG	2.35	0.47
17:N:17:ARG:HB3	17:N:17:ARG:NH1	2.27	0.47
17:N:64:SER:C	17:N:66:LEU:H	2.18	0.47
26:W:149:LEU:HG	26:W:153:MET:HE2	1.96	0.47
1:0:1681:G:H5''	1:0:1682:A:H5'	1.97	0.47
1:0:447:A:O2'	1:0:448:G:H5'	2.15	0.47
5:A:69:LEU:HD23	5:A:107:ASN:CB	2.45	0.47
40:0:5212:HOH:O	6:B:300:SER:HB3	2.15	0.47
9:E:5:LEU:HD21	9:E:66:GLN:HG3	1.95	0.47
9:E:77:THR:OG1	9:E:78:GLU:N	2.47	0.47
14:K:7:ASP:OD2	14:K:81:ARG:NH2	2.48	0.47
15:L:97:VAL:HB	15:L:100:ALA:HB2	1.97	0.47
15:L:21:ARG:N	40:L:9425:HOH:O	2.47	0.47
24:U:52:THR:HG22	24:U:54:THR:H	1.79	0.47
27:X:80:GLU:HG2	27:X:80:GLU:O	2.15	0.47
1:0:1299:G:N7	15:L:6:ARG:NH1	2.63	0.47
1:0:1634:G:H3'	40:0:4467:HOH:O	2.14	0.47
1:0:1641:A:C2'	1:0:1642:A:H5'	2.43	0.47
1:0:1783:A:O2'	1:0:1784:U:H5'	2.15	0.47
1:0:2506:A:O2'	1:0:2507:G:O5'	2.33	0.47
9:E:157:LYS:HD2	9:E:162:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:58:GLU:HA	10:F:61:MET:HG3	1.97	0.47
33:I:72:VAL:CG1	33:I:73:PRO:HD2	2.45	0.47
13:J:52:GLN:HG3	13:J:53:ILE:N	2.30	0.47
22:S:53:ASN:ND2	40:S:9479:HOH:O	2.49	0.47
1:0:1268:C:O2'	28:Y:169:ARG:HB2	2.15	0.47
1:0:1192:A:H3'	1:0:1193:A:H5'	1.96	0.46
1:0:1794:G:N2	1:0:1796:A:H3'	2.30	0.46
1:0:2374:A:H2'	1:0:2375:G:C8	2.51	0.46
1:0:451:C:O2'	1:0:452:G:H5'	2.15	0.46
1:0:657:G:OP1	7:C:27:ARG:NH2	2.30	0.46
7:C:153:VAL:O	7:C:157:LEU:HG	2.15	0.46
1:0:894:A:N1	7:C:87:ARG:NH2	2.63	0.46
8:D:154:LYS:HD2	8:D:154:LYS:N	2.30	0.46
8:D:65:GLU:HG3	40:D:6752:HOH:O	2.14	0.46
33:I:100:LEU:O	33:I:139:ILE:HG23	2.15	0.46
17:N:38:LYS:HD3	17:N:107:ASN:ND2	2.29	0.46
28:Y:155:ARG:NH1	40:Y:9355:HOH:O	2.49	0.46
1:0:1180:U:H1'	40:I:1549:HOH:O	2.14	0.46
1:0:136:C:H2'	1:0:137:U:O4'	2.14	0.46
1:0:1406:A:H5'	1:0:1407:A:C8	2.51	0.46
1:0:2256:G:H2'	1:0:2257:G:C5'	2.46	0.46
1:0:2270:G:H4'	5:A:223:ARG:NH1	2.30	0.46
1:0:449:A:N7	7:C:43:LYS:HG2	2.31	0.46
1:0:603:A:H1'	1:0:605:C:C2	2.50	0.46
32:3:65:THR:HG22	32:3:67:LEU:CG	2.42	0.46
7:C:35:VAL:HG21	7:C:227:GLY:HA2	1.96	0.46
8:D:166:ILE:HB	40:D:6326:HOH:O	2.14	0.46
8:D:88:LEU:HB2	8:D:89:PRO:HD3	1.97	0.46
10:F:102:GLY:O	10:F:103:GLU:HB2	2.15	0.46
33:I:112:LYS:C	33:I:114:PRO:HD2	2.35	0.46
14:K:81:ARG:HD3	14:K:87:ARG:CZ	2.44	0.46
23:T:75:GLU:O	23:T:76:ASP:HB2	2.16	0.46
1:0:56:G:H5''	25:V:50:ARG:NH1	2.31	0.46
40:0:5814:HOH:O	26:W:122:ARG:NH2	2.47	0.46
1:0:1307:A:H2'	1:0:1308:A:C8	2.49	0.46
1:0:1679:C:H5'	40:0:9938:HOH:O	2.16	0.46
5:A:65:ARG:HH11	5:A:65:ARG:HG2	1.80	0.46
8:D:60:GLU:O	8:D:60:GLU:HG3	2.15	0.46
10:F:105:ASP:O	10:F:109:GLU:HB2	2.16	0.46
10:F:56:PRO:HB2	10:F:58:GLU:OE1	2.16	0.46
15:L:57:VAL:HG12	15:L:57:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:W:88:THR:HG23	26:W:110:GLN:HB3	1.97	0.46
1:O:1799:G:H21	19:P:88:GLN:NE2	2.14	0.46
1:O:2453:G:H5'	40:O:5233:HOH:O	2.16	0.46
40:O:3854:HOH:O	6:B:222:LYS:HE2	2.16	0.46
6:B:62:ARG:HG2	6:B:65:MET:HE3	1.97	0.46
7:C:218:VAL:HG12	40:C:9232:HOH:O	2.16	0.46
8:D:172:VAL:CG1	8:D:173:GLU:N	2.78	0.46
13:J:131:THR:HG22	13:J:133:GLY:N	2.30	0.46
25:V:29:ASN:O	25:V:33:VAL:HG23	2.16	0.46
25:V:4:HIS:O	25:V:8:ILE:HG13	2.15	0.46
1:O:1435:U:H5'	40:O:3203:HOH:O	2.15	0.46
1:O:2072:G:H3'	1:O:2073:G:C5'	2.45	0.46
4:5:78:ACA:H61	4:5:79:BTN:H101	1.60	0.46
6:B:41:PHE:HA	6:B:79:MET:CE	2.45	0.46
8:D:58:VAL:N	8:D:62:ASP:O	2.45	0.46
10:F:57:GLU:O	10:F:61:MET:HG3	2.15	0.46
24:U:45:GLU:HB2	24:U:48:ASN:HD22	1.78	0.46
27:X:72:VAL:CG2	27:X:85:VAL:HG12	2.42	0.46
28:Y:102:LEU:HD11	28:Y:225:GLY:HA2	1.97	0.46
1:O:1014:A:H2'	1:O:1015:C:H5'	1.97	0.46
1:O:2587:OMU:H6	1:O:2587:OMU:O5'	2.16	0.46
1:O:702:G:O2'	1:O:703:G:H5'	2.16	0.46
30:1:56:GLU:HG2	30:1:56:GLU:OXT	2.16	0.46
6:B:14:GLY:HA2	6:B:15:PRO:C	2.36	0.46
18:O:26:TRP:N	40:O:3062:HOH:O	2.49	0.46
26:W:4:LEU:CD2	26:W:52:VAL:HG21	2.39	0.46
1:O:1636:G:O2'	1:O:1637:A:H5'	2.15	0.46
1:O:1789:G:O6	19:P:73:HIS:HE1	1.99	0.46
1:O:2511:A:H2'	1:O:2512:U:O4'	2.15	0.46
1:O:319:A:H4'	1:O:338:C:C5	2.49	0.46
6:B:215:VAL:HB	6:B:234:ARG:HH12	1.81	0.46
7:C:236:THR:O	7:C:237:GLU:C	2.53	0.46
8:D:10:PHE:CG	8:D:11:HIS:N	2.84	0.46
12:H:45:VAL:HA	12:H:167:PRO:O	2.15	0.46
12:H:58:ARG:HG3	12:H:58:ARG:NH1	2.30	0.46
33:I:103:ASP:HA	33:I:106:LYS:HD2	1.97	0.46
21:R:39:THR:CG2	21:R:107:GLU:O	2.63	0.46
23:T:71:VAL:HG13	23:T:91:LEU:O	2.16	0.46
28:Y:99:ALA:HB2	28:Y:233:TYR:CZ	2.51	0.46
29:Z:17:ARG:HD3	40:Z:9220:HOH:O	2.15	0.46
29:Z:39:CYS:SG	29:Z:41:ASN:HB3	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1778:A:H2'	1:0:1779:A:H5'	1.97	0.46
1:0:2524:G:H21	1:0:2526:C:N4	2.13	0.46
2:9:3057:A:H8	8:D:141:VAL:HG21	1.80	0.46
6:B:87:TYR:HD1	40:B:9575:HOH:O	1.99	0.46
7:C:236:THR:O	7:C:239:ALA:N	2.49	0.46
1:0:894:A:C2	7:C:87:ARG:NH2	2.83	0.46
33:I:99:ASP:O	33:I:100:LEU:HD23	2.16	0.46
13:J:71:TYR:CG	13:J:72:PRO:HD2	2.51	0.46
15:L:79:ASP:HB3	40:L:9453:HOH:O	2.15	0.46
17:N:183:ASP:O	17:N:184:ILE:O	2.34	0.46
21:R:114:VAL:HG13	21:R:114:VAL:O	2.15	0.46
26:W:142:ASP:HB2	40:W:6373:HOH:O	2.15	0.46
27:X:34:ARG:NH1	27:X:48:VAL:O	2.48	0.46
27:X:43:VAL:CG1	27:X:44:ASP:N	2.79	0.46
1:0:1015:C:H2'	1:0:1016:U:C6	2.51	0.46
1:0:2011:A:H4'	1:0:2012:U:O5'	2.16	0.46
1:0:2487:C:H5	40:0:5422:HOH:O	1.98	0.46
6:B:51:VAL:HG21	6:B:327:VAL:HG13	1.94	0.46
12:H:9:ILE:HD12	12:H:54:THR:HG22	1.97	0.46
14:K:87:ARG:NH1	40:K:4066:HOH:O	2.49	0.46
15:L:91:VAL:CG1	15:L:120:LEU:HD23	2.46	0.46
27:X:20:GLU:HG3	27:X:21:PRO:HD2	1.98	0.46
1:0:1200:A:H3'	40:0:6272:HOH:O	2.15	0.46
1:0:1298:U:H2'	1:0:1299:G:C8	2.50	0.46
1:0:1730:G:H5'	1:0:1731:C:C6	2.51	0.46
1:0:1799:G:H21	19:P:88:GLN:HE22	1.64	0.46
1:0:2372:A:H2'	1:0:2373:U:C6	2.51	0.46
1:0:2505:G:C2'	1:0:2506:A:H5'	2.46	0.46
1:0:802:G:H2'	1:0:803:C:C6	2.50	0.46
1:0:951:A:O2'	1:0:952:G:H5'	2.16	0.46
2:9:3064:C:H2'	2:9:3065:A:H5'	1.97	0.46
2:9:3092:G:H2'	2:9:3093:A:C8	2.51	0.46
1:0:1654:U:H2'	5:A:47:HIS:CD2	2.51	0.46
6:B:217:ARG:HG3	6:B:257:THR:CG2	2.46	0.46
7:C:107:ARG:NE	40:C:9266:HOH:O	2.32	0.46
10:F:107:ASP:O	10:F:111:ILE:HG13	2.16	0.46
25:V:45:ARG:HA	25:V:48:GLU:HB2	1.98	0.46
1:0:2904:U:H4'	27:X:8:ARG:NH1	2.31	0.46
28:Y:152:LYS:HB3	28:Y:160:LYS:HG3	1.98	0.46
1:0:1250:C:O2'	1:0:1251:C:H5'	2.16	0.45
1:0:1878:G:O2'	1:0:1879:U:C5	2.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:3:6:ARG:HA	32:3:20:HIS:O	2.16	0.45
5:A:217:ARG:NH1	5:A:217:ARG:CG	2.78	0.45
5:A:232:ARG:NH2	5:A:236:GLY:O	2.45	0.45
5:A:39:ALA:HB3	5:A:61:GLU:OE2	2.16	0.45
1:0:2346:C:H4'	8:D:52:THR:CG2	2.47	0.45
12:H:54:THR:O	12:H:55:VAL:HG13	2.16	0.45
14:K:101:ASN:O	14:K:102:GLU:HB2	2.17	0.45
26:W:21:LEU:HD13	26:W:26:ILE:HD11	1.99	0.45
26:W:3:ALA:O	26:W:54:PHE:HA	2.16	0.45
1:0:1067:A:H5'	40:0:4906:HOH:O	2.15	0.45
1:0:2338:G:H2'	8:D:129:ASP:OD1	2.16	0.45
6:B:42:ALA:H	6:B:79:MET:HE2	1.81	0.45
6:B:86:ALA:HA	40:B:9575:HOH:O	2.15	0.45
7:C:5:ILE:HG13	7:C:15:GLU:HA	1.99	0.45
7:C:78:ARG:CG	7:C:78:ARG:NH1	2.76	0.45
13:J:8:ALA:HA	13:J:35:THR:HG22	1.98	0.45
26:W:11:VAL:O	26:W:12:ASN:HB2	2.15	0.45
26:W:59:GLN:NE2	26:W:97:ALA:HB3	2.32	0.45
28:Y:117:LEU:HA	28:Y:174:VAL:HG11	1.98	0.45
1:0:1942:A:H3'	40:0:7785:HOH:O	2.16	0.45
1:0:1980:U:H5'	1:0:2626:C:H1'	1.98	0.45
1:0:2356:A:H2'	1:0:2357:G:O4'	2.16	0.45
5:A:130:THR:HB	5:A:137:VAL:HB	1.97	0.45
12:H:43:TYR:HA	12:H:44:PRO:HD3	1.77	0.45
17:N:110:THR:HB	17:N:113:SER:HG	1.80	0.45
19:P:10:ALA:HA	19:P:13:VAL:HG12	1.98	0.45
1:0:1182:C:H1'	1:0:1192:A:C8	2.45	0.45
1:0:1205:U:H2'	1:0:1206:U:H5''	1.99	0.45
1:0:1441:G:H1'	40:0:8275:HOH:O	2.16	0.45
1:0:1603:A:H5''	1:0:1605:G:H5'	1.98	0.45
1:0:2003:U:H4'	1:0:2004:U:H5	1.80	0.45
1:0:2072:G:C6	1:0:2533:C:H1'	2.52	0.45
1:0:558:C:H2'	1:0:559:U:H5''	1.97	0.45
1:0:737:A:H2'	1:0:738:G:O4'	2.16	0.45
6:B:168:GLY:O	6:B:169:GLY:O	2.35	0.45
8:D:167:GLU:C	8:D:169:THR:H	2.20	0.45
33:I:116:LEU:HD22	33:I:127:GLU:OE1	2.17	0.45
16:M:66:SER:HB3	16:M:128:TRP:CD1	2.51	0.45
28:Y:107:PRO:HB3	28:Y:182:PHE:CE2	2.51	0.45
1:0:2672:C:O2'	1:0:2673:U:H5'	2.16	0.45
1:0:2747:C:H4'	40:0:8429:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:27:U:H2'	1:0:28:G:O4'	2.17	0.45
1:0:447:A:OP1	23:T:2:LYS:HG2	2.16	0.45
6:B:97:LEU:HD21	40:B:9637:HOH:O	2.17	0.45
1:0:2101:A:H2'	7:C:63:SER:OG	2.16	0.45
15:L:90:ARG:NH2	15:L:121:ILE:HD11	2.32	0.45
16:M:68:ARG:O	16:M:68:ARG:HD3	2.17	0.45
17:N:154:LEU:CG	17:N:155:GLU:H	2.25	0.45
17:N:73:ALA:HB1	17:N:74:PRO:CD	2.46	0.45
1:0:1180:U:H2'	1:0:1181:A:C8	2.51	0.45
2:9:3041:C:C6	8:D:50:VAL:HG21	2.51	0.45
2:9:3045:A:H4'	8:D:143:LYS:O	2.16	0.45
9:E:95:VAL:HG11	9:E:131:LEU:HD11	1.97	0.45
9:E:31:ARG:HH12	9:E:68:HIS:CE1	2.35	0.45
9:E:69:ILE:HA	9:E:72:MET:CE	2.47	0.45
12:H:136:ALA:HB3	12:H:146:VAL:HG21	1.97	0.45
33:I:89:SER:HB2	33:I:95:ASP:HB2	1.99	0.45
13:J:131:THR:HB	13:J:134:GLU:OE1	2.16	0.45
15:L:143:THR:CG2	15:L:144:ASP:H	2.23	0.45
15:L:77:ALA:C	15:L:79:ASP:H	2.20	0.45
23:T:78:THR:HB	23:T:87:VAL:O	2.17	0.45
22:S:10:VAL:HG11	25:V:36:ALA:CA	2.45	0.45
25:V:8:ILE:HG21	25:V:59:ILE:HG13	1.98	0.45
1:0:1163:G:H2'	1:0:1164:U:C5	2.52	0.45
5:A:223:ARG:CZ	40:A:9562:HOH:O	2.64	0.45
33:I:75:THR:OG1	33:I:112:LYS:HE2	2.17	0.45
15:L:101:ASP:C	15:L:103:ALA:H	2.20	0.45
20:Q:30:VAL:HG12	20:Q:30:VAL:O	2.17	0.45
40:0:6180:HOH:O	23:T:68:ASP:HB2	2.16	0.45
23:T:85:GLU:CG	23:T:86:GLU:N	2.79	0.45
24:U:14:GLU:OE1	24:U:15:PRO:HD2	2.17	0.45
26:W:108:ARG:CG	26:W:114:PRO:HG3	2.44	0.45
26:W:85:ALA:HB2	26:W:91:ASP:O	2.17	0.45
26:W:88:THR:CG2	26:W:90:TYR:HD1	2.29	0.45
1:0:1167:G:H2'	1:0:1168:C:O4'	2.17	0.45
1:0:1201:C:C2'	1:0:1202:A:H5'	2.43	0.45
1:0:1574:C:H2'	1:0:1575:C:C6	2.52	0.45
1:0:2256:G:H2'	1:0:2257:G:H5'	1.99	0.45
1:0:962:C:H5'	40:0:7430:HOH:O	2.16	0.45
5:A:131:HIS:O	5:A:132:ASP:HB2	2.17	0.45
7:C:133:ARG:NE	7:C:138:VAL:HG22	2.30	0.45
7:C:119:ALA:HA	7:C:137:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:44:ILE:HG23	8:D:45:THR:HG23	1.99	0.45
20:Q:53:HIS:CE1	20:Q:55:ARG:HB2	2.52	0.45
23:T:71:VAL:HG12	23:T:72:ILE:H	1.82	0.45
1:0:1477:C:H5'	1:0:1868:G:C5'	2.47	0.45
1:0:790:A:H1'	1:0:1710:A:H2'	1.99	0.45
1:0:2250:G:OP1	5:A:31:LYS:HD3	2.17	0.45
1:0:1168:C:H5''	33:I:87:THR:HG23	1.99	0.45
14:K:80:ILE:O	14:K:87:ARG:HA	2.16	0.45
15:L:149:ARG:O	15:L:150:GLN:HB2	2.16	0.45
16:M:46:LEU:HD22	16:M:50:ARG:HG3	1.98	0.45
20:Q:40:HIS:HD2	20:Q:60:THR:HG23	1.82	0.45
21:R:119:VAL:CG1	21:R:119:VAL:O	2.64	0.45
28:Y:187:VAL:HG23	28:Y:192:ASP:HB3	1.98	0.45
1:0:1015:C:H2'	1:0:1016:U:H6	1.81	0.45
1:0:1180:U:H2'	1:0:1181:A:O4'	2.17	0.45
1:0:2256:G:C2'	1:0:2257:G:H5'	2.47	0.45
1:0:2541:U:C6	1:0:2541:U:C3'	3.00	0.45
1:0:622:G:P	28:Y:148:GLY:HA3	2.57	0.45
1:0:816:G:H5'	1:0:1598:A:H4'	1.97	0.45
1:0:907:A:H2'	1:0:908:A:C8	2.51	0.45
5:A:206:ARG:N	5:A:206:ARG:HD3	2.27	0.45
12:H:146:VAL:HG22	40:H:9543:HOH:O	2.17	0.45
16:M:120:VAL:CG1	16:M:130:GLU:HG3	2.46	0.45
16:M:158:ARG:HB2	16:M:163:LEU:HB2	1.97	0.45
18:O:47:ARG:HG3	18:O:47:ARG:NH1	2.32	0.45
19:P:16:VAL:HG12	19:P:17:GLY:H	1.80	0.45
24:U:4:ARG:NH1	24:U:4:ARG:HG2	2.32	0.45
28:Y:144:ARG:CG	28:Y:144:ARG:NH1	2.71	0.45
5:A:167:LYS:HE3	29:Z:26:VAL:HG13	1.99	0.45
1:0:1350:U:H2'	1:0:1351:G:O4'	2.17	0.44
1:0:2724:U:H2'	1:0:2725:G:O4'	2.17	0.44
1:0:2769:C:H2'	1:0:2770:G:O4'	2.17	0.44
4:5:76:A:OP1	4:5:76:A:H4'	2.17	0.44
5:A:105:VAL:HG12	5:A:106:CYS:H	1.82	0.44
6:B:175:LEU:C	6:B:175:LEU:HD23	2.37	0.44
6:B:41:PHE:CB	6:B:190:MET:HE3	2.47	0.44
9:E:170:ARG:HE	9:E:170:ARG:HB2	1.67	0.44
10:F:33:THR:HG21	10:F:59:ILE:O	2.17	0.44
15:L:89:PHE:CD1	15:L:89:PHE:N	2.85	0.44
17:N:49:THR:HG22	17:N:56:ASP:CB	2.39	0.44
18:O:24:ALA:O	18:O:28:ASP:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2365:G:H4'	20:Q:45:PRO:O	2.17	0.44
27:X:21:PRO:HG2	27:X:24:LYS:HD3	1.98	0.44
28:Y:163:THR:HB	40:Y:9397:HOH:O	2.16	0.44
1:0:1163:G:H1	1:0:1184:C:N4	2.15	0.44
1:0:2443:C:H5'	15:L:57:VAL:HG21	1.99	0.44
1:0:603:A:H4'	1:0:604:G:O5'	2.16	0.44
2:9:3001:U:H5''	2:9:3003:A:OP1	2.17	0.44
2:9:3049:G:H2'	2:9:3050:G:O4'	2.17	0.44
2:9:3056:A:C3'	2:9:3057:A:H5''	2.47	0.44
9:E:31:ARG:NH1	40:E:5919:HOH:O	2.49	0.44
10:F:28:ALA:HB3	10:F:99:THR:O	2.18	0.44
12:H:58:ARG:HG3	40:H:9520:HOH:O	2.18	0.44
14:K:115:ARG:O	14:K:118:ALA:HB3	2.16	0.44
15:L:145:LEU:C	15:L:145:LEU:HD23	2.38	0.44
1:0:1593:C:OP1	19:P:117:SER:HB3	2.17	0.44
25:V:42:ASN:O	25:V:44:GLY:N	2.50	0.44
1:0:2726:U:O2	1:0:2749:U:O5'	2.34	0.44
1:0:656:G:H1'	40:C:9267:HOH:O	2.17	0.44
1:0:794:U:H3	1:0:819:A:H61	1.64	0.44
6:B:113:LEU:HD21	6:B:161:VAL:HG21	1.98	0.44
6:B:185:GLY:HA2	40:B:9628:HOH:O	2.16	0.44
6:B:41:PHE:HA	6:B:79:MET:HE1	1.99	0.44
6:B:8:LYS:HG3	6:B:220:VAL:HG12	1.99	0.44
7:C:107:ARG:NH1	40:C:9238:HOH:O	2.50	0.44
7:C:115:LEU:O	7:C:118:THR:HB	2.17	0.44
9:E:22:VAL:O	9:E:28:SER:HA	2.17	0.44
33:I:97:VAL:N	33:I:136:GLY:O	2.51	0.44
13:J:39:VAL:CG1	13:J:40:ASN:N	2.81	0.44
27:X:41:PHE:O	27:X:43:VAL:HG23	2.16	0.44
27:X:73:ARG:HB2	27:X:88:GLU:OE2	2.17	0.44
1:0:1380:U:O4	1:0:2043:U:H4'	2.17	0.44
5:A:179:MET:HG2	5:A:186:TRP:CG	2.52	0.44
8:D:78:GLU:O	8:D:82:GLU:HG3	2.18	0.44
10:F:5:ASP:O	10:F:119:ARG:NH1	2.50	0.44
13:J:42:GLU:O	13:J:131:THR:HG23	2.18	0.44
15:L:35:ARG:HB2	15:L:35:ARG:HH11	1.82	0.44
1:0:154:C:P	16:M:188:ARG:HH12	2.40	0.44
19:P:143:ALA:HA	40:P:164:HOH:O	2.17	0.44
1:0:2100:A:H4'	7:C:64:GLY:O	2.16	0.44
1:0:2541:U:C2	1:0:2620:U:O4	2.71	0.44
1:0:2857:C:H2'	1:0:2858:U:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:407:A:H5'	40:0:6529:HOH:O	2.18	0.44
1:0:82:C:OP1	23:T:67:LEU:HB2	2.18	0.44
2:9:3114:G:O6	17:N:11:ARG:HD3	2.17	0.44
12:H:29:ALA:C	12:H:30:GLN:HG3	2.38	0.44
1:0:1104:C:H4'	13:J:88:PRO:HD3	1.99	0.44
1:0:1185:U:H5'	40:0:7899:HOH:O	2.18	0.44
1:0:1278:A:H4'	1:0:1279:U:C4	2.52	0.44
1:0:1552:G:H2'	1:0:1553:C:C6	2.52	0.44
1:0:2019:A:H5'	40:0:5087:HOH:O	2.17	0.44
1:0:256:C:H2'	1:0:257:G:O4'	2.17	0.44
6:B:53:LEU:CD1	6:B:327:VAL:HG22	2.46	0.44
6:B:85:ARG:HB2	6:B:99:GLU:HG2	1.99	0.44
33:I:92:PRO:O	33:I:94:GLU:N	2.50	0.44
18:O:60:VAL:HG12	18:O:62:GLY:H	1.81	0.44
23:T:71:VAL:CG1	23:T:72:ILE:N	2.80	0.44
25:V:56:ILE:HG22	25:V:60:GLN:NE2	2.32	0.44
40:0:3165:HOH:O	26:W:119:HIS:HE1	2.01	0.44
1:0:1266:U:H4'	28:Y:115:ARG:HH21	1.82	0.44
1:0:1162:G:H1'	33:I:117:LEU:CD1	2.47	0.44
1:0:1666:C:C2'	1:0:1667:A:C5'	2.96	0.44
1:0:2296:C:H2'	1:0:2297:U:C6	2.52	0.44
1:0:2533:C:H6	1:0:2533:C:C5'	2.25	0.44
1:0:2748:G:H4'	1:0:2749:U:C5'	2.47	0.44
1:0:371:U:H2'	1:0:372:A:H8	1.82	0.44
31:2:5:LYS:O	31:2:9:LYS:HG3	2.17	0.44
2:9:3012:C:H5'	2:9:3070:U:O4'	2.18	0.44
6:B:217:ARG:HD3	6:B:218:TRP:NE1	2.33	0.44
6:B:66:GLU:OE1	6:B:328:ARG:HD2	2.18	0.44
6:B:96:PRO:HG3	40:B:9629:HOH:O	2.17	0.44
7:C:1:MET:HG2	7:C:2:GLN:NE2	2.33	0.44
8:D:60:GLU:O	8:D:61:PHE:C	2.55	0.44
33:I:139:ILE:HG22	33:I:140:GLU:N	2.32	0.44
1:0:645:U:OP2	15:L:4:LYS:HE2	2.18	0.44
16:M:98:GLN:O	16:M:102:GLU:HG3	2.17	0.44
16:M:82:ARG:O	16:M:83:SER:C	2.56	0.44
25:V:5:VAL:HG23	40:V:2271:HOH:O	2.18	0.44
26:W:122:ARG:NE	40:W:5817:HOH:O	2.50	0.44
27:X:18:ARG:NH1	40:X:4132:HOH:O	2.50	0.44
27:X:9:VAL:HG13	27:X:88:GLU:OE2	2.17	0.44
28:Y:203:VAL:CG1	28:Y:228:VAL:HG22	2.48	0.44
1:0:1044:C:H5''	40:0:9648:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1350:U:H1'	40:0:3273:HOH:O	2.17	0.44
1:0:2335:C:H2'	1:0:2336:G:H8	1.83	0.44
1:0:2712:G:H5'	40:K:4183:HOH:O	2.17	0.44
1:0:2895:C:H4'	40:X:4132:HOH:O	2.18	0.44
1:0:29:C:O2'	1:0:30:U:H5'	2.18	0.44
1:0:656:G:H4'	40:C:9167:HOH:O	2.18	0.44
5:A:103:VAL:O	5:A:105:VAL:HG23	2.18	0.44
1:0:1119:G:H8	13:J:52:GLN:HE22	1.66	0.44
1:0:1771:U:C4'	29:Z:20:ARG:HE	2.30	0.44
1:0:1139:U:H2'	1:0:1140:C:C6	2.53	0.44
1:0:1244:U:H2'	13:J:47:THR:HG21	1.99	0.44
1:0:1592:G:O2'	1:0:1593:C:O4'	2.34	0.44
1:0:2472:C:O2'	1:0:2634:G:H4'	2.18	0.44
1:0:960:G:N3	1:0:960:G:C2'	2.81	0.44
6:B:71:VAL:CG1	6:B:296:LEU:HD22	2.48	0.44
12:H:55:VAL:HG12	40:H:9540:HOH:O	2.18	0.44
18:O:4:ASN:HA	18:O:5:PRO:HD3	1.90	0.44
40:0:4557:HOH:O	23:T:82:THR:HA	2.17	0.44
27:X:31:ILE:O	27:X:35:GLU:HG3	2.16	0.44
1:0:1053:G:OP1	12:H:12:PRO:HG3	2.18	0.43
1:0:2044:G:OP1	27:X:23:HIS:HE1	2.01	0.43
1:0:213:G:N2	1:0:225:G:H2'	2.33	0.43
1:0:556:C:H2'	1:0:557:C:C6	2.53	0.43
5:A:132:ASP:HB3	5:A:135:VAL:H	1.83	0.43
7:C:219:ASN:N	7:C:222:ASP:OD1	2.44	0.43
13:J:75:PRO:HB3	13:J:132:LEU:HB3	2.00	0.43
15:L:144:ASP:O	15:L:147:GLU:HB2	2.18	0.43
21:R:61:GLN:NE2	40:R:9449:HOH:O	2.50	0.43
23:T:38:ARG:HG3	23:T:38:ARG:NH1	2.32	0.43
1:0:1086:A:C6	26:W:11:VAL:HG11	2.52	0.43
27:X:61:ARG:HG3	27:X:61:ARG:NH1	2.33	0.43
29:Z:30:GLU:HA	29:Z:33:MET:HB3	1.99	0.43
1:0:157:G:H4'	16:M:95:LYS:HE2	1.99	0.43
1:0:2401:A:H2'	1:0:2402:A:C8	2.53	0.43
1:0:2503:A:OP1	12:H:151:ARG:NH2	2.42	0.43
1:0:338:C:H5''	40:C:9230:HOH:O	2.16	0.43
5:A:29:HIS:CD2	5:A:153:ARG:NH1	2.86	0.43
5:A:105:VAL:HG13	5:A:155:THR:O	2.18	0.43
6:B:279:THR:CG2	6:B:280:VAL:N	2.80	0.43
1:0:2548:C:OP2	6:B:5:ARG:NH2	2.51	0.43
19:P:55:LYS:CG	19:P:56:GLY:N	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Q:25:PRO:HA	20:Q:26:PRO:HD3	1.85	0.43
23:T:30:ASP:O	23:T:33:GLU:HB3	2.18	0.43
23:T:96:VAL:HG13	23:T:97:ARG:N	2.32	0.43
28:Y:106:THR:HG23	28:Y:107:PRO:HD2	1.98	0.43
28:Y:151:SER:HB3	28:Y:154:ARG:HB3	2.00	0.43
31:2:41:HIS:CD2	31:2:44:ARG:H	2.35	0.43
2:9:3057:A:C8	8:D:141:VAL:HG21	2.52	0.43
6:B:181:ILE:HG22	6:B:186:GLY:HA2	1.98	0.43
6:B:243:ASN:HA	6:B:244:PRO:C	2.37	0.43
8:D:88:LEU:N	8:D:89:PRO:CD	2.81	0.43
12:H:169:GLY:C	12:H:170:ASN:HD22	2.20	0.43
28:Y:216:ARG:HD2	40:Y:9368:HOH:O	2.16	0.43
29:Z:60:CYS:O	29:Z:61:ASP:HB2	2.18	0.43
1:0:1174:A:H62	1:0:1200:A:H2'	1.83	0.43
1:0:2568:A:H2'	1:0:2569:A:O4'	2.18	0.43
1:0:2787:C:H5	40:0:5178:HOH:O	2.01	0.43
1:0:661:G:C5	1:0:686:A:C2	3.06	0.43
5:A:123:GLY:HA2	5:A:159:VAL:O	2.18	0.43
40:0:5154:HOH:O	5:A:206:ARG:HD3	2.18	0.43
15:L:130:ARG:O	15:L:131:GLU:C	2.57	0.43
16:M:49:ALA:C	16:M:54:TYR:HB3	2.39	0.43
16:M:72:ALA:HB2	16:M:93:ARG:HG2	2.01	0.43
1:0:1289:C:O2'	1:0:1290:G:H5'	2.19	0.43
1:0:1482:A:O2'	1:0:1483:C:H5'	2.19	0.43
1:0:1928:C:C2'	1:0:1929:G:H5'	2.47	0.43
2:9:3042:C:H5'	2:9:3043:G:OP2	2.17	0.43
2:9:3044:A:O4'	8:D:76:ARG:NE	2.51	0.43
1:0:1884:G:O6	5:A:190:ARG:HD2	2.16	0.43
6:B:36:PRO:HB3	6:B:174:ARG:HB2	1.99	0.43
7:C:123:LEU:HA	7:C:123:LEU:HD23	1.86	0.43
7:C:142:ASP:CG	7:C:237:GLU:HB3	2.39	0.43
7:C:79:ARG:O	7:C:87:ARG:HG2	2.18	0.43
9:E:84:MET:CE	9:E:148:ILE:HD12	2.45	0.43
17:N:11:ARG:CG	17:N:14:ARG:NH1	2.73	0.43
17:N:71:TRP:CE3	17:N:175:LEU:HD22	2.53	0.43
20:Q:59:GLN:HB3	40:Q:6286:HOH:O	2.17	0.43
20:Q:64:GLU:OE1	20:Q:64:GLU:HA	2.18	0.43
26:W:106:THR:OG1	26:W:109:GLU:HG3	2.18	0.43
1:0:1181:A:N1	1:0:1192:A:O2'	2.51	0.43
1:0:1511:U:O2'	1:0:1512:G:H5'	2.18	0.43
1:0:1657:A:H2'	1:0:1658:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2363:G:O3'	20:Q:11:ARG:NH1	2.51	0.43
1:0:2478:U:O2'	1:0:2479:A:H5'	2.19	0.43
1:0:2776:A:H2'	1:0:2777:G:O4'	2.18	0.43
1:0:415:A:O2'	1:0:416:G:H5'	2.19	0.43
1:0:588:G:O6	26:W:154:ARG:NH1	2.52	0.43
7:C:51:TYR:CD1	30:1:56:GLU:HB2	2.54	0.43
9:E:35:TYR:HB2	40:E:5715:HOH:O	2.18	0.43
10:F:11:ASP:O	10:F:14:ASP:HB2	2.17	0.43
12:H:47:ILE:HG21	40:H:9543:HOH:O	2.18	0.43
1:0:903:U:O4	15:L:18:HIS:HB2	2.17	0.43
21:R:104:PHE:HB3	21:R:109:MET:CE	2.49	0.43
26:W:110:GLN:HE21	26:W:110:GLN:HA	1.84	0.43
40:O:6985:HOH:O	28:Y:141:THR:HG23	2.19	0.43
1:0:1218:U:H2'	1:0:1219:U:H6	1.83	0.43
1:0:1878:G:O2'	1:0:1879:U:H6	1.98	0.43
1:0:542:A:H2'	1:0:543:G:O4'	2.19	0.43
30:1:53:LYS:HA	30:1:53:LYS:HD3	1.84	0.43
7:C:194:PHE:HA	7:C:234:VAL:HG13	2.01	0.43
10:F:60:VAL:HG13	10:F:63:ILE:HG13	2.01	0.43
12:H:56:GLN:HG2	12:H:126:ARG:HG2	2.00	0.43
12:H:83:TYR:C	12:H:83:TYR:CD1	2.92	0.43
33:I:132:CYS:C	33:I:134:SER:H	2.21	0.43
15:L:12:THR:HG21	15:L:16:GLY:O	2.18	0.43
16:M:107:ARG:CG	16:M:107:ARG:NH1	2.77	0.43
16:M:24:GLN:O	16:M:28:GLN:HG3	2.19	0.43
7:C:27:ARG:HD2	18:O:5:PRO:HD2	2.01	0.43
19:P:13:VAL:HG21	19:P:41:ARG:HG2	2.01	0.43
23:T:79:LEU:HG	23:T:89:ARG:HB2	2.01	0.43
26:W:146:ILE:HA	26:W:146:ILE:HD13	1.92	0.43
1:0:2856:A:P	27:X:15:ARG:HH22	2.42	0.43
1:0:1236:A:H2'	1:0:1237:U:O4'	2.19	0.43
1:0:2001:G:O2'	1:0:2002:C:H5'	2.19	0.43
1:0:2015:A:O2'	1:0:2016:U:H5'	2.19	0.43
1:0:830:G:H2'	1:0:831:U:C6	2.54	0.43
6:B:109:LEU:HD11	6:B:113:LEU:HD11	2.00	0.43
10:F:49:PHE:CB	10:F:83:LEU:HD11	2.49	0.43
10:F:52:GLU:HG3	10:F:77:VAL:O	2.19	0.43
33:I:132:CYS:C	33:I:134:SER:N	2.71	0.43
40:C:9167:HOH:O	18:O:3:THR:HG21	2.18	0.43
28:Y:112:GLU:OE2	28:Y:115:ARG:NH1	2.52	0.43
1:0:1979:G:HO2'	1:0:1980:U:P	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2676:C:H4'	13:J:70:PHE:HD1	1.83	0.43
1:0:660:A:H4'	1:0:661:G:O5'	2.19	0.43
1:0:710:G:N2	1:0:719:C:C2	2.87	0.43
1:0:907:A:H2'	1:0:908:A:H8	1.84	0.43
40:0:4966:HOH:O	5:A:11:ARG:CZ	2.67	0.43
5:A:217:ARG:HH11	5:A:217:ARG:HG3	1.84	0.43
12:H:166:SER:HB2	12:H:167:PRO:CD	2.48	0.43
1:0:1185:U:H4'	33:I:123:ASN:HB3	2.00	0.43
17:N:48:VAL:HG11	17:N:55:ASP:HB3	1.99	0.43
17:N:74:PRO:HG2	17:N:159:TYR:CE1	2.54	0.43
24:U:52:THR:CG2	24:U:54:THR:HB	2.49	0.43
26:W:108:ARG:HE	26:W:114:PRO:CG	2.32	0.43
1:0:2515:C:H2'	1:0:2516:G:O4'	2.19	0.43
1:0:821:U:H2'	1:0:822:C:H6	1.84	0.43
1:0:883:U:C2'	1:0:883:U:O2	2.65	0.43
7:C:46:TYR:CE2	7:C:98:ARG:NH1	2.87	0.43
10:F:101:ALA:HA	40:F:5413:HOH:O	2.19	0.43
12:H:2:PRO:HD2	12:H:5:MET:SD	2.58	0.43
13:J:39:VAL:HG21	13:J:107:ASN:ND2	2.34	0.43
14:K:13:GLU:OE1	14:K:44:LEU:HD12	2.19	0.43
19:P:105:LEU:CD2	19:P:137:LEU:HD21	2.49	0.43
19:P:55:LYS:HG2	19:P:56:GLY:N	2.33	0.43
25:V:5:VAL:HG11	25:V:9:ARG:NH1	2.33	0.43
28:Y:107:PRO:HB3	28:Y:182:PHE:CD2	2.54	0.43
1:0:818:A:O2'	29:Z:13:ARG:HD2	2.19	0.43
1:0:1008:C:H2'	1:0:1009:U:C6	2.54	0.42
1:0:185:G:H4'	1:0:186:A:H4'	2.00	0.42
1:0:2072:G:N2	40:0:7335:HOH:O	2.50	0.42
1:0:2088:C:H1'	1:0:2841:A:N1	2.34	0.42
1:0:2851:G:H4'	6:B:157:LYS:NZ	2.34	0.42
1:0:292:G:H2'	1:0:358:G:N2	2.33	0.42
5:A:207:GLN:O	5:A:208:HIS:HB3	2.19	0.42
6:B:102:THR:HG23	6:B:182:VAL:HG12	1.99	0.42
6:B:190:MET:CE	6:B:194:PHE:CD1	3.01	0.42
7:C:246:ARG:HB3	7:C:246:ARG:NH1	2.33	0.42
22:S:37:VAL:O	22:S:41:VAL:HG23	2.18	0.42
25:V:12:THR:OG1	25:V:13:PRO:HD2	2.19	0.42
1:0:797:A:O4'	29:Z:10:ARG:N	2.51	0.42
1:0:1151:G:OP1	11:G:63:ARG:NH1	2.52	0.42
1:0:1926:G:H2'	1:0:1927:A:C8	2.54	0.42
1:0:2748:G:H5'	40:0:7972:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:461:C:N3	1:0:479:G:H5'	2.34	0.42
1:0:920:C:H5'	1:0:921:G:C4	2.54	0.42
1:0:958:G:H2'	1:0:959:C:C6	2.53	0.42
31:2:44:ARG:HA	31:2:44:ARG:HD3	1.78	0.42
33:I:102:VAL:HG23	33:I:140:GLU:O	2.18	0.42
15:L:91:VAL:HG12	15:L:120:LEU:HD23	2.01	0.42
16:M:42:ARG:HA	16:M:43:PRO:HD3	1.87	0.42
40:9:5851:HOH:O	17:N:115:VAL:HG13	2.19	0.42
1:0:2866:U:C4	24:U:50:GLU:HB3	2.55	0.42
26:W:142:ASP:HB3	26:W:145:GLY:H	1.84	0.42
1:0:1182:C:C1'	1:0:1192:A:H8	2.30	0.42
1:0:1315:G:C4	28:Y:212:ARG:HB2	2.55	0.42
1:0:1363:G:OP1	7:C:76:ARG:NH2	2.48	0.42
1:0:1947:G:H2'	1:0:1948:G:H8	1.84	0.42
1:0:2134:G:C6	1:0:2258:A:C8	3.08	0.42
1:0:2663:U:O2	40:0:8435:HOH:O	2.22	0.42
1:0:37:A:H2'	1:0:38:G:C8	2.54	0.42
1:0:709:G:O2'	18:O:25:VAL:CG1	2.67	0.42
1:0:816:G:C6	1:0:817:G:N1	2.87	0.42
1:0:952:G:N3	1:0:2302:A:H2'	2.34	0.42
31:2:48:ASP:O	31:2:49:GLU:HB2	2.19	0.42
10:F:111:ILE:O	10:F:115:VAL:HG23	2.19	0.42
12:H:154:TYR:C	12:H:154:TYR:CD1	2.92	0.42
1:0:1819:G:H2'	1:0:1820:G:C4'	2.50	0.42
1:0:2415:A:O2'	17:N:29:SER:HB3	2.19	0.42
1:0:483:C:C4	1:0:484:A:C6	3.07	0.42
1:0:945:U:H2'	1:0:946:C:C6	2.55	0.42
32:3:18:GLN:OE1	32:3:73:GLU:HB3	2.19	0.42
6:B:69:VAL:HA	6:B:70:PRO:HD3	1.84	0.42
7:C:127:ARG:HG2	7:C:127:ARG:HH11	1.85	0.42
11:G:64:ASN:N	11:G:64:ASN:ND2	2.67	0.42
17:N:181:ASP:O	17:N:184:ILE:HG22	2.19	0.42
18:O:98:LEU:O	18:O:102:ILE:HG13	2.19	0.42
1:0:1257:C:H2'	1:0:1258:G:O4'	2.19	0.42
1:0:2064:U:H4'	1:0:2653:A:OP1	2.19	0.42
40:0:7289:HOH:O	7:C:175:LYS:HE3	2.19	0.42
13:J:132:LEU:HA	13:J:132:LEU:HD23	1.82	0.42
16:M:167:GLY:O	16:M:171:ARG:HG3	2.20	0.42
18:O:59:VAL:HG21	18:O:111:VAL:HG21	2.02	0.42
19:P:13:VAL:HG11	19:P:40:VAL:HG12	2.01	0.42
21:R:122:GLN:HB3	21:R:138:SER:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:33:SER:OG	22:S:36:GLU:HG3	2.19	0.42
22:S:51:GLN:HE21	22:S:53:ASN:ND2	1.90	0.42
23:T:14:ALA:HA	23:T:15:PRO:HD3	1.95	0.42
27:X:20:GLU:CG	27:X:21:PRO:HD2	2.49	0.42
29:Z:32:GLU:HA	29:Z:35:GLU:HG3	2.01	0.42
1:O:1342:C:O2'	1:O:1343:C:H5'	2.20	0.42
1:O:1574:C:H6	1:O:1574:C:O5'	2.02	0.42
1:O:2248:C:H3'	40:O:5967:HOH:O	2.18	0.42
1:O:2506:A:O2'	1:O:2507:G:P	2.77	0.42
1:O:2713:G:O2'	1:O:2714:U:H5'	2.20	0.42
1:O:2793:A:H2'	1:O:2794:G:H5'	2.00	0.42
1:O:325:U:H2'	1:O:326:G:H8	1.84	0.42
5:A:109:GLU:HG2	5:A:116:GLY:H	1.85	0.42
5:A:113:GLY:HA2	5:A:153:ARG:NH2	2.34	0.42
14:K:49:LEU:CD1	14:K:80:ILE:HD13	2.49	0.42
16:M:15:PRO:HA	16:M:20:LEU:HD23	2.02	0.42
2:9:3004:G:O2'	17:N:44:ARG:NH2	2.53	0.42
1:O:710:G:H5'	18:O:25:VAL:CG1	2.49	0.42
1:O:107:U:H2'	1:O:108:U:H5'	2.02	0.42
1:O:1298:U:H2'	1:O:1299:G:H8	1.85	0.42
1:O:1422:U:H2'	1:O:1423:C:C6	2.55	0.42
1:O:2911:C:O2'	1:O:2912:C:H5'	2.20	0.42
1:O:470:U:O2'	30:1:16:HIS:CD2	2.70	0.42
1:O:564:G:H1'	40:O:6803:HOH:O	2.18	0.42
2:9:3023:U:O2'	2:9:3024:U:H4'	2.19	0.42
7:C:133:ARG:HE	7:C:138:VAL:HG22	1.85	0.42
13:J:74:ARG:HH12	13:J:76:ASP:CB	2.30	0.42
17:N:36:ALA:HB1	17:N:118:ILE:HD12	2.02	0.42
18:O:38:ARG:NH1	40:O:7674:HOH:O	2.53	0.42
23:T:12:ARG:NH1	40:T:3035:HOH:O	2.47	0.42
25:V:1:THR:CG2	25:V:2:VAL:N	2.82	0.42
26:W:73:LEU:HA	26:W:73:LEU:HD12	1.83	0.42
1:O:1205:U:C2'	1:O:1206:U:H5''	2.50	0.42
1:O:271:C:C2	1:O:273:G:O4'	2.73	0.42
1:O:2821:C:H4'	6:B:116:PRO:HG3	2.01	0.42
1:O:64:G:H2'	1:O:65:C:O4'	2.20	0.42
2:9:3096:C:H2'	2:9:3097:U:C6	2.55	0.42
5:A:51:ARG:NH1	5:A:120:ARG:O	2.53	0.42
6:B:17:LYS:O	6:B:260:HIS:CD2	2.70	0.42
7:C:218:VAL:N	40:C:9232:HOH:O	2.52	0.42
10:F:67:ALA:HB1	10:F:72:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:14:TYR:CD2	12:H:94:VAL:HB	2.54	0.42
33:I:118:SER:HB2	33:I:123:ASN:HB2	2.02	0.42
15:L:6:ARG:NH2	40:L:9444:HOH:O	2.53	0.42
20:Q:94:GLN:O	20:Q:95:GLU:HB2	2.20	0.42
27:X:7:GLU:HA	27:X:75:ALA:HA	2.00	0.42
1:O:1733:A:H4'	6:B:212:GLN:HA	2.02	0.42
1:O:2716:G:H5''	6:B:206:THR:CG2	2.45	0.42
1:O:380:A:H2'	40:O:7673:HOH:O	2.19	0.42
1:O:695:C:H2'	1:O:696:C:C6	2.54	0.42
5:A:33:GLU:OE1	5:A:33:GLU:N	2.36	0.42
6:B:277:GLU:N	6:B:278:PRO:CD	2.82	0.42
10:F:99:THR:HG23	10:F:99:THR:O	2.19	0.42
11:G:23:ILE:O	11:G:27:ILE:HG13	2.20	0.42
12:H:51:VAL:CG1	12:H:53:GLU:O	2.67	0.42
14:K:20:CYS:HB2	14:K:29:LEU:HG	2.01	0.42
15:L:133:VAL:HB	40:L:9452:HOH:O	2.19	0.42
16:M:47:ASP:CG	16:M:48:LYS:N	2.73	0.42
17:N:173:ASP:O	17:N:177:GLU:HB2	2.20	0.42
2:9:3006:C:H4'	17:N:35:VAL:HG11	2.02	0.42
17:N:61:ALA:CB	17:N:88:ALA:HB2	2.48	0.42
22:S:51:GLN:NE2	22:S:53:ASN:HD21	1.90	0.42
29:Z:46:ARG:O	29:Z:57:CYS:HA	2.19	0.42
1:O:1314:U:H2'	40:O:6383:HOH:O	2.20	0.42
1:O:1367:A:H2'	1:O:1368:U:O4'	2.19	0.42
1:O:1940:C:H4'	40:O:7785:HOH:O	2.19	0.42
1:O:2089:A:O2'	1:O:2090:G:H5'	2.20	0.42
1:O:2456:A:H2'	1:O:2457:U:H6	1.85	0.42
1:O:2642:G:H2'	1:O:2643:G:O4'	2.20	0.42
1:O:1739:G:H1'	1:O:2726:U:O4	2.20	0.42
32:3:48:ASN:ND2	32:3:50:GLY:H	2.18	0.42
1:O:1363:G:P	7:C:76:ARG:HH22	2.43	0.42
8:D:10:PHE:CD1	8:D:11:HIS:N	2.88	0.42
11:G:63:ARG:HB2	11:G:66:LEU:HG	2.02	0.42
33:I:92:PRO:HD3	40:I:1549:HOH:O	2.19	0.42
15:L:104:ASP:HB2	40:L:9460:HOH:O	2.19	0.42
27:X:80:GLU:HB3	40:X:5564:HOH:O	2.19	0.42
1:O:1311:G:O2'	1:O:1312:G:H5'	2.20	0.41
1:O:1473:U:O2'	1:O:1474:C:H5''	2.20	0.41
1:O:226:A:H1'	1:O:393:G:C5	2.54	0.41
1:O:629:A:H2'	1:O:630:A:O4'	2.20	0.41
32:3:55:VAL:HB	32:3:56:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:3:69:TYR:O	32:3:77:ALA:HA	2.19	0.41
5:A:122:SER:O	5:A:124:VAL:HG13	2.20	0.41
6:B:62:ARG:CA	6:B:65:MET:HE3	2.49	0.41
7:C:21:VAL:C	7:C:23:GLU:H	2.23	0.41
8:D:167:GLU:OE2	8:D:173:GLU:HB3	2.20	0.41
33:I:74:PRO:C	33:I:112:LYS:HZ1	2.23	0.41
1:0:1242:A:OP2	13:J:60:ARG:NH2	2.46	0.41
1:0:1380:U:O4	1:0:2748:G:O2'	2.28	0.41
1:0:1406:A:H4'	1:0:1407:A:H5''	2.01	0.41
1:0:1902:G:H2'	1:0:1903:U:O4'	2.20	0.41
1:0:2256:G:O2'	1:0:2257:G:H5'	2.21	0.41
1:0:2445:U:H2'	1:0:2446:G:H8	1.85	0.41
1:0:396:U:OP2	32:3:38:ARG:HD2	2.19	0.41
32:3:62:THR:HB	40:3:9487:HOH:O	2.20	0.41
5:A:36:ASP:O	5:A:36:ASP:CG	2.59	0.41
6:B:115:VAL:HA	6:B:116:PRO:HD3	1.93	0.41
40:0:7470:HOH:O	6:B:264:GLU:HG3	2.19	0.41
10:F:70:LYS:C	10:F:72:VAL:H	2.22	0.41
40:0:7460:HOH:O	20:Q:9:GLY:HA2	2.20	0.41
25:V:45:ARG:O	25:V:48:GLU:N	2.53	0.41
5:A:75:GLY:HA2	29:Z:64:PHE:HA	2.02	0.41
1:0:553:G:O4'	1:0:1325:G:H5'	2.20	0.41
1:0:1826:C:O2'	1:0:1827:G:H5'	2.20	0.41
1:0:195:C:H2'	1:0:196:G:H5'	2.01	0.41
6:B:171:VAL:HG23	6:B:172:SER:N	2.35	0.41
6:B:56:ASP:OD1	6:B:322:ARG:HB3	2.21	0.41
8:D:163:VAL:HA	40:D:6326:HOH:O	2.20	0.41
8:D:170:TYR:CD1	8:D:170:TYR:N	2.89	0.41
8:D:173:GLU:O	8:D:174:VAL:C	2.59	0.41
12:H:169:GLY:HA3	40:H:9557:HOH:O	2.20	0.41
33:I:80:LYS:HD3	33:I:86:GLU:O	2.20	0.41
19:P:16:VAL:CG1	19:P:17:GLY:N	2.83	0.41
26:W:38:THR:HG22	26:W:39:ASP:H	1.85	0.41
1:0:1086:A:N6	26:W:11:VAL:HG11	2.35	0.41
1:0:1120:U:H5'	1:0:1121:G:OP2	2.20	0.41
1:0:1174:A:C6	1:0:1201:C:H4'	2.55	0.41
1:0:1451:C:H5'	1:0:1505:U:C4	2.56	0.41
1:0:2015:A:H2'	1:0:2016:U:O4'	2.19	0.41
1:0:2362:A:H2'	1:0:2363:G:C8	2.56	0.41
16:M:81:ARG:HG2	16:M:85:ARG:O	2.19	0.41
18:O:14:LEU:HG	18:O:102:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:89:ASN:HB3	19:P:92:GLU:HB2	2.01	0.41
20:Q:28:ARG:HG2	40:Q:4350:HOH:O	2.20	0.41
24:U:47:ARG:HG2	24:U:54:THR:HG21	2.03	0.41
28:Y:154:ARG:HH11	28:Y:154:ARG:CG	2.34	0.41
1:0:1181:A:H2'	1:0:1182:C:H5'	2.03	0.41
1:0:1183:C:H5	1:0:1192:A:OP1	2.04	0.41
1:0:162:C:H2'	1:0:163:U:H5'	2.02	0.41
1:0:790:A:H1'	1:0:1710:A:O2'	2.21	0.41
1:0:1730:G:H5''	1:0:1731:C:C6	2.55	0.41
1:0:20:G:H5''	1:0:510:U:O4	2.21	0.41
5:A:29:HIS:CD2	5:A:153:ARG:HH12	2.37	0.41
5:A:53:ALA:HB3	40:A:9591:HOH:O	2.20	0.41
15:L:145:LEU:C	15:L:147:GLU:H	2.23	0.41
15:L:73:VAL:HG23	15:L:74:THR:N	2.32	0.41
21:R:96:VAL:O	21:R:99:ALA:HB3	2.20	0.41
26:W:5:VAL:O	26:W:52:VAL:CG2	2.68	0.41
1:0:1524:U:HO2'	1:0:1525:G:P	2.44	0.41
1:0:1979:G:O2'	1:0:1980:U:OP1	2.30	0.41
1:0:2324:G:N2	1:0:2377:U:H1'	2.36	0.41
1:0:407:A:H8	40:0:5010:HOH:O	2.03	0.41
5:A:6:GLY:HA3	40:A:9557:HOH:O	2.20	0.41
5:A:36:ASP:HA	5:A:83:GLY:HA3	2.02	0.41
6:B:294:TYR:C	6:B:294:TYR:CD1	2.93	0.41
6:B:305:ASP:O	6:B:306:LYS:CB	2.67	0.41
6:B:81:ALA:HB1	6:B:142:LEU:HD13	2.03	0.41
33:I:110:GLU:HA	33:I:113:HIS:CD2	2.55	0.41
14:K:2:GLU:O	14:K:3:ALA:C	2.58	0.41
14:K:41:LYS:O	14:K:42:ASN:HB2	2.20	0.41
17:N:170:GLU:O	17:N:174:GLU:HG3	2.21	0.41
26:W:21:LEU:HD22	26:W:26:ILE:HD11	2.02	0.41
1:0:1535:G:H2'	1:0:1536:C:C6	2.56	0.41
1:0:2351:C:H2'	1:0:2352:G:O4'	2.21	0.41
1:0:440:C:H2'	1:0:441:A:C8	2.54	0.41
1:0:447:A:OP1	23:T:1:SER:HB2	2.21	0.41
30:1:8:GLN:HE22	30:1:11:LYS:HZ2	1.65	0.41
2:9:3039:U:O2'	2:9:3042:C:H5	2.03	0.41
5:A:30:ARG:HB3	5:A:30:ARG:HE	1.64	0.41
5:A:95:PRO:HA	5:A:153:ARG:HA	2.03	0.41
15:L:35:ARG:HD3	15:L:35:ARG:C	2.41	0.41
15:L:66:VAL:HG23	15:L:67:ARG:N	2.35	0.41
16:M:164:THR:CG2	16:M:166:ALA:H	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:108:SER:HA	17:N:109:PRO:HD3	1.80	0.41
18:O:45:LEU:CD1	18:O:88:LYS:HD2	2.51	0.41
29:Z:30:GLU:HG2	29:Z:33:MET:CE	2.51	0.41
1:O:1076:G:C2	1:O:1084:C:C2	3.09	0.41
1:O:1427:A:N6	1:O:1440:U:H1'	2.33	0.41
1:O:1594:C:O2'	1:O:1607:A:H4'	2.21	0.41
1:O:1849:G:H1'	1:O:2011:A:N1	2.35	0.41
1:O:2335:C:H2'	1:O:2336:G:C8	2.56	0.41
31:2:11:LEU:HA	31:2:11:LEU:HD23	1.91	0.41
31:2:39:ARG:HG2	40:2:3143:HOH:O	2.21	0.41
6:B:18:ARG:HE	6:B:256:GLN:NE2	2.19	0.41
7:C:61:PHE:HB3	40:C:9251:HOH:O	2.20	0.41
9:E:69:ILE:HA	9:E:72:MET:HE3	2.01	0.41
10:F:12:LEU:HD23	10:F:12:LEU:O	2.21	0.41
13:J:143:LYS:HA	13:J:145:TRP:CZ3	2.55	0.41
15:L:124:ASP:OD1	15:L:149:ARG:NH2	2.54	0.41
15:L:94:ARG:NH1	15:L:143:THR:HG21	2.36	0.41
16:M:76:ARG:HG3	16:M:88:VAL:HG21	2.03	0.41
40:O:3646:HOH:O	19:P:91:LYS:HA	2.21	0.41
21:R:33:ARG:NH1	40:R:9452:HOH:O	2.51	0.41
40:O:4333:HOH:O	23:T:9:LYS:HD2	2.20	0.41
25:V:43:PRO:O	25:V:46:ILE:HG22	2.19	0.41
1:O:1025:C:H5'	26:W:23:MET:O	2.21	0.41
26:W:5:VAL:O	26:W:52:VAL:HG23	2.20	0.41
29:Z:39:CYS:HA	29:Z:40:PRO:HD3	1.97	0.41
1:O:1821:A:O2'	1:O:1822:A:H5'	2.21	0.41
1:O:271:C:H41	1:O:378:A:H2	1.68	0.41
1:O:2748:G:H4'	1:O:2749:U:H5'	2.02	0.41
1:O:2819:C:O4'	6:B:96:PRO:HB2	2.21	0.41
1:O:2820:A:H2'	1:O:2821:C:C6	2.56	0.41
40:O:3421:HOH:O	6:B:252:PRO:HD3	2.21	0.41
6:B:27:ASN:H	6:B:27:ASN:HD22	1.69	0.41
6:B:41:PHE:CD1	6:B:79:MET:CE	3.04	0.41
8:D:23:VAL:O	8:D:23:VAL:HG23	2.21	0.41
10:F:79:GLN:HB2	10:F:82:ASP:OD2	2.21	0.41
33:I:92:PRO:C	33:I:94:GLU:N	2.72	0.41
33:I:93:GLN:HA	33:I:96:PHE:CE2	2.54	0.41
14:K:98:VAL:HG11	14:K:102:GLU:HA	1.99	0.41
1:O:392:U:H5''	16:M:193:LYS:HB3	2.01	0.41
19:P:134:VAL:O	19:P:137:LEU:HB3	2.21	0.41
23:T:81:LYS:HD2	23:T:87:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:45:GLU:HG3	40:X:6178:HOH:O	2.21	0.41
1:0:1414:A:H2'	1:0:1415:G:O4'	2.20	0.41
1:0:2336:G:H1'	40:D:5675:HOH:O	2.20	0.41
1:0:284:C:H4'	1:0:285:A:H8	1.86	0.41
1:0:737:A:H3'	1:0:737:A:C8	2.56	0.41
1:0:1882:C:OP1	5:A:192:VAL:HG23	2.21	0.41
1:0:875:A:C2	5:A:194:MET:SD	3.14	0.41
5:A:65:ARG:NH1	5:A:65:ARG:HG2	2.36	0.41
5:A:66:ARG:HH11	5:A:66:ARG:CB	2.33	0.41
6:B:312:ARG:HG2	6:B:313:PRO:N	2.34	0.41
9:E:84:MET:HB2	9:E:131:LEU:HB2	2.03	0.41
1:0:1181:A:H4'	33:I:92:PRO:HG2	2.03	0.41
14:K:107:THR:HG22	14:K:108:GLU:CG	2.44	0.41
14:K:118:ALA:O	14:K:119:GLN:C	2.59	0.41
17:N:33:ARG:NH1	17:N:103:ASP:OD2	2.47	0.41
17:N:24:LEU:HD13	20:Q:26:PRO:HB3	2.02	0.41
26:W:54:PHE:CZ	26:W:140:LYS:HB2	2.55	0.41
27:X:30:MET:CE	27:X:58:ALA:HB3	2.50	0.41
29:Z:36:ASP:HB3	29:Z:45:ASP:O	2.21	0.41
1:0:1453:G:H2'	1:0:1454:U:O4'	2.21	0.41
1:0:1834:C:H2'	1:0:1840:A:N6	2.36	0.41
1:0:2767:C:OP1	6:B:318:ASN:ND2	2.54	0.41
1:0:2828:G:H2'	1:0:2829:G:O4'	2.21	0.41
1:0:791:A:H2'	1:0:792:G:O4'	2.21	0.41
30:1:28:HIS:O	30:1:32:LYS:N	2.49	0.41
31:2:20:ARG:HG3	31:2:21:VAL:H	1.86	0.41
2:9:3014:G:H2'	2:9:3015:C:H5'	2.03	0.41
15:L:120:LEU:HD12	15:L:133:VAL:HG21	2.02	0.41
18:O:14:LEU:HD23	18:O:102:ILE:HD11	2.02	0.41
18:O:60:VAL:C	18:O:62:GLY:H	2.24	0.41
21:R:68:HIS:CD2	21:R:76:ASP:HB2	2.56	0.41
24:U:17:THR:HG21	40:U:3194:HOH:O	2.21	0.41
26:W:4:LEU:HD23	26:W:54:PHE:HB3	2.03	0.41
28:Y:178:HIS:CG	28:Y:179:PRO:HD2	2.56	0.41
1:0:1724:U:H5''	40:0:4311:HOH:O	2.19	0.40
1:0:1816:C:H2'	1:0:1817:U:O4'	2.21	0.40
1:0:185:G:O3'	1:0:186:A:H4'	2.21	0.40
1:0:2720:C:O2	14:K:87:ARG:NH2	2.54	0.40
1:0:556:C:H2'	1:0:557:C:H6	1.86	0.40
1:0:932:U:H2'	1:0:933:C:C6	2.56	0.40
5:A:135:VAL:HG13	5:A:135:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:140:VAL:HG12	7:C:141:SER:N	2.36	0.40
7:C:72:LYS:HG2	7:C:77:ALA:HA	2.02	0.40
9:E:7:ILE:HD11	9:E:11:VAL:C	2.41	0.40
12:H:114:ARG:O	12:H:115:ALA:C	2.60	0.40
40:O:9644:HOH:O	15:L:30:ARG:HD2	2.20	0.40
25:V:1:THR:OG1	25:V:2:VAL:N	2.53	0.40
28:Y:186:ARG:HG2	28:Y:186:ARG:NH1	2.36	0.40
1:O:1119:G:C6	1:O:1244:U:C5	3.09	0.40
1:O:2329:C:O2'	1:O:2330:U:H5'	2.21	0.40
1:O:2361:A:H2'	1:O:2362:A:O4'	2.21	0.40
1:O:2748:G:C5'	40:O:7972:HOH:O	2.69	0.40
5:A:38:ILE:HD13	5:A:38:ILE:HA	1.92	0.40
6:B:278:PRO:HD3	6:B:294:TYR:CE2	2.56	0.40
8:D:21:VAL:HA	8:D:131:THR:O	2.21	0.40
8:D:23:VAL:CG2	8:D:73:VAL:HB	2.51	0.40
10:F:72:VAL:HA	10:F:73:PRO:HD3	1.92	0.40
17:N:37:ARG:HA	17:N:37:ARG:HD3	1.69	0.40
20:Q:43:ILE:HG13	20:Q:52:PHE:CZ	2.56	0.40
25:V:1:THR:O	25:V:2:VAL:C	2.59	0.40
26:W:4:LEU:CD1	26:W:24:LEU:HD13	2.51	0.40
1:O:120:A:H2'	1:O:120:A:N3	2.37	0.40
1:O:1589:G:N2	1:O:1605:G:H1'	2.35	0.40
1:O:1829:A:C8	1:O:1885:A:C8	3.09	0.40
1:O:2824:C:C5'	1:O:2825:C:H5'	2.51	0.40
5:A:43:VAL:O	5:A:44:ASP:HB2	2.21	0.40
5:A:81:GLN:H	5:A:92:ASN:CG	2.24	0.40
5:A:85:SER:O	5:A:86:ALA:C	2.60	0.40
6:B:81:ALA:O	6:B:186:GLY:HA3	2.22	0.40
6:B:279:THR:HG23	6:B:280:VAL:N	2.35	0.40
6:B:60:SER:HA	6:B:61:PRO:HD3	1.92	0.40
1:O:2101:A:H5'	7:C:63:SER:HB3	2.04	0.40
7:C:84:VAL:HG12	7:C:85:LYS:HG2	2.04	0.40
8:D:91:ALA:HB2	8:D:106:PHE:CD2	2.56	0.40
8:D:67:ASP:O	8:D:69:ILE:HG13	2.21	0.40
12:H:78:GLY:C	12:H:80:GLU:H	2.25	0.40
17:N:103:ASP:OD1	17:N:103:ASP:C	2.60	0.40
23:T:18:GLU:O	23:T:21:LYS:HG2	2.22	0.40
25:V:42:ASN:HB3	40:V:7247:HOH:O	2.21	0.40
25:V:8:ILE:CG2	25:V:59:ILE:HG13	2.51	0.40
28:Y:115:ARG:NE	40:Y:9353:HOH:O	2.55	0.40
28:Y:187:VAL:CG1	28:Y:205:ILE:HG12	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:96:GLU:O	28:Y:235:GLU:HA	2.21	0.40
1:0:1235:G:C1'	13:J:63:ILE:HG23	2.51	0.40
1:0:1299:G:N2	40:0:5226:HOH:O	2.53	0.40
1:0:1462:C:H2'	1:0:1463:A:H8	1.85	0.40
1:0:2070:G:H2'	1:0:2072:G:OP1	2.21	0.40
1:0:294:C:H2'	1:0:295:C:O4'	2.21	0.40
40:0:7989:HOH:O	32:3:60:LYS:HG3	2.21	0.40
15:L:65:ASP:CG	15:L:111:ALA:HB3	2.42	0.40
18:O:59:VAL:HG23	18:O:111:VAL:HG23	2.02	0.40
1:0:1007:A:H2'	12:H:19:TYR:CZ	2.56	0.40
1:0:1081:A:H5''	40:0:3742:HOH:O	2.21	0.40
1:0:1626:A:H2'	1:0:1627:G:C5'	2.52	0.40
1:0:2819:C:H2'	1:0:2820:A:C8	2.56	0.40
1:0:423:A:O2'	1:0:424:C:H5'	2.21	0.40
1:0:565:A:OP2	1:0:592:G:N1	2.49	0.40
30:1:25:LYS:CG	31:2:49:GLU:H	2.35	0.40
32:3:30:GLN:HE21	32:3:30:GLN:HB3	1.61	0.40
2:9:3002:U:OP2	2:9:3003:A:H5'	2.22	0.40
2:9:3008:G:OP1	17:N:23:ARG:NH1	2.51	0.40
2:9:3091:C:H2'	2:9:3092:G:O4'	2.22	0.40
1:0:1881:A:OP1	5:A:199:HIS:HE1	2.04	0.40
6:B:24:PRO:CG	6:B:204:GLY:HA2	2.52	0.40
7:C:57:PRO:HG2	7:C:73:LEU:CD1	2.51	0.40
11:G:16:LYS:O	11:G:20:VAL:HG23	2.22	0.40
13:J:103:VAL:HG12	40:J:5907:HOH:O	2.21	0.40
13:J:80:LYS:HE2	13:J:98:PHE:CZ	2.56	0.40
15:L:67:ARG:HB2	15:L:112:GLY:HA3	2.03	0.40
18:O:23:GLY:C	40:O:3062:HOH:O	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	A	235/240 (98%)	207 (88%)	25 (11%)	3 (1%)	12	17
6	B	335/338 (99%)	309 (92%)	21 (6%)	5 (2%)	10	14
7	C	244/246 (99%)	223 (91%)	19 (8%)	2 (1%)	19	29
8	D	134/177 (76%)	104 (78%)	19 (14%)	11 (8%)	1	0
9	E	170/178 (96%)	162 (95%)	8 (5%)	0	100	100
10	F	117/120 (98%)	103 (88%)	11 (9%)	3 (3%)	5	5
11	G	25/348 (7%)	25 (100%)	0	0	100	100
12	H	156/171 (91%)	136 (87%)	16 (10%)	4 (3%)	5	5
13	J	140/145 (97%)	130 (93%)	6 (4%)	4 (3%)	4	4
14	K	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	19	29
15	L	141/165 (86%)	118 (84%)	21 (15%)	2 (1%)	11	15
16	M	192/194 (99%)	178 (93%)	13 (7%)	1 (0%)	29	41
17	N	184/187 (98%)	161 (88%)	14 (8%)	9 (5%)	2	1
18	O	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
19	P	141/149 (95%)	137 (97%)	4 (3%)	0	100	100
20	Q	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
21	R	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
22	S	79/85 (93%)	73 (92%)	6 (8%)	0	100	100
23	T	117/120 (98%)	107 (92%)	8 (7%)	2 (2%)	9	11
24	U	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
25	V	63/71 (89%)	59 (94%)	1 (2%)	3 (5%)	2	1
26	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
27	X	80/92 (87%)	72 (90%)	8 (10%)	0	100	100
28	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
29	Z	71/83 (86%)	58 (82%)	10 (14%)	3 (4%)	3	2
30	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
31	2	42/50 (84%)	41 (98%)	0	1 (2%)	6	6
32	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	14	20
33	I	68/162 (42%)	54 (79%)	12 (18%)	2 (3%)	4	4
All	All	3705/4430 (84%)	3385 (91%)	263 (7%)	57 (2%)	10	14

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	169	GLY
8	D	60	GLU
8	D	137	PRO
10	F	101	ALA
12	H	166	SER
13	J	143	LYS
15	L	80	ASP
17	N	154	LEU
17	N	184	ILE
29	Z	81	ARG
5	A	37	VAL
6	B	34	GLY
8	D	27	ILE
8	D	61	PHE
8	D	65	GLU
12	H	168	ALA
15	L	143	THR
16	M	83	SER
23	T	53	GLY
25	V	43	PRO
29	Z	20	ARG
31	2	37	HIS
33	I	129	VAL
5	A	86	ALA
6	B	185	GLY
8	D	28	GLY
8	D	56	ARG
8	D	164	ALA
10	F	71	GLY
17	N	183	ASP
23	T	46	ASP
5	A	34	ASP
7	C	8	LEU
7	C	58	ALA
8	D	171	ASP
12	H	16	ARG
12	H	81	GLY
13	J	5	GLU
13	J	7	ASP
17	N	65	ASP
17	N	155	GLU
17	N	162	ASP
8	D	77	ASP

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Mol	Chain	Res	Type
10	F	100	ASP
14	K	126	SER
17	N	164	ASP
17	N	167	ASP
29	Z	42	CYS
32	3	56	PRO
6	B	2	GLN
8	D	16	PRO
13	J	65	ASN
17	N	68	GLU
25	V	40	PRO
25	V	2	VAL
6	B	181	ILE
33	I	73	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	A	179/182 (98%)	165 (92%)	14 (8%)	12	19
6	B	282/283 (100%)	267 (95%)	15 (5%)	22	37
7	C	193/193 (100%)	173 (90%)	20 (10%)	7	10
8	D	117/148 (79%)	112 (96%)	5 (4%)	29	46
9	E	152/156 (97%)	146 (96%)	6 (4%)	32	50
10	F	93/94 (99%)	91 (98%)	2 (2%)	52	71
11	G	27/283 (10%)	27 (100%)	0	100	100
12	H	132/138 (96%)	127 (96%)	5 (4%)	33	51
13	J	118/121 (98%)	108 (92%)	10 (8%)	10	16
14	K	106/106 (100%)	101 (95%)	5 (5%)	26	42
15	L	113/127 (89%)	110 (97%)	3 (3%)	44	65
16	M	158/158 (100%)	153 (97%)	5 (3%)	39	59
17	N	149/150 (99%)	142 (95%)	7 (5%)	26	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	O	93/94 (99%)	92 (99%)	1 (1%)	73	87
19	P	113/117 (97%)	110 (97%)	3 (3%)	44	65
20	Q	79/80 (99%)	75 (95%)	4 (5%)	24	39
21	R	117/122 (96%)	114 (97%)	3 (3%)	46	66
22	S	71/74 (96%)	71 (100%)	0	100	100
23	T	105/106 (99%)	101 (96%)	4 (4%)	33	51
24	U	44/52 (85%)	44 (100%)	0	100	100
25	V	51/57 (90%)	50 (98%)	1 (2%)	55	74
26	W	130/130 (100%)	124 (95%)	6 (5%)	27	43
27	X	66/74 (89%)	63 (96%)	3 (4%)	27	44
28	Y	120/196 (61%)	109 (91%)	11 (9%)	9	13
29	Z	60/68 (88%)	59 (98%)	1 (2%)	60	78
30	1	46/47 (98%)	45 (98%)	1 (2%)	52	71
31	2	42/46 (91%)	41 (98%)	1 (2%)	49	68
32	3	79/79 (100%)	77 (98%)	2 (2%)	47	67
33	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3611 (86%)	2955 (96%)	138 (4%)	27	44

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	3	ARG
5	A	26	ASP
5	A	33	GLU
5	A	36	ASP
5	A	62	ASP
5	A	78	ASP
5	A	94	LEU
5	A	120	ARG
5	A	131	HIS
5	A	151	GLN
5	A	165	THR
5	A	179	MET
5	A	206	ARG
5	A	217	ARG
6	B	11	LEU

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Mol	Chain	Res	Type
6	B	27	ASN
6	B	82	VAL
6	B	84	LEU
6	B	98	THR
6	B	103	ASP
6	B	113	LEU
6	B	149	ASP
6	B	162	MET
6	B	190	MET
6	B	254	GLN
6	B	277	GLU
6	B	279	THR
6	B	307	ARG
6	B	312	ARG
7	C	2	GLN
7	C	16	VAL
7	C	27	ARG
7	C	67	GLN
7	C	76	ARG
7	C	78	ARG
7	C	91	PRO
7	C	94	THR
7	C	101	ASP
7	C	115	LEU
7	C	136	VAL
7	C	162	VAL
7	C	187	ARG
7	C	214	THR
7	C	222	ASP
7	C	223	LEU
7	C	234	VAL
7	C	236	THR
7	C	240	LEU
7	C	243	VAL
8	D	24	HIS
8	D	61	PHE
8	D	100	ASP
8	D	133	ASN
8	D	137	PRO
9	E	7	ILE
9	E	102	VAL
9	E	108	LEU

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Mol	Chain	Res	Type
9	E	155	ASN
9	E	156	ASP
9	E	164	ASP
10	F	12	LEU
10	F	46	GLU
12	H	18	GLU
12	H	84	LYS
12	H	88	ARG
12	H	154	TYR
12	H	159	PRO
13	J	7	ASP
13	J	45	VAL
13	J	46	ILE
13	J	52	GLN
13	J	70	PHE
13	J	74	ARG
13	J	79	PHE
13	J	107	ASN
13	J	127	ILE
13	J	131	THR
14	K	4	LEU
14	K	10	GLN
14	K	56	SER
14	K	84	ASP
14	K	100	GLU
15	L	35	ARG
15	L	43	HIS
15	L	140	VAL
16	M	46	LEU
16	M	68	ARG
16	M	93	ARG
16	M	99	ARG
16	M	116	ASN
17	N	17	ARG
17	N	23	ARG
17	N	26	LEU
17	N	49	THR
17	N	65	ASP
17	N	139	TRP
17	N	152	GLU
18	O	111	VAL
19	P	52	LYS

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Mol	Chain	Res	Type
19	P	98	ILE
19	P	117	SER
20	Q	11	ARG
20	Q	16	ASN
20	Q	57	ASP
20	Q	95	GLU
21	R	13	THR
21	R	132	ARG
21	R	143	VAL
23	T	5	ASP
23	T	39	ASN
23	T	80	GLU
23	T	89	ARG
25	V	65	ASP
26	W	26	ILE
26	W	35	VAL
26	W	78	ASP
26	W	122	ARG
26	W	142	ASP
26	W	146	ILE
27	X	72	VAL
27	X	79	GLU
27	X	82	GLU
28	Y	103	THR
28	Y	141	THR
28	Y	144	ARG
28	Y	154	ARG
28	Y	163	THR
28	Y	174	VAL
28	Y	187	VAL
28	Y	189	ASN
28	Y	200	THR
28	Y	231	PRO
28	Y	235	GLU
29	Z	44	GLU
30	1	47	ASP
31	2	18	ASN
32	3	11	CYS
32	3	65	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	29	HIS
5	A	199	HIS
6	B	27	ASN
6	B	145	HIS
6	B	221	GLN
6	B	238	ASN
6	B	256	GLN
6	B	260	HIS
6	B	320	GLN
6	B	332	ASN
7	C	2	GLN
7	C	39	GLN
7	C	129	HIS
8	D	47	GLN
8	D	103	ASN
8	D	133	ASN
9	E	106	ASN
9	E	143	GLN
11	G	64	ASN
12	H	56	GLN
12	H	59	HIS
12	H	70	ASN
12	H	170	ASN
13	J	52	GLN
13	J	107	ASN
14	K	10	GLN
15	L	18	HIS
15	L	41	HIS
15	L	42	ASN
16	M	24	GLN
16	M	77	HIS
16	M	170	ASN
17	N	93	GLN
17	N	107	ASN
17	N	153	GLN
18	O	100	GLN
19	P	50	GLN
19	P	66	GLN
19	P	73	HIS
19	P	88	GLN
19	P	89	ASN
19	P	118	GLN
20	Q	16	ASN

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Mol	Chain	Res	Type
20	Q	40	HIS
21	R	61	GLN
21	R	94	ASN
21	R	98	ASN
21	R	113	HIS
21	R	117	HIS
22	S	44	GLN
22	S	53	ASN
22	S	55	GLN
23	T	37	GLN
23	T	39	ASN
24	U	39	ASN
24	U	48	ASN
25	V	60	GLN
26	W	2	HIS
26	W	28	HIS
26	W	110	GLN
26	W	119	HIS
26	W	125	HIS
26	W	141	HIS
27	X	22	ASN
27	X	23	HIS
28	Y	119	GLN
28	Y	134	HIS
28	Y	149	GLN
28	Y	189	ASN
29	Z	41	ASN
30	1	8	GLN
30	1	16	HIS
30	1	28	HIS
31	2	16	ASN
31	2	18	ASN
31	2	41	HIS
31	2	45	ASN
32	3	30	GLN
32	3	48	ASN
33	I	113	HIS

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	233 (8%)	32 (1%)
2	9	121/122 (99%)	15 (12%)	1 (0%)
3	4	1/4 (25%)	0	0
4	5	2/6 (33%)	1 (50%)	0
All	All	2869/3054 (93%)	249 (8%)	33 (1%)

All (249) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	86	A
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	186	A
1	0	191	A
1	0	192	A
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	308	U
1	0	309	C
1	0	318	C
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G
1	0	397	A

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Mol	Chain	Res	Type
1	0	417	G
1	0	457	U
1	0	461	C
1	0	473	A
1	0	487	G
1	0	497	A
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	581	G
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	698	A
1	0	701	U
1	0	702	G
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	875	A
1	0	877	G
1	0	878	G

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Mol	Chain	Res	Type
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1087	G
1	0	1088	A
1	0	1100	G
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C

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Mol	Chain	Res	Type
1	0	1378	G
1	0	1407	A
1	0	1409	G
1	0	1474	C
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1528	A
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2006	C
1	0	2008	U

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Mol	Chain	Res	Type
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2103	A
1	0	2110	G
1	0	2238	A
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2317	C
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2467	A
1	0	2469	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2542	C
1	0	2553	A
1	0	2564	G
1	0	2589	U

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Mol	Chain	Res	Type
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2634	G
1	0	2637	A
1	0	2644	C
1	0	2645	U
1	0	2648	U
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2783	A
1	0	2786	G
1	0	2800	A
1	0	2811	A
1	0	2812	A
1	0	2825	C
1	0	2852	A
1	0	2853	U
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3007	G
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3041	C
2	9	3043	G

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Mol	Chain	Res	Type
2	9	3044	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C
4	5	76	A

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A
1	0	129	A
1	0	169	A
1	0	603	A
1	0	644	G
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1232	A
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1506	U
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1730	G
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2536	C
1	0	2541	U
1	0	2637	A
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2761	A

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Mol	Chain	Res	Type
1	0	2852	A
2	9	3065	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	PSU	0	2621	1	17,21,22	1.65	3 (17%)	20,30,33	5.47	4 (20%)
1	1MA	0	628	1,36	15,25,26	0.70	0	15,37,40	1.37	1 (6%)
4	ACA	5	78	4	7,7,8	1.98	1 (14%)	6,6,8	0.91	0
1	OMG	0	2588	1,3	18,26,27	1.12	2 (11%)	20,38,41	2.60	4 (20%)
1	OMU	0	2587	1	14,22,23	1.02	2 (14%)	14,31,34	1.14	1 (7%)
3	PPU	4	76	1,3	18,26,41	0.81	0	15,38,60	0.77	0
3	HFA	4	77	3	10,11,12	0.91	1 (10%)	12,13,15	0.61	0
1	UR3	0	2619	1,38	14,22,23	0.95	1 (7%)	15,32,35	0.58	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1,36	-	0/3/25/26	0/3/3/3
4	ACA	5	78	4	-	0/4/5/6	-
1	OMG	0	2588	1,3	-	0/5/27/28	0/3/3/3
1	OMU	0	2587	1	-	0/7/27/28	0/2/2/2
3	PPU	4	76	1,3	-	0/7/29/44	0/3/3/4
3	HFA	4	77	3	-	0/5/6/8	0/1/1/1
1	UR3	0	2619	1,38	-	0/5/25/26	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	78	ACA	C3-C2	-4.87	1.32	1.52
1	0	2621	PSU	C5-C1'	-4.79	1.48	1.52
1	0	2588	OMG	C6-N1	3.42	1.39	1.33
1	0	2621	PSU	C4-N3	3.27	1.38	1.33
1	0	2587	OMU	C4-N3	2.74	1.37	1.33
1	0	2621	PSU	C2-N1	2.58	1.43	1.38
3	4	77	HFA	OA-CA	2.25	1.48	1.43
1	0	2588	OMG	C8-N7	-2.24	1.30	1.34
1	0	2619	UR3	C6-N1	2.15	1.38	1.35
1	0	2587	OMU	C6-C5	-2.07	1.33	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-17.45	114.56	128.43
1	0	2621	PSU	C4-N3-C2	14.33	127.24	115.14
1	0	2588	OMG	C5-C6-N1	-8.59	111.69	123.43
1	0	2621	PSU	C5-C4-N3	-8.31	114.65	125.36
1	0	2588	OMG	C6-N1-C2	5.80	125.14	115.93
1	0	628	1MA	C2-N3-C4	-4.60	110.83	116.58
1	0	2587	OMU	C5-C4-N3	-3.86	114.82	123.31
1	0	2588	OMG	C2-N3-C4	-3.02	111.91	115.36
1	0	2621	PSU	C6-N1-C2	2.69	119.80	115.36
1	0	2588	OMG	N3-C2-N1	-2.49	123.91	127.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	5	78	ACA	1	0
1	0	2587	OMU	3	0
3	4	76	PPU	1	0
1	0	2619	UR3	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 312 ligands modelled in this entry, 312 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2922 (94%)	-0.63	62 (2%) 60 58	24, 49, 93, 153	0
2	9	122/122 (100%)	-0.24	6 (4%) 29 28	41, 69, 93, 152	0
3	4	2/4 (50%)	-1.10	0 100 100	43, 43, 43, 52	0
4	5	4/6 (66%)	-0.08	1 (25%) 0 0	55, 57, 58, 66	0
5	A	237/240 (98%)	0.33	13 (5%) 25 24	31, 54, 86, 106	0
6	B	337/338 (99%)	0.14	11 (3%) 46 45	31, 55, 79, 93	0
7	C	246/246 (100%)	-0.06	1 (0%) 92 91	27, 49, 70, 87	0
8	D	140/177 (79%)	1.71	44 (31%) 0 0	64, 96, 125, 132	0
9	E	172/178 (96%)	0.74	24 (13%) 2 2	44, 66, 86, 92	0
10	F	119/120 (99%)	1.00	27 (22%) 0 0	49, 74, 100, 112	0
11	G	29/348 (8%)	2.39	18 (62%) 0 0	74, 92, 103, 105	0
12	H	160/171 (93%)	0.60	16 (10%) 7 6	47, 65, 96, 103	0
13	J	142/145 (97%)	-0.01	3 (2%) 63 61	37, 52, 72, 93	0
14	K	132/132 (100%)	-0.15	2 (1%) 73 72	37, 48, 71, 84	0
15	L	145/165 (87%)	0.60	15 (10%) 6 6	29, 69, 112, 121	0
16	M	194/194 (100%)	0.52	19 (9%) 7 7	37, 48, 85, 93	0
17	N	186/187 (99%)	0.90	33 (17%) 1 1	49, 68, 112, 119	0
18	O	115/116 (99%)	0.16	2 (1%) 70 68	40, 59, 73, 81	0
19	P	143/149 (95%)	0.24	3 (2%) 63 61	39, 55, 66, 79	0
20	Q	95/96 (98%)	0.05	4 (4%) 36 35	42, 52, 67, 76	0
21	R	150/155 (96%)	-0.14	0 100 100	33, 47, 66, 75	0
22	S	81/85 (95%)	0.30	3 (3%) 41 41	43, 61, 84, 97	0
23	T	119/120 (99%)	0.67	11 (9%) 9 8	41, 59, 85, 110	0
24	U	53/66 (80%)	0.26	2 (3%) 40 39	42, 56, 73, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	V	65/71 (91%)	1.61	16 (24%) 0 0	56, 78, 115, 120	0
26	W	154/154 (100%)	0.02	2 (1%) 77 75	40, 53, 74, 82	0
27	X	82/92 (89%)	0.67	13 (15%) 1 1	44, 58, 84, 103	0
28	Y	142/241 (58%)	0.10	8 (5%) 24 23	29, 45, 68, 90	0
29	Z	73/83 (87%)	1.74	29 (39%) 0 0	52, 83, 97, 105	0
30	1	56/57 (98%)	-0.43	0 100 100	31, 36, 46, 55	0
31	2	46/50 (92%)	1.44	15 (32%) 0 0	41, 68, 96, 102	0
32	3	92/92 (100%)	0.33	6 (6%) 18 17	41, 61, 73, 86	0
33	I	70/162 (43%)	5.01	57 (81%) 0 0	111, 125, 142, 144	0
All	All	6652/7484 (88%)	0.03	466 (7%) 16 15	24, 54, 100, 153	0

All (466) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	I	71	GLY	15.4
25	V	1	THR	14.2
33	I	79	ILE	12.3
33	I	76	ALA	12.1
33	I	133	THR	11.9
8	D	63	ILE	11.6
29	Z	11	SER	11.4
23	T	119	ALA	10.9
2	9	3001	U	10.2
33	I	85	PHE	10.0
17	N	166	ALA	9.5
8	D	57	THR	9.2
16	M	70	GLY	9.0
29	Z	22	SER	8.9
31	2	49	GLU	8.8
33	I	88	GLY	8.5
25	V	40	PRO	8.5
25	V	39	ALA	8.2
33	I	121	LEU	8.2
33	I	81	ASP	8.1
33	I	75	THR	8.1
33	I	77	GLU	7.9
33	I	137	VAL	7.9
33	I	116	LEU	7.8
33	I	91	GLU	7.8

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Mol	Chain	Res	Type	RSRZ
33	I	105	VAL	7.7
16	M	79	ALA	7.7
33	I	118	SER	7.4
33	I	129	VAL	7.4
33	I	109	ALA	7.4
33	I	87	THR	7.2
33	I	96	PHE	7.1
8	D	90	LEU	7.1
33	I	78	LEU	7.0
5	A	37	VAL	6.8
33	I	126	LYS	6.8
31	2	48	ASP	6.6
2	9	3024	U	6.4
33	I	113	HIS	6.4
33	I	132	CYS	6.3
5	A	237	GLY	6.3
33	I	89	SER	6.3
1	0	282	C	6.1
29	Z	20	ARG	6.0
33	I	93	GLN	5.9
33	I	108	ILE	5.9
23	T	118	SER	5.8
31	2	39	ARG	5.8
29	Z	45	ASP	5.7
33	I	74	PRO	5.5
33	I	111	GLN	5.5
8	D	69	ILE	5.5
25	V	38	GLY	5.5
33	I	107	GLN	5.4
16	M	74	LYS	5.4
27	X	88	GLU	5.4
8	D	64	ARG	5.3
2	9	3023	U	5.2
33	I	83	ALA	5.2
29	Z	18	TYR	5.2
33	I	104	GLN	5.1
31	2	41	HIS	5.1
33	I	80	LYS	5.1
16	M	75	ARG	5.0
27	X	80	GLU	5.0
29	Z	25	ARG	5.0
14	K	132	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
17	N	155	GLU	5.0
29	Z	12	GLY	5.0
33	I	98	ALA	5.0
11	G	26	MET	4.9
11	G	69	ARG	4.9
16	M	86	GLN	4.9
25	V	41	GLU	4.8
29	Z	32	GLU	4.8
1	0	1951	G	4.8
1	0	1199	A	4.8
8	D	61	PHE	4.8
29	Z	21	VAL	4.8
17	N	68	GLU	4.7
33	I	125	ALA	4.7
16	M	71	SER	4.6
29	Z	14	PHE	4.6
16	M	87	GLY	4.6
33	I	138	THR	4.6
15	L	81	VAL	4.6
29	Z	23	ARG	4.6
11	G	23	ILE	4.6
11	G	71	LEU	4.5
31	2	44	ARG	4.5
31	2	47	THR	4.5
33	I	86	GLU	4.5
33	I	102	VAL	4.5
17	N	163	PHE	4.4
8	D	66	GLY	4.4
8	D	170	TYR	4.4
17	N	175	LEU	4.4
2	9	3002	U	4.3
23	T	117	ASP	4.3
1	0	1177	A	4.3
1	0	1172	G	4.3
1	0	2237	G	4.3
1	0	497	A	4.3
1	0	1169	U	4.3
11	G	27	ILE	4.2
17	N	147	ILE	4.2
23	T	116	ASP	4.2
11	G	66	LEU	4.2
9	E	10	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
33	I	114	PRO	4.2
27	X	77	PHE	4.2
12	H	138	CYS	4.2
8	D	44	ILE	4.1
9	E	45	ASP	4.1
1	0	2004	U	4.1
29	Z	37	HIS	4.0
1	0	2508	C	4.0
29	Z	34	ASN	4.0
12	H	73	LEU	4.0
15	L	80	ASP	4.0
12	H	74	ILE	4.0
8	D	26	GLY	4.0
1	0	280	C	4.0
28	Y	216	ARG	4.0
12	H	78	GLY	3.9
33	I	112	LYS	3.9
15	L	93	VAL	3.9
31	2	38	LYS	3.9
28	Y	235	GLU	3.9
8	D	134	LEU	3.9
33	I	122	THR	3.8
10	F	107	ASP	3.8
27	X	41	PHE	3.8
29	Z	24	ARG	3.8
10	F	28	ALA	3.8
8	D	92	GLU	3.7
5	A	31	LYS	3.7
8	D	56	ARG	3.7
15	L	76	LEU	3.7
5	A	133	ARG	3.7
1	0	285	A	3.7
29	Z	33	MET	3.7
1	0	2511	A	3.6
16	M	78	LYS	3.6
25	V	59	ILE	3.6
8	D	154	LYS	3.6
33	I	119	TYR	3.6
12	H	146	VAL	3.6
8	D	10	PHE	3.5
29	Z	19	GLY	3.5
8	D	73	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
9	E	100	ASP	3.5
25	V	37	GLY	3.5
16	M	77	HIS	3.5
1	0	970	U	3.5
9	E	87	PHE	3.5
33	I	134	SER	3.5
1	0	1173	A	3.5
31	2	42	TRP	3.5
29	Z	31	SER	3.5
25	V	36	ALA	3.4
9	E	86	VAL	3.4
10	F	117	GLU	3.4
8	D	40	ILE	3.4
8	D	128	LEU	3.4
31	2	35	ARG	3.4
33	I	99	ASP	3.4
8	D	166	ILE	3.4
17	N	185	GLU	3.4
15	L	97	VAL	3.4
27	X	7	GLU	3.4
17	N	178	THR	3.4
1	0	960	G	3.4
1	0	1198	U	3.4
15	L	100	ALA	3.4
15	L	91	VAL	3.4
33	I	84	GLY	3.3
8	D	88	LEU	3.3
32	3	92	GLU	3.3
1	0	1202	A	3.3
25	V	63	GLU	3.3
22	S	81	ILE	3.3
25	V	8	ILE	3.3
23	T	82	THR	3.3
5	A	36	ASP	3.3
1	0	1948	G	3.3
1	0	2645	U	3.3
1	0	514	G	3.3
16	M	81	ARG	3.3
8	D	18	ILE	3.3
10	F	16	ALA	3.3
8	D	27	ILE	3.3
17	N	95	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
5	A	35	GLY	3.3
16	M	80	GLY	3.2
16	M	72	ALA	3.2
22	S	20	PHE	3.2
33	I	117	LEU	3.2
29	Z	29	ILE	3.2
1	0	1163	G	3.2
8	D	68	PRO	3.2
1	0	2238	A	3.2
8	D	62	ASP	3.2
1	0	1965	C	3.2
27	X	85	VAL	3.2
1	0	272	A	3.2
8	D	41	LEU	3.2
1	0	1966	U	3.2
17	N	184	ILE	3.2
17	N	134	ASP	3.2
15	L	60	GLU	3.2
29	Z	30	GLU	3.2
15	L	145	LEU	3.2
33	I	120	ASP	3.1
8	D	172	VAL	3.1
9	E	124	VAL	3.1
10	F	100	ASP	3.1
15	L	120	LEU	3.1
31	2	27	LEU	3.1
31	2	26	MET	3.1
12	H	171	ALA	3.1
33	I	123	ASN	3.1
8	D	53	LYS	3.1
6	B	104	GLU	3.1
10	F	17	LEU	3.1
33	I	73	PRO	3.1
16	M	76	ARG	3.1
17	N	2	THR	3.1
5	A	32	VAL	3.1
8	D	11	HIS	3.1
13	J	70	PHE	3.1
29	Z	10	ARG	3.1
9	E	127	ASP	3.0
1	0	1950	G	3.0
5	A	65	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
17	N	139	TRP	3.0
17	N	180	LEU	3.0
20	Q	95	GLU	3.0
1	0	735	C	3.0
9	E	88	TYR	3.0
1	0	716	G	3.0
6	B	2	GLN	3.0
10	F	49	PHE	3.0
8	D	107	GLY	3.0
15	L	102	ASP	2.9
33	I	82	GLU	2.9
31	2	37	HIS	2.9
11	G	22	ALA	2.9
28	Y	95	THR	2.9
33	I	72	VAL	2.9
1	0	1180	U	2.9
1	0	284	C	2.9
8	D	173	GLU	2.9
10	F	44	SER	2.9
1	0	1168	C	2.9
17	N	179	LEU	2.9
1	0	358	G	2.9
9	E	6	GLU	2.9
12	H	47	ILE	2.9
29	Z	59	TYR	2.9
8	D	85	GLN	2.9
11	G	73	ASP	2.9
10	F	106	ALA	2.9
12	H	149	ALA	2.9
10	F	22	VAL	2.9
33	I	94	GLU	2.9
1	0	1981	A	2.8
25	V	3	LEU	2.8
10	F	119	ARG	2.8
24	U	47	ARG	2.8
10	F	99	THR	2.8
29	Z	16	ALA	2.8
11	G	72	ASP	2.8
29	Z	26	VAL	2.8
29	Z	36	ASP	2.8
33	I	115	ASP	2.8
1	0	281	U	2.8

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Mol	Chain	Res	Type	RSRZ
10	F	110	ASP	2.8
17	N	67	ALA	2.8
24	U	43	GLY	2.8
11	G	63	ARG	2.8
23	T	112	LEU	2.8
19	P	18	LYS	2.8
8	D	51	ARG	2.8
16	M	82	ARG	2.8
1	0	1200	A	2.8
17	N	138	ASP	2.8
32	3	41	GLU	2.8
8	D	93	LEU	2.8
8	D	89	PRO	2.8
9	E	4	GLU	2.7
1	0	138	U	2.7
1	0	1171	A	2.7
8	D	91	ALA	2.7
8	D	106	PHE	2.7
10	F	12	LEU	2.7
11	G	12	ILE	2.7
17	N	156	GLU	2.7
1	0	1170	U	2.7
13	J	5	GLU	2.7
17	N	71	TRP	2.7
1	0	999	C	2.7
6	B	117	GLU	2.7
25	V	2	VAL	2.7
17	N	165	ALA	2.7
11	G	67	LEU	2.7
12	H	130	GLY	2.7
1	0	1625	U	2.7
11	G	24	VAL	2.7
1	0	10	U	2.7
8	D	167	GLU	2.7
25	V	14	ALA	2.7
27	X	71	ARG	2.7
9	E	11	VAL	2.6
10	F	108	VAL	2.6
12	H	143	ALA	2.6
1	0	1164	U	2.6
12	H	37	GLN	2.6
6	B	180	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
17	N	160	SER	2.6
1	0	1192	A	2.6
16	M	89	THR	2.6
9	E	99	GLY	2.6
27	X	10	VAL	2.6
1	0	1967	U	2.6
28	Y	102	LEU	2.6
10	F	25	ASP	2.6
10	F	98	VAL	2.6
16	M	73	ARG	2.6
17	N	1	ALA	2.6
33	I	97	VAL	2.6
25	V	43	PRO	2.6
10	F	21	GLU	2.6
17	N	159	TYR	2.6
20	Q	18	PRO	2.6
7	C	61	PHE	2.6
8	D	65	GLU	2.6
5	A	85	SER	2.5
11	G	25	GLU	2.5
16	M	84	LYS	2.5
9	E	118	ILE	2.5
17	N	172	PHE	2.5
28	Y	234	VAL	2.5
10	F	70	LYS	2.5
6	B	1	PRO	2.5
17	N	137	ALA	2.5
1	0	2769	C	2.5
10	F	75	ILE	2.5
9	E	44	GLY	2.5
19	P	114	LEU	2.5
6	B	183	GLU	2.5
13	J	4	ALA	2.5
8	D	104	PHE	2.5
20	Q	76	VAL	2.4
1	0	1525	G	2.4
33	I	135	LEU	2.4
27	X	43	VAL	2.4
23	T	77	VAL	2.4
1	0	283	U	2.4
11	G	70	ALA	2.4
5	A	99	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	0	370	G	2.4
11	G	15	TRP	2.4
28	Y	96	GLU	2.4
15	L	79	ASP	2.4
17	N	65	ASP	2.4
12	H	66	ARG	2.4
6	B	128	ILE	2.4
5	A	97	ALA	2.4
23	T	109	GLU	2.4
9	E	126	ILE	2.4
9	E	154	ILE	2.4
32	3	62	THR	2.4
8	D	84	LEU	2.4
9	E	5	LEU	2.4
9	E	48	VAL	2.3
10	F	29	VAL	2.3
1	0	288	A	2.3
2	9	3072	C	2.3
1	0	2748	G	2.3
33	I	103	ASP	2.3
33	I	124	ALA	2.3
8	D	81	GLU	2.3
29	Z	28	GLU	2.3
20	Q	17	LYS	2.3
16	M	85	ARG	2.3
31	2	36	ASN	2.3
1	0	1929	G	2.3
1	0	1947	G	2.3
10	F	15	ASP	2.3
17	N	158	LEU	2.3
31	2	20	ARG	2.3
31	2	43	ARG	2.3
6	B	105	PHE	2.3
1	0	1203	G	2.3
29	Z	35	GLU	2.3
12	H	35	ARG	2.3
27	X	72	VAL	2.3
12	H	111	ASP	2.3
22	S	72	ASP	2.3
11	G	68	GLU	2.3
23	T	115	GLU	2.3
1	0	362	G	2.2

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Mol	Chain	Res	Type	RSRZ
9	E	94	GLN	2.2
17	N	167	ASP	2.2
6	B	134	ALA	2.2
16	M	132	ILE	2.2
27	X	76	ARG	2.2
27	X	65	ASN	2.2
6	B	57	GLU	2.2
28	Y	236	VAL	2.2
8	D	87	ALA	2.2
10	F	24	ARG	2.2
9	E	1	PRO	2.2
14	K	119	GLN	2.2
17	N	106	LEU	2.2
17	N	183	ASP	2.2
28	Y	108	ASP	2.2
12	H	83	TYR	2.2
9	E	161	VAL	2.2
26	W	86	GLU	2.2
15	L	75	LEU	2.2
10	F	19	ALA	2.2
4	5	77	PHE	2.2
17	N	161	GLY	2.2
29	Z	15	GLY	2.2
6	B	119	HIS	2.2
5	A	82	VAL	2.2
8	D	58	VAL	2.2
23	T	110	ALA	2.2
29	Z	27	ALA	2.2
32	3	6	ARG	2.2
15	L	105	TYR	2.1
1	0	359	U	2.1
1	0	371	U	2.1
10	F	11	ASP	2.1
25	V	5	VAL	2.1
27	X	44	ASP	2.1
18	O	23	GLY	2.1
2	9	3122	C	2.1
15	L	148	GLU	2.1
17	N	152	GLU	2.1
18	O	22	GLY	2.1
1	0	2344	G	2.1
10	F	23	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
9	E	105	GLU	2.1
10	F	118	LEU	2.1
25	V	60	GLN	2.1
1	0	1181	A	2.1
1	0	2345	A	2.1
17	N	177	GLU	2.1
9	E	7	ILE	2.1
23	T	59	GLU	2.1
32	3	20	HIS	2.1
29	Z	44	GLU	2.1
1	0	2239	C	2.0
1	0	2747	C	2.0
19	P	110	ASP	2.0
26	W	78	ASP	2.0
5	A	38	ILE	2.0
33	I	110	GLU	2.0
8	D	23	VAL	2.0
9	E	53	GLU	2.0
12	H	137	TYR	2.0
32	3	56	PRO	2.0
11	G	20	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ACA	5	78	8/9	0.88	0.30	66,72,83,86	0
3	HFA	4	77	11/12	0.95	0.20	42,44,47,48	0
1	UR3	0	2619	21/22	0.97	0.15	39,42,45,48	0
1	OMG	0	2588	24/25	0.98	0.13	31,34,39,41	0
1	OMU	0	2587	21/22	0.98	0.13	32,37,40,40	0
3	PPU	4	76	24/38	0.98	0.13	41,44,45,49	0
1	1MA	0	628	23/24	0.98	0.12	32,35,37,38	0
1	PSU	0	2621	20/21	0.98	0.14	36,38,43,43	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
38	SR	0	9529	1/1	-0.08	0.27	131,131,131,131	0
38	SR	0	9484	1/1	0.32	0.14	149,149,149,149	0
36	NA	0	9184	1/1	0.40	0.41	87,87,87,87	0
38	SR	0	9537	1/1	0.50	0.23	157,157,157,157	0
38	SR	0	9547	1/1	0.52	0.39	194,194,194,194	0
34	MG	0	8047	1/1	0.56	0.54	107,107,107,107	0
36	NA	0	9122	1/1	0.57	0.40	90,90,90,90	0
38	SR	9	9588	1/1	0.59	0.14	143,143,143,143	0
38	SR	B	9521	1/1	0.59	0.63	200,200,200,200	0
34	MG	0	8101	1/1	0.61	0.29	80,80,80,80	0
36	NA	0	9182	1/1	0.63	0.39	90,90,90,90	0
38	SR	0	9501	1/1	0.65	0.20	159,159,159,159	0
34	MG	0	8108	1/1	0.68	0.14	103,103,103,103	0
36	NA	D	9151	1/1	0.70	0.23	68,68,68,68	0
36	NA	0	9181	1/1	0.72	0.16	54,54,54,54	0
36	NA	0	9135	1/1	0.72	0.30	55,55,55,55	0
36	NA	0	9141	1/1	0.74	0.13	73,73,73,73	0
36	NA	9	9183	1/1	0.75	0.38	75,75,75,75	0
35	K	0	9002	1/1	0.75	0.18	88,88,88,88	0
39	CD	Z	9203	1/1	0.75	0.13	84,84,84,84	0
36	NA	0	9114	1/1	0.76	0.20	65,65,65,65	0
36	NA	0	9116	1/1	0.77	0.35	52,52,52,52	0
36	NA	0	9152	1/1	0.77	1.03	83,83,83,83	0
36	NA	0	9126	1/1	0.78	0.11	63,63,63,63	0
34	MG	0	8093	1/1	0.79	0.13	49,49,49,49	0
36	NA	J	9146	1/1	0.79	0.11	55,55,55,55	0
36	NA	0	9129	1/1	0.80	0.13	72,72,72,72	0
34	MG	0	8090	1/1	0.80	0.35	68,68,68,68	0
34	MG	0	8092	1/1	0.82	0.34	77,77,77,77	0
34	MG	0	8065	1/1	0.82	0.34	107,107,107,107	0
34	MG	0	8059	1/1	0.83	0.42	84,84,84,84	0
34	MG	0	8052	1/1	0.83	0.25	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	NA	0	9172	1/1	0.83	0.35	76,76,76,76	0
34	MG	0	8037	1/1	0.84	0.10	46,46,46,46	0
34	MG	0	8104	1/1	0.84	0.13	57,57,57,57	0
36	NA	R	9186	1/1	0.84	0.38	80,80,80,80	0
34	MG	0	8107	1/1	0.84	0.17	65,65,65,65	0
34	MG	0	8013	1/1	0.84	0.34	25,25,25,25	0
34	MG	0	8102	1/1	0.85	0.12	68,68,68,68	0
36	NA	0	9158	1/1	0.85	0.44	66,66,66,66	0
36	NA	0	9185	1/1	0.85	0.61	54,54,54,54	0
34	MG	0	8022	1/1	0.85	0.94	112,112,112,112	0
36	NA	0	9132	1/1	0.86	0.22	68,68,68,68	0
36	NA	0	9161	1/1	0.86	0.72	68,68,68,68	0
34	MG	0	8061	1/1	0.86	0.19	87,87,87,87	0
36	NA	0	9169	1/1	0.86	0.39	116,116,116,116	0
36	NA	0	9164	1/1	0.87	0.57	61,61,61,61	0
34	MG	0	8113	1/1	0.87	0.12	52,52,52,52	0
36	NA	0	9102	1/1	0.87	0.22	63,63,63,63	0
36	NA	S	9112	1/1	0.87	0.23	80,80,80,80	0
35	K	0	9001	1/1	0.87	0.31	74,74,74,74	0
34	MG	0	8030	1/1	0.87	0.08	37,37,37,37	0
38	SR	0	9581	1/1	0.87	0.08	130,130,130,130	0
38	SR	0	9500	1/1	0.88	1.54	200,200,200,200	0
34	MG	0	8089	1/1	0.88	0.17	61,61,61,61	0
34	MG	0	8024	1/1	0.88	0.41	86,86,86,86	0
34	MG	5	8118	1/1	0.88	0.34	45,45,45,45	0
34	MG	0	8050	1/1	0.88	0.22	89,89,89,89	0
34	MG	0	8106	1/1	0.88	0.09	51,51,51,51	0
38	SR	0	9539	1/1	0.88	0.38	157,157,157,157	0
34	MG	0	8091	1/1	0.89	0.15	64,64,64,64	0
38	SR	0	9532	1/1	0.89	0.05	120,120,120,120	0
34	MG	0	8072	1/1	0.89	0.65	89,89,89,89	0
36	NA	0	9143	1/1	0.89	0.14	40,40,40,40	0
36	NA	0	9165	1/1	0.89	0.30	45,45,45,45	0
36	NA	0	9140	1/1	0.89	0.15	57,57,57,57	0
34	MG	0	8103	1/1	0.89	0.17	67,67,67,67	0
36	NA	0	9170	1/1	0.89	0.28	77,77,77,77	0
36	NA	0	9166	1/1	0.89	0.09	74,74,74,74	0
38	SR	0	9590	1/1	0.89	0.12	131,131,131,131	0
34	MG	0	8040	1/1	0.90	0.21	92,92,92,92	0
34	MG	0	8058	1/1	0.90	0.21	41,41,41,41	0
34	MG	0	8025	1/1	0.90	0.42	27,27,27,27	0
36	NA	0	9131	1/1	0.90	0.14	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
38	SR	0	9482	1/1	0.90	0.35	135,135,135,135	0
36	NA	0	9128	1/1	0.90	0.15	49,49,49,49	0
34	MG	0	8014	1/1	0.90	0.38	73,73,73,73	0
34	MG	0	8051	1/1	0.90	0.21	36,36,36,36	0
38	SR	9	9503	1/1	0.90	0.05	122,122,122,122	0
36	NA	0	9168	1/1	0.90	0.17	69,69,69,69	0
38	SR	0	9626	1/1	0.91	0.25	154,154,154,154	0
34	MG	0	8055	1/1	0.91	0.31	97,97,97,97	0
36	NA	0	9111	1/1	0.91	0.31	63,63,63,63	0
36	NA	0	9167	1/1	0.91	0.10	65,65,65,65	0
38	SR	0	9504	1/1	0.91	0.11	108,108,108,108	0
36	NA	0	9177	1/1	0.91	0.35	77,77,77,77	0
34	MG	0	8099	1/1	0.91	0.14	75,75,75,75	0
38	SR	0	9459	1/1	0.91	0.10	103,103,103,103	0
38	SR	0	9468	1/1	0.91	0.05	128,128,128,128	0
34	MG	0	8043	1/1	0.91	0.06	52,52,52,52	0
36	NA	0	9174	1/1	0.91	0.38	65,65,65,65	0
36	NA	0	9179	1/1	0.91	0.60	121,121,121,121	0
37	CL	L	9310	1/1	0.92	0.12	58,58,58,58	0
34	MG	0	8094	1/1	0.92	0.50	72,72,72,72	0
36	NA	0	9101	1/1	0.92	0.13	46,46,46,46	0
34	MG	0	8019	1/1	0.92	0.06	51,51,51,51	0
34	MG	0	8063	1/1	0.92	0.10	65,65,65,65	0
38	SR	0	9465	1/1	0.92	0.10	107,107,107,107	0
38	SR	0	9509	1/1	0.92	0.15	95,95,95,95	0
37	CL	A	9309	1/1	0.92	0.19	66,66,66,66	0
34	MG	0	8032	1/1	0.92	0.10	48,48,48,48	0
34	MG	9	8095	1/1	0.92	0.35	55,55,55,55	0
37	CL	J	9301	1/1	0.93	0.18	60,60,60,60	0
36	NA	0	9113	1/1	0.93	0.11	60,60,60,60	0
36	NA	M	9147	1/1	0.93	0.18	42,42,42,42	0
36	NA	0	9159	1/1	0.93	0.35	58,58,58,58	0
36	NA	0	9173	1/1	0.93	0.34	69,69,69,69	0
36	NA	0	9117	1/1	0.93	0.07	51,51,51,51	0
34	MG	0	8085	1/1	0.93	0.21	63,63,63,63	0
36	NA	0	9106	1/1	0.93	0.44	44,44,44,44	0
34	MG	0	8115	1/1	0.93	0.09	59,59,59,59	0
36	NA	0	9171	1/1	0.93	0.31	61,61,61,61	0
36	NA	0	9124	1/1	0.93	0.19	50,50,50,50	0
34	MG	0	8054	1/1	0.93	0.16	63,63,63,63	0
36	NA	0	9175	1/1	0.93	0.33	55,55,55,55	0
36	NA	0	9120	1/1	0.93	0.21	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	MG	0	8036	1/1	0.94	0.11	65,65,65,65	0
34	MG	0	8097	1/1	0.94	0.13	57,57,57,57	0
38	SR	0	9452	1/1	0.94	0.16	106,106,106,106	0
38	SR	0	9508	1/1	0.94	0.08	97,97,97,97	0
34	MG	T	8073	1/1	0.94	0.11	43,43,43,43	0
36	NA	0	9157	1/1	0.94	0.18	47,47,47,47	0
36	NA	0	9150	1/1	0.94	0.21	47,47,47,47	0
36	NA	0	9163	1/1	0.94	0.17	73,73,73,73	0
34	MG	2	8076	1/1	0.94	0.17	64,64,64,64	0
36	NA	0	9110	1/1	0.94	0.33	46,46,46,46	0
39	CD	O	9205	1/1	0.94	0.05	132,132,132,132	0
38	SR	0	9570	1/1	0.94	0.07	111,111,111,111	0
36	NA	0	9149	1/1	0.94	0.29	49,49,49,49	0
34	MG	0	8057	1/1	0.94	0.20	77,77,77,77	0
38	SR	0	9522	1/1	0.95	0.04	114,114,114,114	0
36	NA	0	9155	1/1	0.95	0.18	60,60,60,60	0
34	MG	0	8003	1/1	0.95	0.13	35,35,35,35	0
37	CL	0	9317	1/1	0.95	0.06	52,52,52,52	0
34	MG	0	8068	1/1	0.95	0.14	48,48,48,48	0
34	MG	0	8004	1/1	0.95	0.10	35,35,35,35	0
37	CL	0	9322	1/1	0.95	0.38	61,61,61,61	0
36	NA	0	9125	1/1	0.95	0.81	92,92,92,92	0
38	SR	H	9486	1/1	0.95	0.15	125,125,125,125	0
38	SR	0	9517	1/1	0.95	0.06	110,110,110,110	0
34	MG	0	8082	1/1	0.95	0.20	82,82,82,82	0
38	SR	0	9505	1/1	0.95	0.07	106,106,106,106	0
38	SR	0	9483	1/1	0.95	0.06	77,77,77,77	0
37	CL	J	9321	1/1	0.95	0.11	66,66,66,66	0
34	MG	0	8045	1/1	0.95	0.26	72,72,72,72	0
38	SR	0	9560	1/1	0.95	0.08	101,101,101,101	0
34	MG	0	8116	1/1	0.95	0.10	64,64,64,64	0
34	MG	0	8083	1/1	0.95	0.11	53,53,53,53	0
36	NA	C	9104	1/1	0.95	0.16	33,33,33,33	0
38	SR	0	9495	1/1	0.95	0.14	111,111,111,111	0
37	CL	M	9318	1/1	0.95	0.17	41,41,41,41	0
34	MG	0	8098	1/1	0.95	0.07	45,45,45,45	0
34	MG	0	8079	1/1	0.95	0.13	33,33,33,33	0
36	NA	0	9139	1/1	0.95	0.10	43,43,43,43	0
34	MG	0	8029	1/1	0.95	0.22	35,35,35,35	0
34	MG	0	8067	1/1	0.95	0.11	40,40,40,40	0
34	MG	0	8021	1/1	0.95	0.16	56,56,56,56	0
34	MG	0	8070	1/1	0.96	0.14	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	NA	0	9162	1/1	0.96	0.15	52,52,52,52	0
37	CL	J	9302	1/1	0.96	0.07	53,53,53,53	0
36	NA	R	9137	1/1	0.96	0.08	36,36,36,36	0
38	SR	F	9595	1/1	0.96	0.16	109,109,109,109	0
36	NA	0	9156	1/1	0.96	0.16	57,57,57,57	0
38	SR	0	9490	1/1	0.96	0.13	116,116,116,116	0
38	SR	0	9530	1/1	0.96	0.11	72,72,72,72	0
34	MG	0	8060	1/1	0.96	0.07	82,82,82,82	0
38	SR	0	9440	1/1	0.96	0.05	72,72,72,72	0
37	CL	Y	9320	1/1	0.96	0.08	47,47,47,47	0
36	NA	0	9178	1/1	0.96	0.45	54,54,54,54	0
38	SR	0	9585	1/1	0.96	0.08	94,94,94,94	0
37	CL	3	9304	1/1	0.96	0.07	61,61,61,61	0
36	NA	0	9107	1/1	0.96	0.40	71,71,71,71	0
38	SR	0	9433	1/1	0.96	0.12	75,75,75,75	0
36	NA	0	9115	1/1	0.96	0.18	41,41,41,41	0
34	MG	0	8042	1/1	0.96	0.11	48,48,48,48	0
34	MG	Y	8109	1/1	0.96	0.12	45,45,45,45	0
34	MG	0	8112	1/1	0.96	0.06	46,46,46,46	0
36	NA	0	9105	1/1	0.96	0.09	44,44,44,44	0
37	CL	N	9307	1/1	0.96	0.16	65,65,65,65	0
38	SR	0	9447	1/1	0.97	0.07	73,73,73,73	0
34	MG	0	8027	1/1	0.97	0.24	36,36,36,36	0
37	CL	0	9316	1/1	0.97	0.26	78,78,78,78	0
34	MG	0	8002	1/1	0.97	0.09	34,34,34,34	0
34	MG	A	8066	1/1	0.97	0.10	57,57,57,57	0
37	CL	0	9311	1/1	0.97	0.15	71,71,71,71	0
38	SR	0	9426	1/1	0.97	0.08	71,71,71,71	0
34	MG	0	8009	1/1	0.97	0.10	21,21,21,21	0
34	MG	0	8114	1/1	0.97	0.47	83,83,83,83	0
38	SR	0	9466	1/1	0.97	0.06	96,96,96,96	0
38	SR	0	9545	1/1	0.97	0.06	85,85,85,85	0
38	SR	A	9437	1/1	0.97	0.10	70,70,70,70	0
37	CL	0	9315	1/1	0.97	0.09	52,52,52,52	0
34	MG	0	8012	1/1	0.97	0.22	39,39,39,39	0
38	SR	0	9601	1/1	0.97	0.06	119,119,119,119	0
38	SR	0	9438	1/1	0.97	0.09	70,70,70,70	0
34	MG	0	8117	1/1	0.97	0.12	46,46,46,46	0
38	SR	0	9446	1/1	0.97	0.07	88,88,88,88	0
34	MG	0	8044	1/1	0.97	0.06	35,35,35,35	0
38	SR	0	9534	1/1	0.97	0.14	111,111,111,111	0
36	NA	0	9127	1/1	0.97	0.10	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
38	SR	0	9442	1/1	0.97	0.10	66,66,66,66	0
38	SR	A	9436	1/1	0.97	0.06	60,60,60,60	0
34	MG	0	8088	1/1	0.97	0.11	28,28,28,28	0
34	MG	0	8046	1/1	0.97	0.05	39,39,39,39	0
36	NA	0	9108	1/1	0.97	0.10	34,34,34,34	0
36	NA	0	9160	1/1	0.97	0.17	46,46,46,46	0
36	NA	0	9138	1/1	0.97	0.07	62,62,62,62	0
38	SR	0	9568	1/1	0.97	0.07	80,80,80,80	0
34	MG	K	8069	1/1	0.97	0.17	25,25,25,25	0
38	SR	0	9405	1/1	0.97	0.16	59,59,59,59	0
38	SR	0	9432	1/1	0.97	0.14	68,68,68,68	0
34	MG	0	8041	1/1	0.97	0.09	55,55,55,55	0
36	NA	0	9134	1/1	0.97	0.10	47,47,47,47	0
34	MG	0	8084	1/1	0.97	0.40	89,89,89,89	0
37	CL	R	9306	1/1	0.97	0.10	45,45,45,45	0
34	MG	0	8110	1/1	0.97	0.11	45,45,45,45	0
38	SR	0	9489	1/1	0.98	0.11	94,94,94,94	0
34	MG	0	8075	1/1	0.98	0.07	47,47,47,47	0
38	SR	0	9464	1/1	0.98	0.05	81,81,81,81	0
38	SR	0	9477	1/1	0.98	0.10	86,86,86,86	0
38	SR	0	9421	1/1	0.98	0.10	78,78,78,78	0
34	MG	0	8001	1/1	0.98	0.19	22,22,22,22	0
38	SR	0	9629	1/1	0.98	0.08	75,75,75,75	0
38	SR	0	9566	1/1	0.98	0.04	80,80,80,80	0
38	SR	9	9481	1/1	0.98	0.08	89,89,89,89	0
34	MG	0	8020	1/1	0.98	0.16	36,36,36,36	0
34	MG	0	8056	1/1	0.98	0.23	44,44,44,44	0
38	SR	0	9454	1/1	0.98	0.10	82,82,82,82	0
38	SR	0	9435	1/1	0.98	0.08	76,76,76,76	0
37	CL	0	9305	1/1	0.98	0.07	61,61,61,61	0
38	SR	0	9427	1/1	0.98	0.12	56,56,56,56	0
38	SR	0	9443	1/1	0.98	0.10	63,63,63,63	0
34	MG	0	8031	1/1	0.98	0.12	49,49,49,49	0
38	SR	0	9475	1/1	0.98	0.13	83,83,83,83	0
38	SR	0	9445	1/1	0.98	0.09	57,57,57,57	0
36	NA	0	9118	1/1	0.98	0.21	66,66,66,66	0
38	SR	0	9506	1/1	0.98	0.04	68,68,68,68	0
36	NA	0	9154	1/1	0.98	0.15	54,54,54,54	0
36	NA	0	9130	1/1	0.98	0.15	50,50,50,50	0
38	SR	0	9461	1/1	0.98	0.06	82,82,82,82	0
34	MG	0	8039	1/1	0.98	0.17	49,49,49,49	0
34	MG	0	8096	1/1	0.98	0.05	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
38	SR	0	9456	1/1	0.98	0.10	67,67,67,67	0
38	SR	0	9469	1/1	0.98	0.05	85,85,85,85	0
38	SR	0	9455	1/1	0.98	0.10	88,88,88,88	0
36	NA	0	9136	1/1	0.98	0.12	34,34,34,34	0
34	MG	0	8005	1/1	0.98	0.06	29,29,29,29	0
38	SR	0	9457	1/1	0.98	0.08	51,51,51,51	0
38	SR	0	9414	1/1	0.98	0.12	57,57,57,57	0
38	SR	0	9441	1/1	0.98	0.07	68,68,68,68	0
34	MG	0	8017	1/1	0.98	0.14	31,31,31,31	0
36	NA	Q	9148	1/1	0.98	0.09	49,49,49,49	0
38	SR	0	9462	1/1	0.98	0.10	74,74,74,74	0
34	MG	0	8080	1/1	0.98	0.17	57,57,57,57	0
38	SR	A	9497	1/1	0.98	0.09	96,96,96,96	0
37	CL	0	9312	1/1	0.99	0.10	57,57,57,57	0
38	SR	0	9478	1/1	0.99	0.06	77,77,77,77	0
34	MG	0	8026	1/1	0.99	0.15	30,30,30,30	0
34	MG	0	8028	1/1	0.99	0.13	37,37,37,37	0
38	SR	0	9428	1/1	0.99	0.07	55,55,55,55	0
37	CL	0	9314	1/1	0.99	0.06	51,51,51,51	0
38	SR	0	9449	1/1	0.99	0.09	67,67,67,67	0
38	SR	0	9473	1/1	0.99	0.03	82,82,82,82	0
38	SR	0	9467	1/1	0.99	0.10	86,86,86,86	0
34	MG	0	8008	1/1	0.99	0.19	16,16,16,16	0
38	SR	0	9410	1/1	0.99	0.14	41,41,41,41	0
38	SR	0	9431	1/1	0.99	0.13	65,65,65,65	0
38	SR	0	9430	1/1	0.99	0.10	49,49,49,49	0
38	SR	0	9515	1/1	0.99	0.14	100,100,100,100	0
37	CL	B	9319	1/1	0.99	0.17	54,54,54,54	0
38	SR	0	9488	1/1	0.99	0.11	86,86,86,86	0
39	CD	1	9202	1/1	0.99	0.05	54,54,54,54	0
38	SR	0	9451	1/1	0.99	0.12	60,60,60,60	0
38	SR	0	9413	1/1	0.99	0.12	49,49,49,49	0
38	SR	0	9408	1/1	0.99	0.12	36,36,36,36	0
36	NA	0	9123	1/1	0.99	0.09	52,52,52,52	0
38	SR	L	9409	1/1	0.99	0.07	37,37,37,37	0
38	SR	0	9425	1/1	0.99	0.15	56,56,56,56	0
38	SR	0	9434	1/1	0.99	0.14	64,64,64,64	0
39	CD	3	9204	1/1	0.99	0.03	64,64,64,64	0
38	SR	1	9419	1/1	0.99	0.09	40,40,40,40	0
38	SR	0	9480	1/1	0.99	0.05	93,93,93,93	0
38	SR	3	9439	1/1	0.99	0.05	72,72,72,72	0
34	MG	0	8015	1/1	0.99	0.09	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
38	SR	0	9417	1/1	0.99	0.08	63,63,63,63	0
38	SR	0	9474	1/1	0.99	0.08	73,73,73,73	0
37	CL	0	9313	1/1	0.99	0.10	59,59,59,59	0
38	SR	1	9460	1/1	0.99	0.10	52,52,52,52	0
37	CL	O	9308	1/1	0.99	0.09	67,67,67,67	0
34	MG	0	8074	1/1	0.99	0.18	27,27,27,27	0
34	MG	0	8038	1/1	0.99	0.25	25,25,25,25	0
37	CL	0	9303	1/1	0.99	0.13	53,53,53,53	0
38	SR	S	9470	1/1	0.99	0.16	101,101,101,101	0
38	SR	0	9411	1/1	0.99	0.14	43,43,43,43	0
38	SR	0	9450	1/1	0.99	0.07	72,72,72,72	0
38	SR	0	9429	1/1	0.99	0.10	72,72,72,72	0
38	SR	0	9453	1/1	0.99	0.06	72,72,72,72	0
38	SR	R	9418	1/1	0.99	0.15	57,57,57,57	0
38	SR	0	9444	1/1	0.99	0.05	55,55,55,55	0
38	SR	0	9422	1/1	0.99	0.10	58,58,58,58	0
38	SR	0	9412	1/1	0.99	0.13	45,45,45,45	0
38	SR	0	9498	1/1	0.99	0.05	63,63,63,63	0
38	SR	B	9458	1/1	0.99	0.05	82,82,82,82	0
38	SR	0	9407	1/1	1.00	0.13	47,47,47,47	0
38	SR	0	9424	1/1	1.00	0.16	49,49,49,49	0
38	SR	0	9448	1/1	1.00	0.07	63,63,63,63	0
38	SR	0	9423	1/1	1.00	0.05	64,64,64,64	0
38	SR	0	9406	1/1	1.00	0.13	35,35,35,35	0
38	SR	0	9415	1/1	1.00	0.10	56,56,56,56	0
38	SR	0	9416	1/1	1.00	0.08	43,43,43,43	0
39	CD	U	9201	1/1	1.00	0.09	53,53,53,53	0
38	SR	0	9420	1/1	1.00	0.17	70,70,70,70	0

6.5 Other polymers

There are no such residues in this entry.