



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 05:22 AM GMT

PDB ID : 1VQ5  
Title : The structure of the transition state analogue "RAA" bound to the large ribosomal subunit of haloarcula marismortui  
Authors : Schmeing, T.M.; Steitz, T.A.  
Deposited on : 2004-12-16  
Resolution : 2.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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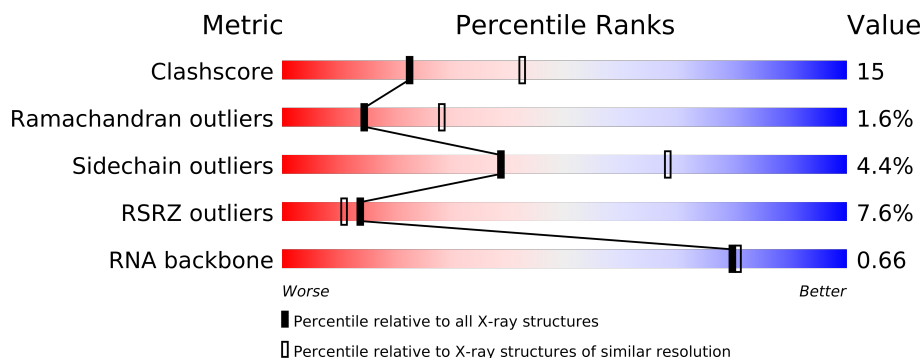
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.60 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	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)
RNA backbone	1838	1002 (3.12-2.08)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	0	2922	
2	9	122	
3	4	8	
4	A	240	
5	B	338	
6	C	246	
7	D	177	
8	E	178	
9	F	120	
10	G	348	
11	H	171	
12	J	145	
13	K	132	
14	L	165	

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Mol	Chain	Length	Quality of chain
15	M	194	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	
30	2	50	
31	3	92	
32	I	162	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
33	MG	0	8011	-	X
33	MG	0	8016	-	X
33	MG	0	8023	-	X
33	MG	0	8041	-	X
33	MG	0	8049	-	X
33	MG	0	8053	-	X
33	MG	0	8060	-	X
33	MG	0	8080	-	X
33	MG	0	8087	-	X
33	MG	0	8090	-	X
33	MG	0	8092	-	X
33	MG	0	8100	-	X
33	MG	0	8101	-	X
33	MG	0	8113	-	X
33	MG	Y	8109	-	X
35	NA	0	9103	-	X
35	NA	0	9105	-	X
35	NA	0	9106	-	X
35	NA	0	9107	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
35	NA	0	9110	-	X
35	NA	0	9113	-	X
35	NA	0	9118	-	X
35	NA	0	9120	-	X
35	NA	0	9121	-	X
35	NA	0	9123	-	X
35	NA	0	9125	-	X
35	NA	0	9129	-	X
35	NA	0	9131	-	X
35	NA	0	9135	-	X
35	NA	0	9142	-	X
35	NA	0	9150	-	X
35	NA	0	9152	-	X
35	NA	0	9153	-	X
35	NA	0	9155	-	X
35	NA	0	9156	-	X
35	NA	0	9160	-	X
35	NA	0	9162	-	X
35	NA	0	9164	-	X
35	NA	0	9165	-	X
35	NA	0	9169	-	X
35	NA	0	9170	-	X
35	NA	0	9173	-	X
35	NA	0	9174	-	X
35	NA	0	9175	-	X
35	NA	0	9176	-	X
35	NA	0	9177	-	X
35	NA	0	9178	-	X
35	NA	0	9179	-	X
35	NA	0	9181	-	X
35	NA	0	9182	-	X
35	NA	0	9184	-	X
35	NA	0	9185	-	X
35	NA	B	9158	-	X
35	NA	L	9180	-	X
35	NA	R	9186	-	X
35	NA	S	9112	-	X
36	CL	0	9315	-	X
36	CL	0	9316	-	X
36	CL	A	9309	-	X
36	CL	N	9307	-	X

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99060 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	modified residue	GB 3377779
0	2587	OMU	U	modified residue	GB 3377779
0	2588	OMG	G	modified residue	GB 3377779
0	2619	UR3	U	modified residue	GB 3377779
0	2621	PSU	U	modified residue	GB 3377779

- 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'-D\*(DC)P\*(DC)P\*(5AA)P\*(2OP)P\*(PO2)P\*AP\*C\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	8	Total	C	N	O	P	0	0	0
			126	61	23	37	5			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	106	Total	Mg	0	0
			106	106		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	2	Total	Mg	0	0
			2	2		
33	A	2	Total	Mg	0	0
			2	2		
33	4	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	2	1	Total	Mg	0	0
			1	1		
33	9	2	Total	Mg	0	0
			2	2		
33	3	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	3	Total K 3 3	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	71	Total Na 71 71	0	0
35	J	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	H	2	Total Na 2 2	0	0
35	B	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	A	1	Total Na 1 1	0	0
35	R	3	Total Na 3 3	0	0
35	9	2	Total Na 2 2	0	0
35	L	1	Total Na 1 1	0	0
35	S	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	10	Total Cl 10 10	0	0
36	J	3	Total Cl 3 3	0	0
36	B	1	Total Cl 1 1	0	0
36	A	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	O	1	Total 1	Cl 1	0	0
36	R	1	Total 1	Cl 1	0	0
36	Y	1	Total 1	Cl 1	0	0
36	L	1	Total 1	Cl 1	0	0
36	3	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	O	1	Total 1	Cd 1	0	0
37	Z	1	Total 1	Cd 1	0	0
37	1	1	Total 1	Cd 1	0	0
37	3	1	Total 1	Cd 1	0	0
37	U	1	Total 1	Cd 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5820	Total 5820	O 5820	0	0
38	9	133	Total 133	O 133	0	0
38	4	8	Total 8	O 8	0	0
38	A	117	Total 117	O 117	0	0
38	B	150	Total 150	O 150	0	0
38	C	165	Total 165	O 165	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	D	49	Total 49	O 49	0	0
38	E	47	Total 47	O 47	0	0
38	F	21	Total 21	O 21	0	0
38	G	16	Total 16	O 16	0	0
38	H	66	Total 66	O 66	0	0
38	J	52	Total 52	O 52	0	0
38	K	54	Total 54	O 54	0	0
38	L	83	Total 83	O 83	0	0
38	M	118	Total 118	O 118	0	0
38	N	66	Total 66	O 66	0	0
38	O	39	Total 39	O 39	0	0
38	P	65	Total 65	O 65	0	0
38	Q	52	Total 52	O 52	0	0
38	R	85	Total 85	O 85	0	0
38	S	31	Total 31	O 31	0	0
38	T	39	Total 39	O 39	0	0
38	U	25	Total 25	O 25	0	0
38	V	13	Total 13	O 13	0	0
38	W	68	Total 68	O 68	0	0
38	X	27	Total 27	O 27	0	0
38	Y	92	Total 92	O 92	0	0

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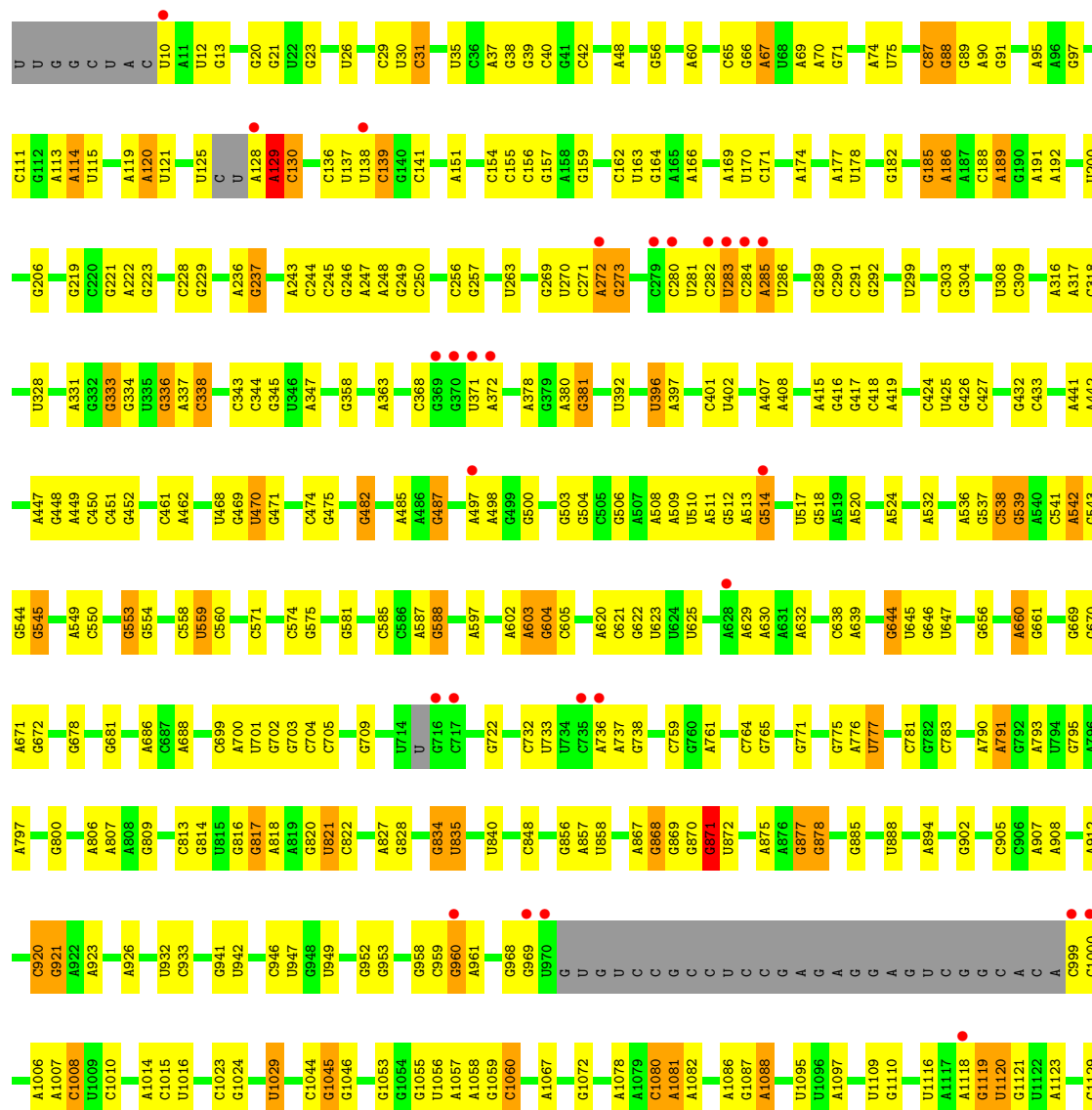
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	Z	30	Total 30	O 30	0	0
38	1	59	Total 59	O 59	0	0
38	2	42	Total 42	O 42	0	0
38	3	74	Total 74	O 74	0	0
38	I	10	Total 10	O 10	0	0

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

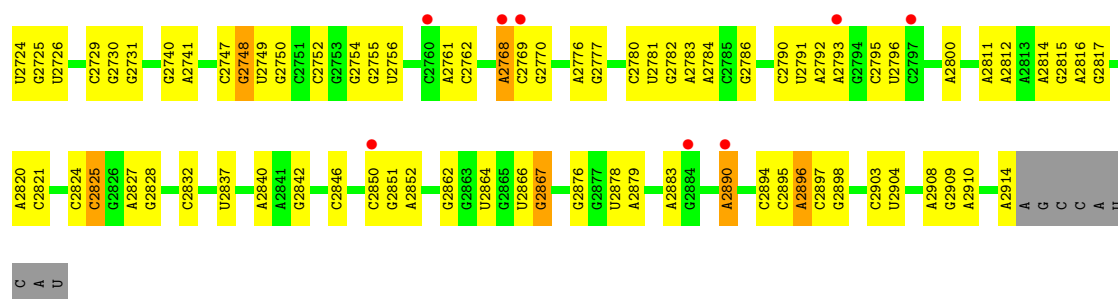
- Molecule 1: 23S ribosomal rna

Chain 0: 



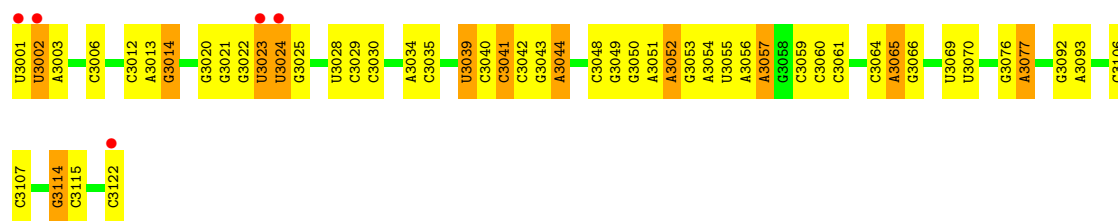
G2634	G2524	G2418	G2324	G2067	G1950	G1806	G1701	G1595	C1450	A1328	C1209	U1130
A2637	G2525	U2419	G2325	G2068	G1951	A1811	U1702	U1596	C1451	A1331	G1210	G1131
G2643	G2526	G2420	C2329	G2072	A	G1819	A1710	A1598	G1452	C1332	C1213	A1132
C2644	U2527	U2421	U2330	G2073	A	G1820	G1711	A1599	G1453	U1333	G1214	U1135
U2645	C2533	C2422	C2331	A2074	C	G1829	A1712	A1603	G1458	C1334	A1215	U1136
U2649	U2534	U2423	G2338	U2076	U	A1829	G1713	G1604	A1458	C1335	G1216	G1137
U2652	C2535	G2426	A	U2077	A	C1830	U1714	G1605	C1462	U1336	G1224	A1150
A2653	U2536	G2427	C	G2080	G	U1834	C1715	C1613	A1463	G1340	C1225	G1151
U2659	G2537	U2428	A	A2081	A	U1835	A1716	G1614	A1341	A1341	C1229	G1158
A2664	U2541	G2438	G	G2083	C	A1839	A1717	A1624	C1474	C1342	C1229	G1159
U2665	C2542	C2439	A2337	G	C	A1840	G1718	U1625	C1477	C1343	U1234	G1160
A2667	U2548	U2443	G2239	A2096	U1964	U1845	U1722	A1626	U1478	G1351	G1235	A1161
U2668	C2549	U2444	U2240	A2101	G	A1846	G1723	A1627	C1479	A1352	A1236	G1162
G2669	U2551	G2445	U2241	A2102	U1972	U1847	U1724	A1631	G1483	C1353	U1237	G1163
U2670	C2552	U2446	C2243	A2103	A1973	G1848	G1725	C1633	G1484	C1360	C1238	U1164
U2671	A2553	A2455	G2248	C2104	G	G1849	G1730	G1634	A1485	G1363	G1239	G1165
C2676	U2563	A2456	G2249	C2105	G1976	G1850	C1731	G1635	A1494	A1372	A1242	A1166
G2679	G2564	U2457	G2250	C2106	U1977	G1855	A1732	G1636	C1495	G1376	C1243	G1167
A2680	U2565	G2462	A2252	G2110	U1978	C1856	C1734	A1637	G1496	C1245	U1244	C1168
G2681	C2566	U2463	G2253	U2115	U1979	G1863	U1741	U1641	U1500	A1375	G1246	A1171
G2682	A2567	A2464	G2254	U2116	U1986	G1867	A1742	A1642	U1503	C1377	A1246	G1172
G2683	G2568	U2465	A2255	G2134	A1997	G1868	G1743	C1644	U1504	U1380	U1249	A1173
A2684	U2569	G2466	G2256	A2135	U2004	G1877	G1744	A1656	U1505	G1385	C1250	A1174
G2685	A2368	U2467	G2257	G2136	U2008	U1878	G1755	A1657	U1506	A1399	C1251	C1176
U2690	G2372	U2468	A2258	C	U2011	U1879	A1756	A1658	C1514	A1406	C1252	C1177
A2691	U2373	G2469	A2259	A	U2012	C1880	G1756	A1659	U1524	A1407	U1270	G1178
G2692	U2377	U2470	C2269	G	G2013	A1904	U1761	G1663	G1525	U1408	C1273	U1180
U2693	G2379	U2471	G2270	G	A2015	U1905	U1762	A1664	A1526	G1409	C1289	C1181
A2694	A2380	G2472	G2271	U	U2016	U1919	U1763	G1665	A1527	G1290	G1290	C1183
G2698	G2385	U2473	G2272	C	U2028	C1920	G1773	C1666	A1528	A1294	A1294	U1185
A2699	U2386	U2474	U2281	A	C2029	A1921	G1774	A1667	G1529	G1299	U1279	C1186
G2708	U2387	U2475	U2282	G	A2030	A1922	U1778	U1668	G1535	G1300	A1189	A1187
U2709	A2388	U2476	A2283	A	G2033	G1926	A1779	C1675	C1536	U1304	G1190	A1188
U2710	A2390	U2477	A2300	U	U2034	A1927	A1780	U1679	U1544	U1305	A1191	C1184
G2711	A2391	U2478	A2301	G	C2036	A1930	A1781	G1681	C1545	A1423	A1294	U1189
U2712	U2392	U2479	A2302	A	G2043	A1931	A1782	C1682	U1559	A1424	A1294	A1192
G2713	A2401	U2480	C2309	C	G2044	G1932	G1785	A1683	U1561	A1427	A1294	A1193
U2714	C2402	U2481	G2312	A	G2050	G1933	C1786	G1684	C1562	A1434	A1294	C1201
G2715	G2403	U2482	C2313	U	A2054	G1934	U1788	A1685	C1564	U1435	A1307	G1202
U2716	A2404	U2483	G2314	C	U2054	C1940	G1789	C1686	U1587	G1436	A1308	G1203
G2717	U2405	U2484	C2315	U	A2061	A1941	C1790	C1687	G1588	U1440	U1310	G1204
U2718	G2412	U2485	C2316	A	C2061	A1942	U1791	G1688	C1592	U1441	G1311	U1205
G2719	A2413	U2486	U2320	G	U2062	C1943	C1798	G1689	C1593	U1442	U1314	U1206
U2720	U2414	U2487	U2321	U	U2063	G1948	G1805	G1690	C1594			C1208
U2721	A2415	U2488	U2322	G	U2064	G1949						
G2723		U2489	U2323	G								





• Molecule 2: 5S ribosomal RNA

Chain 9:



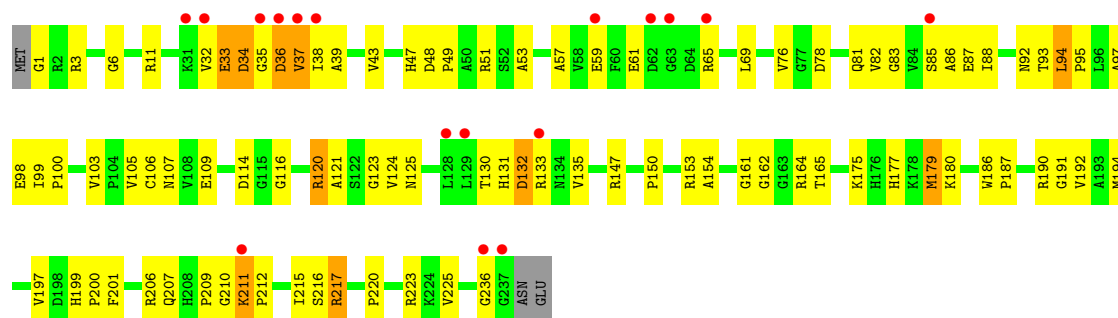
• Molecule 3: 5'-D\*(DC)P\*(DC)P\*(5AA)P\*(2OP)P\*(PO2)P\*AP\*C\*C-3'

Chain 4:



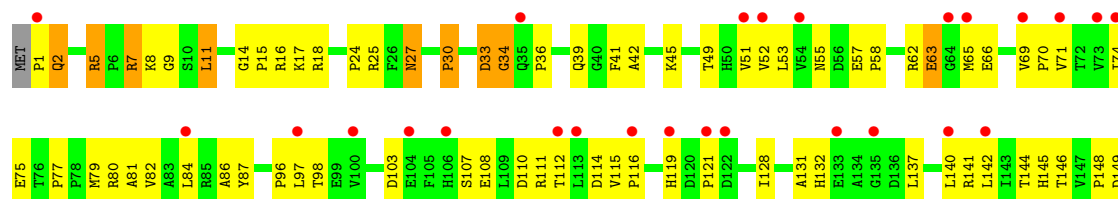
• Molecule 4: 50S ribosomal protein L2P

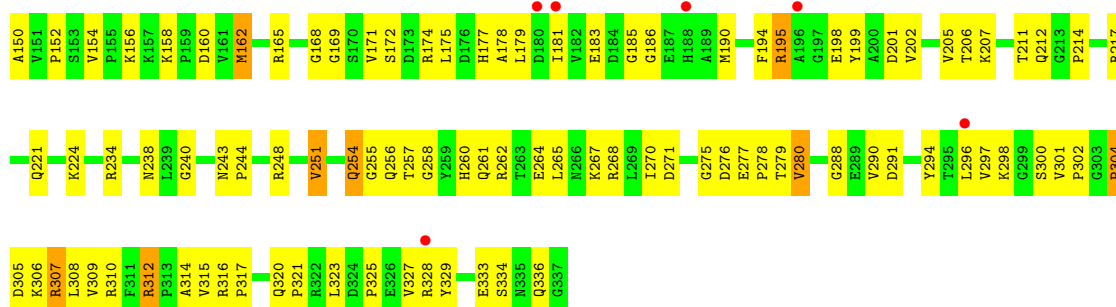
Chain A:



• Molecule 5: 50S ribosomal protein L3P

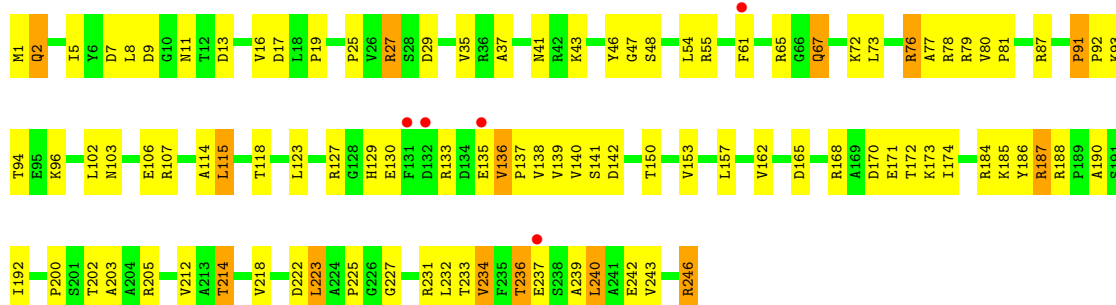
Chain B:





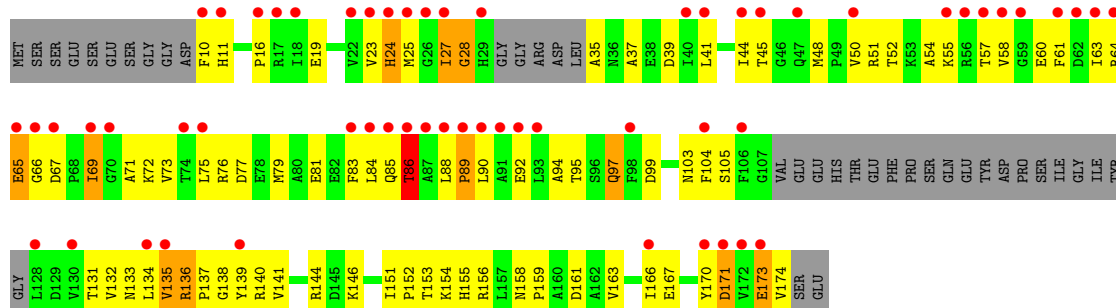
• Molecule 6: 50S ribosomal protein L4E

Chain C:



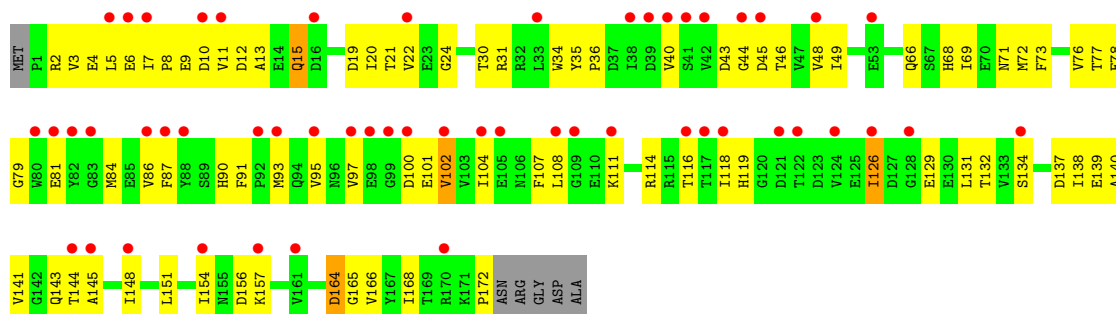
• Molecule 7: 50S ribosomal protein L5P

Chain D:



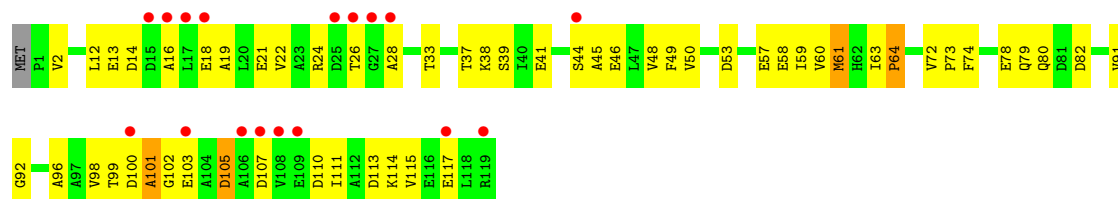
• Molecule 8: 50S ribosomal protein L6P

Chain E:



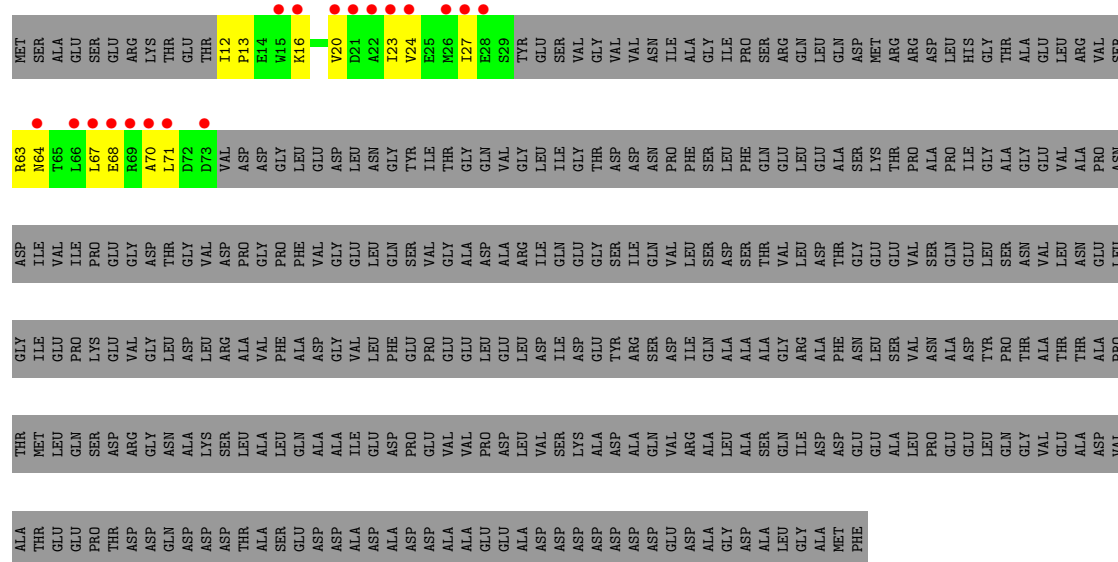
• Molecule 9: 50S ribosomal protein L7AE

Chain F:



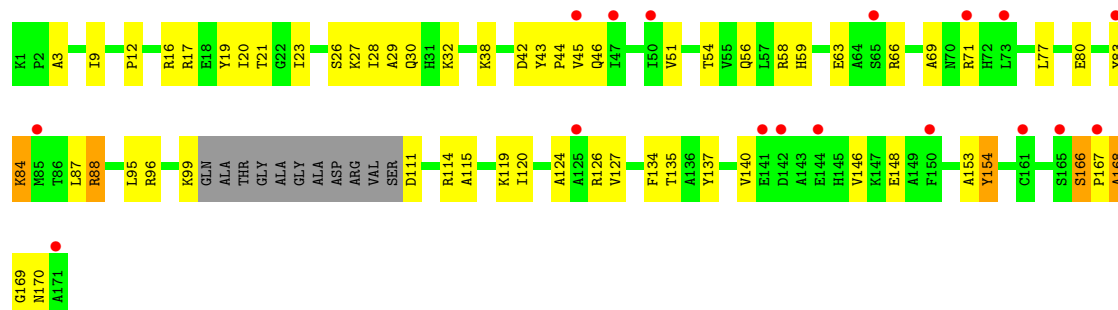
• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

Chain G:



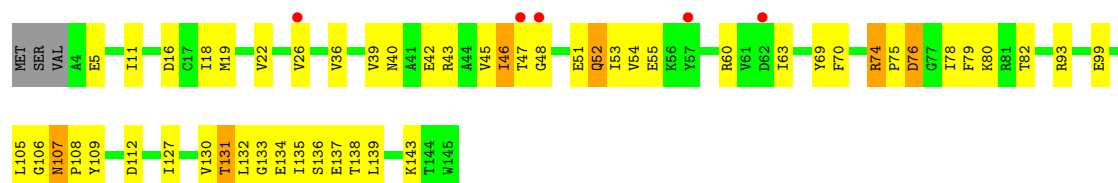
• Molecule 11: 50S RIBOSOMAL PROTEIN L10E

Chain H:



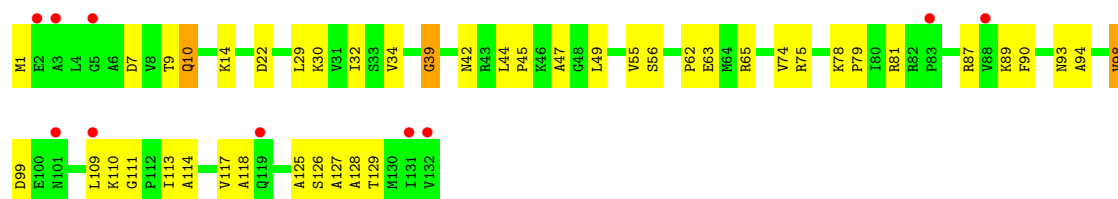
• Molecule 12: 50S ribosomal protein L13P

Chain J:



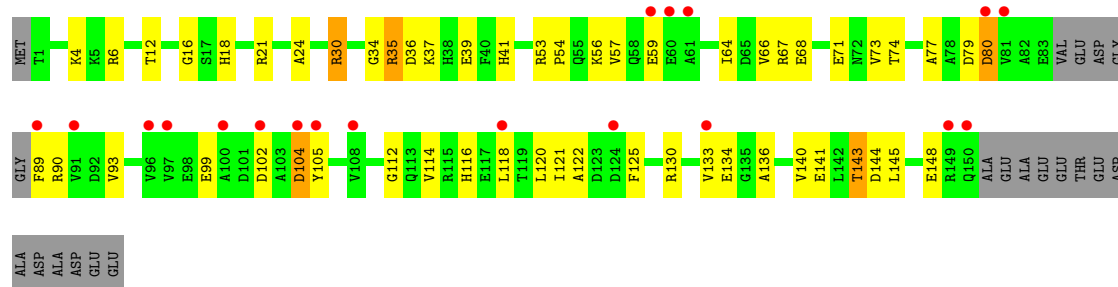
- Molecule 13: 50S ribosomal protein L14P

Chain K:



- Molecule 14: 50S ribosomal protein L15P

Chain L:



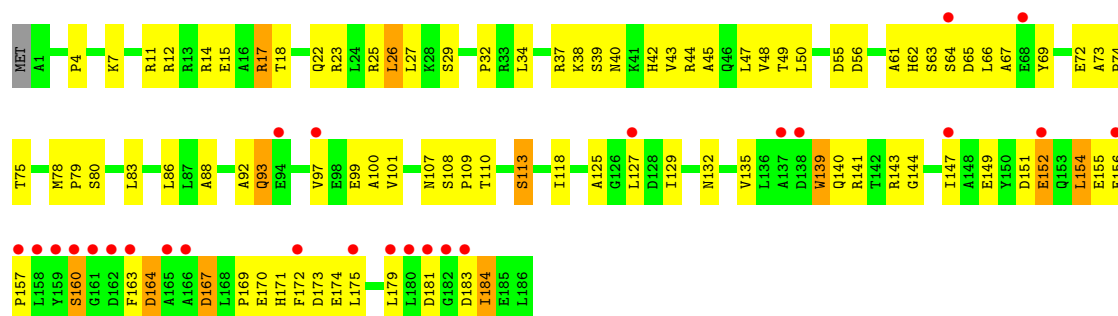
- Molecule 15: 50S Ribosomal Protein L15E

Chain M:



- Molecule 16: 50S ribosomal protein L18P

Chain N:



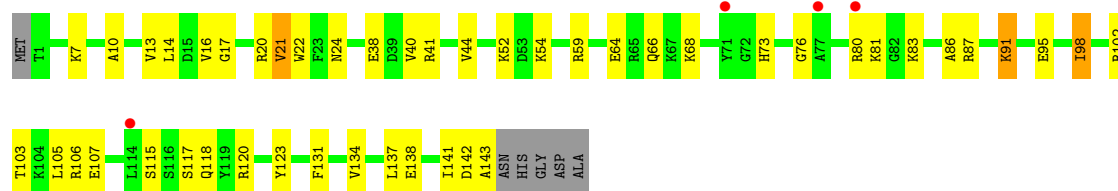
- Molecule 17: 50S ribosomal protein L18e

Chain O:



- Molecule 18: 50S ribosomal protein L19E

Chain P:



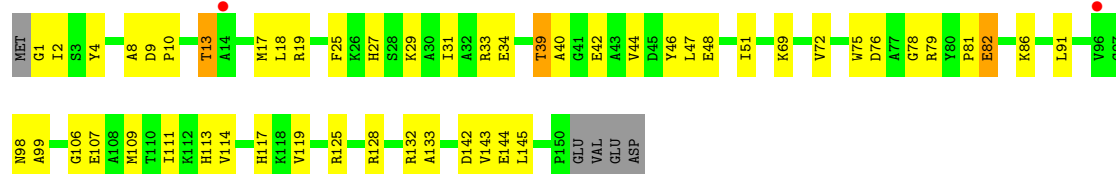
- Molecule 19: 50S ribosomal protein L21e

Chain Q:



- Molecule 20: 50S ribosomal protein L22P

Chain R:



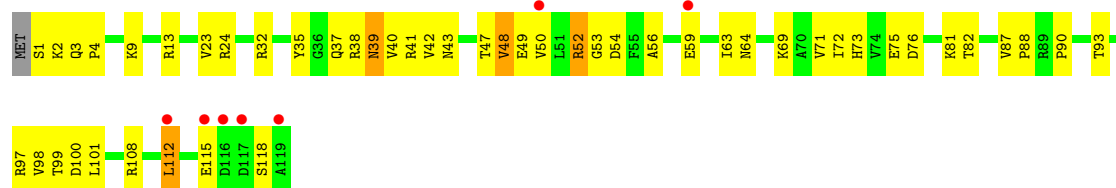
- Molecule 21: 50S ribosomal protein L23P

Chain S:



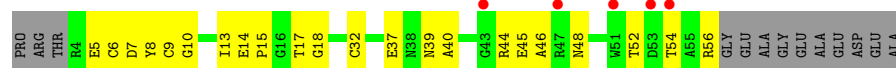
- Molecule 22: 50S ribosomal protein L24P

Chain T:



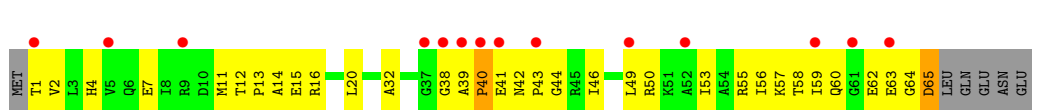
- Molecule 23: 50S ribosomal protein L24E

Chain U:



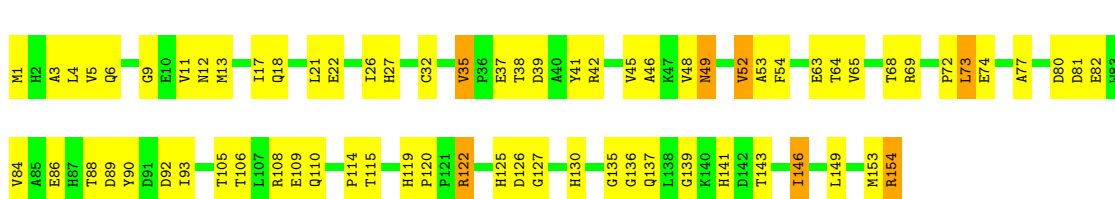
- Molecule 24: 50S ribosomal protein L29P

Chain V:



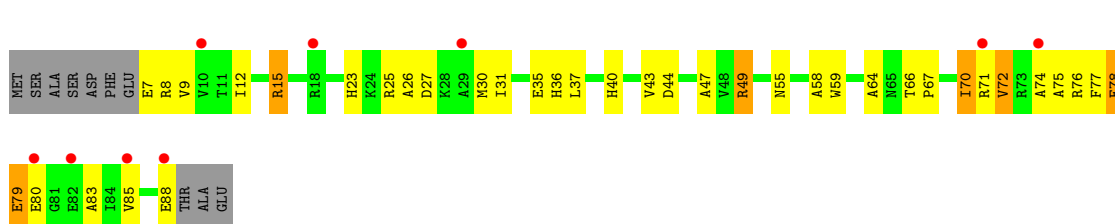
- Molecule 25: 50S ribosomal protein L30P

Chain W:



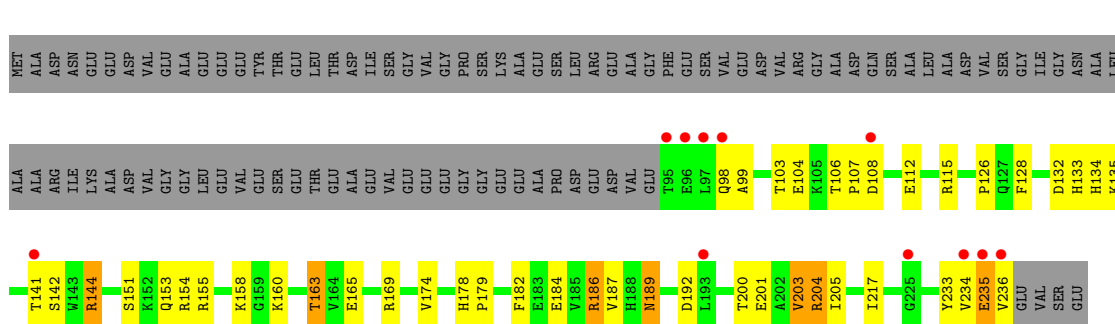
- Molecule 26: 50S ribosomal protein L31e

Chain X:



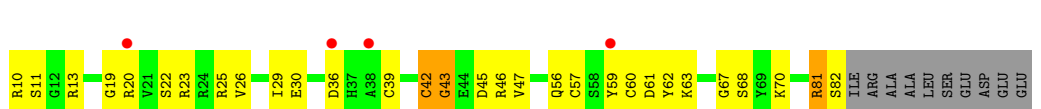
- Molecule 27: 50S ribosomal protein L32E

Chain Y:



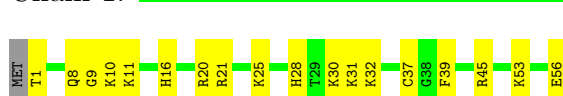
- Molecule 28: 50S ribosomal protein L37Ae

Chain Z:



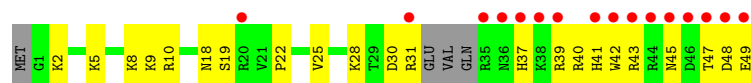
- Molecule 29: 50S ribosomal protein L37e

Chain 1:



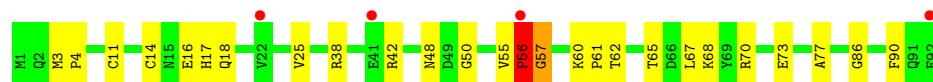
- Molecule 30: 50S ribosomal protein L39e

Chain 2: 



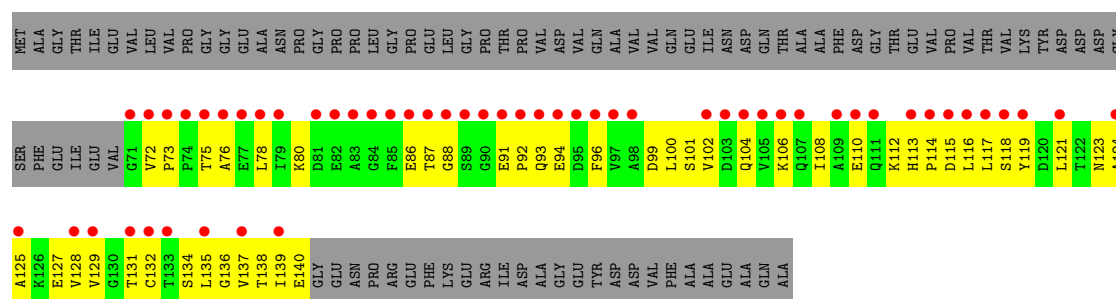
- Molecule 31: 50S ribosomal protein L44E

Chain 3: 



- Molecule 32: 50S RIBOSOMAL PROTEIN L11P

Chain I: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.79Å 300.61Å 573.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 49.67 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.60) 90.1 (49.67-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.197 , 0.237 0.241 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	54.0	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 602690 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	99060	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, NA, K, PO2, CD, 5AA, DCZ, OMU, UR3, 2OP, 1MA, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	0	0.38	0/65959	0.69	20/102870 (0.0%)
2	9	0.33	0/2905	0.70	1/4528 (0.0%)
3	4	0.53	0/83	0.82	0/119
4	A	0.33	0/1786	0.64	0/2408
5	B	0.32	0/2690	0.63	0/3652
6	C	0.39	0/1884	0.66	0/2551
7	D	0.29	0/1111	0.53	0/1498
8	E	0.31	0/1382	0.57	0/1880
9	F	0.30	0/901	0.53	0/1224
10	G	0.29	0/241	0.45	0/324
11	H	0.34	0/1287	0.63	0/1725
12	J	0.35	0/1136	0.60	0/1530
13	K	0.35	0/1001	0.67	0/1347
14	L	0.33	0/1130	0.64	0/1509
15	M	0.35	0/1584	0.61	0/2119
16	N	0.28	0/1474	0.62	0/1999
17	O	0.34	0/874	0.59	0/1181
18	P	0.33	0/1147	0.54	0/1528
19	Q	0.37	0/749	0.68	0/1005
20	R	0.35	0/1172	0.64	0/1578
21	S	0.33	0/648	0.58	0/875
22	T	0.32	0/958	0.65	1/1289 (0.1%)
23	U	0.34	0/417	0.56	0/562
24	V	0.28	0/502	0.51	0/675
25	W	0.33	0/1219	0.62	0/1655
26	X	0.34	0/664	0.59	0/895
27	Y	0.36	0/1146	0.65	0/1536
28	Z	0.37	0/589	0.65	0/787
29	1	0.41	0/438	0.64	0/578
30	2	0.32	0/401	0.55	0/529
31	3	0.38	0/771	0.59	0/1024
32	I	0.29	0/526	0.53	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.37	0/98775	0.67	22/147696 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	1	52
25	W	0	1
All	All	1	53

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.50	130.40	109.50
1	0	1942	A	C5'-C4'-C3'	7.87	128.58	116.00
2	9	3039	U	N1-C1'-C2'	6.80	122.84	114.00
1	0	871	G	C5'-C4'-O4'	-6.76	100.98	109.10
1	0	1819	G	C5'-C4'-C3'	6.21	125.94	116.00
1	0	2467	A	C1'-O4'-C4'	-5.92	105.17	109.90
1	0	2316	G	C5'-C4'-C3'	-5.90	106.56	116.00
1	0	1504	A	C1'-O4'-C4'	-5.79	105.27	109.90
1	0	1120	U	C5'-C4'-C3'	-5.77	106.77	116.00
1	0	1504	A	N9-C1'-C2'	5.76	121.49	114.00
1	0	2291	A	N9-C1'-C2'	5.72	121.43	114.00
1	0	1829	A	N9-C1'-C2'	-5.59	105.85	112.00
1	0	2313	C	C5'-C4'-O4'	5.55	115.76	109.10
1	0	1942	A	C5'-C4'-O4'	5.42	115.60	109.10
1	0	206	G	C5'-C4'-C3'	-5.39	107.38	116.00
1	0	129	A	C2'-C3'-O3'	5.34	122.25	113.70
1	0	1165	G	C1'-O4'-C4'	-5.17	105.76	109.90
22	T	52	ARG	N-CA-C	5.15	124.91	111.00
1	0	1942	A	C4'-C3'-C2'	-5.14	97.46	102.60
1	0	2607	U	N1-C1'-C2'	5.13	120.67	114.00
1	0	2313	C	C5'-C4'-C3'	5.07	124.11	116.00
1	0	1971	G	N9-C1'-C2'	5.01	120.51	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (53) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1055	G	Sidechain
1	0	1078	A	Sidechain
1	0	1340	G	Sidechain
1	0	1342	C	Sidechain
1	0	1351	G	Sidechain
1	0	1417	G	Sidechain
1	0	1458	A	Sidechain
1	0	1718	G	Sidechain
1	0	174	A	Sidechain
1	0	1819	G	Sidechain
1	0	1829	A	Sidechain
1	0	1839	A	Sidechain
1	0	1845	A	Sidechain
1	0	1848	G	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	189	A	Sidechain
1	0	2312	G	Sidechain
1	0	2316	G	Sidechain
1	0	2412	G	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2551	C	Sidechain
1	0	2552	C	Sidechain
1	0	2564	G	Sidechain
1	0	26	U	Sidechain
1	0	2607	U	Sidechain
1	0	2620	U	Sidechain
1	0	2630	G	Sidechain
1	0	2643	G	Sidechain
1	0	2793	A	Sidechain
1	0	2842	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	469	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	48	A	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	554	G	Sidechain
1	0	722	G	Sidechain
1	0	771	G	Sidechain
1	0	781	C	Sidechain
1	0	791	A	Sidechain
1	0	817	G	Sidechain
1	0	867	A	Sidechain
1	0	868	G	Sidechain
1	0	888	U	Sidechain
25	W	90	TYR	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29813	777	1
2	9	2600	0	1326	52	1
3	4	126	0	75	5	0
4	A	1753	0	1766	106	0
5	B	2625	0	2533	158	1
6	C	1859	0	1816	111	0
7	D	1094	0	1085	93	0
8	E	1357	0	1266	78	0
9	F	890	0	843	51	0
10	G	240	0	231	11	0
11	H	1266	0	1268	60	0
12	J	1120	0	1098	62	0
13	K	992	0	1031	51	1
14	L	1118	0	1076	53	0
15	M	1560	0	1568	62	0
16	N	1445	0	1401	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	O	865	0	873	29	0
18	P	1136	0	1123	51	0
19	Q	735	0	729	23	0
20	R	1149	0	1122	55	0
21	S	641	0	605	19	0
22	T	950	0	923	50	0
23	U	410	0	364	21	0
24	V	499	0	511	34	0
25	W	1196	0	1137	95	0
26	X	654	0	653	44	0
27	Y	1130	0	1133	53	0
28	Z	578	0	539	24	0
29	1	431	0	426	27	0
30	2	396	0	413	29	0
31	3	755	0	728	19	0
32	I	519	0	500	58	0
33	0	106	0	0	0	0
33	2	1	0	0	0	0
33	3	1	0	0	0	0
33	4	1	0	0	0	0
33	9	2	0	0	0	0
33	A	2	0	0	0	0
33	B	2	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	3	0	0	0	0
35	0	71	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	1	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	B	1	0	0	0	0
36	J	3	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5820	0	0	111	0
38	1	59	0	0	2	0
38	2	42	0	0	2	0
38	3	74	0	0	3	0
38	4	8	0	0	0	0
38	9	133	0	0	3	0
38	A	117	0	0	9	0
38	B	150	0	0	16	0
38	C	165	0	0	15	0
38	D	49	0	0	11	0
38	E	47	0	0	7	0
38	F	21	0	0	3	0
38	G	16	0	0	0	0
38	H	66	0	0	6	0
38	I	10	0	0	2	0
38	J	52	0	0	1	0
38	K	54	0	0	3	0
38	L	83	0	0	10	0
38	M	118	0	0	3	0
38	N	66	0	0	8	0
38	O	39	0	0	4	0
38	P	65	0	0	3	0
38	Q	52	0	0	5	0
38	R	85	0	0	4	0
38	S	31	0	0	3	0
38	T	39	0	0	1	0
38	U	25	0	0	0	0
38	V	13	0	0	2	0
38	W	68	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	X	27	0	0	2	0
38	Y	92	0	0	5	0
38	Z	30	0	0	2	0
All	All	99060	0	59975	2235	3

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (2235) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1160:G:H5'	1:0:1161:A:H5'	1.26	1.12
15:M:164:THR:HG22	15:M:167:GLY:H	1.13	1.09
1:0:156:C:H5''	15:M:171:ARG:HD3	1.35	1.08
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.30	1.08
11:H:166:SER:HB2	11:H:167:PRO:HD3	1.35	1.07
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.31	1.07
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.37	1.06
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.36	1.06
7:D:25:MET:HE3	7:D:37:ALA:HB1	1.33	1.05
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.75	1.02
2:9:3076:G:H3'	2:9:3077:A:H5''	1.39	1.02
6:C:236:THR:HG22	6:C:239:ALA:H	1.24	1.01
1:0:1242:A:H5'	12:J:82:THR:HG23	1.41	1.01
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.43	0.99
1:0:2717:C:H2'	1:0:2718:C:H5''	1.42	0.99
1:0:1119:G:H2'	12:J:52:GLN:NE2	1.77	0.98
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.29	0.97
30:2:41:HIS:H	30:2:45:ASN:HD22	0.98	0.97
1:0:1119:G:H2'	12:J:52:GLN:HE22	1.32	0.95
4:A:211:LYS:HB3	4:A:212:PRO:HD2	1.49	0.94
1:0:2717:C:C2'	1:0:2718:C:H5''	1.98	0.93
1:0:870:G:H2'	1:0:871:G:H5''	1.48	0.93
1:0:871:G:C8	1:0:871:G:H5'	2.02	0.93
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.51	0.93
13:K:10:GLN:H	13:K:10:GLN:NE2	1.66	0.92
1:0:541:C:H2'	1:0:542:A:H5''	1.52	0.92
1:0:1474:C:H6	1:0:1474:C:H5'	1.34	0.92
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.49	0.91
16:N:17:ARG:HB3	16:N:17:ARG:HH11	1.34	0.91
13:K:10:GLN:H	13:K:10:GLN:HE21	0.94	0.90
1:0:2812:A:H2	1:0:2814:A:H62	1.17	0.89
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.55	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:871:G:H8	1:0:871:G:H5'	1.36	0.89
18:P:115:SER:H	18:P:118:GLN:HE21	0.93	0.89
1:0:1667:A:H8	1:0:1667:A:H5'	1.38	0.89
6:C:236:THR:HG22	6:C:239:ALA:N	1.87	0.88
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.56	0.88
2:9:3056:A:H2'	2:9:3057:A:H5''	1.54	0.88
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.53	0.88
28:Z:10:ARG:HA	38:Z:9215:HOH:O	1.74	0.88
1:0:1835:U:H5	1:0:1840:A:N7	1.72	0.88
22:T:101:LEU:HD13	22:T:112:LEU:HD11	1.54	0.87
1:0:1751:G:H2'	1:0:1752:G:H5''	1.54	0.87
1:0:2364:A:H5''	19:Q:15:LYS:HD3	1.56	0.87
13:K:10:GLN:N	13:K:10:GLN:HE21	1.71	0.87
6:C:1:MET:HG2	6:C:2:GLN:H	1.37	0.87
24:V:1:THR:HG23	24:V:2:VAL:H	1.40	0.86
1:0:1160:G:C5'	1:0:1161:A:H5'	2.04	0.86
1:0:2506:A:HO2'	1:0:2507:G:H8	0.87	0.86
5:B:264:GLU:HG2	5:B:267:LYS:HE2	1.57	0.86
6:C:5:ILE:HD11	6:C:16:VAL:HG23	1.57	0.86
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.89	0.86
5:B:307:ARG:HB2	5:B:307:ARG:HH11	1.39	0.85
25:W:13:MET:HE2	25:W:18:GLN:HA	1.57	0.85
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.57	0.85
4:A:35:GLY:O	4:A:36:ASP:HB3	1.76	0.85
25:W:72:PRO:HG2	25:W:77:ALA:HB3	1.57	0.85
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.06	0.85
15:M:99:ARG:HD2	15:M:167:GLY:HA2	1.59	0.85
1:0:542:A:H5'	1:0:542:A:H8	1.41	0.85
1:0:545:G:H8	1:0:545:G:H5'	1.42	0.84
4:A:153:ARG:HH11	4:A:153:ARG:HB2	1.41	0.84
18:P:115:SER:N	18:P:118:GLN:HE21	1.75	0.84
16:N:144:GLY:O	16:N:147:ILE:HG22	1.77	0.84
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.56	0.84
1:0:2586:U:H3	1:0:2592:G:H22	1.25	0.84
15:M:166:ALA:HA	15:M:169:ARG:NH1	1.93	0.84
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.58	0.84
7:D:57:THR:HG23	7:D:63:ILE:HA	1.60	0.83
13:K:62:PRO:HG3	13:K:65:ARG:HH21	1.43	0.83
18:P:115:SER:H	18:P:118:GLN:NE2	1.76	0.83
26:X:30:MET:HE1	26:X:55:ASN:HA	1.58	0.83
5:B:62:ARG:HA	5:B:65:MET:HE2	1.57	0.83
15:M:164:THR:HG22	15:M:167:GLY:N	1.91	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:N:48:VAL:HG11	16:N:55:ASP:HB3	1.59	0.83
2:9:3006:C:H5"	16:N:37:ARG:NH1	1.94	0.83
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.79	0.82
4:A:191:GLY:HA2	4:A:194:MET:CE	2.09	0.82
24:V:12:THR:HG23	24:V:14:ALA:H	1.42	0.82
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.27	0.82
11:H:56:GLN:HE21	11:H:126:ARG:HE	1.25	0.82
1:0:2904:U:H4'	26:X:8:ARG:NH1	1.95	0.82
1:0:21:G:H5'	20:R:2:ILE:HA	1.61	0.82
1:0:1159:G:H21	1:0:1189:A:H8	1.27	0.82
23:U:9:CYS:HA	23:U:52:THR:HG23	1.62	0.82
11:H:166:SER:HB2	11:H:167:PRO:CD	2.10	0.82
30:2:41:HIS:N	30:2:45:ASN:HD22	1.77	0.82
5:B:36:PRO:HA	5:B:168:GLY:HA3	1.60	0.82
1:0:381:G:H5"	38:0:4610:HOH:O	1.79	0.81
1:0:282:C:H1'	1:0:368:C:N4	1.94	0.81
4:A:192:VAL:HG12	4:A:207:GLN:HB3	1.62	0.81
1:0:2506:A:O2'	1:0:2507:G:H8	1.64	0.81
12:J:107:ASN:ND2	12:J:109:TYR:H	1.79	0.81
1:0:21:G:C5'	20:R:2:ILE:HA	2.12	0.80
25:W:88:THR:HB	38:W:6679:HOH:O	1.80	0.80
7:D:154:LYS:HD2	7:D:154:LYS:H	1.46	0.80
20:R:39:THR:HG22	20:R:42:GLU:H	1.46	0.80
5:B:217:ARG:HG3	5:B:257:THR:HG22	1.62	0.80
1:0:2533:C:H5'	1:0:2533:C:H6	1.46	0.80
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.63	0.79
1:0:506:G:H22	1:0:509:A:H5"	1.47	0.79
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.63	0.79
1:0:541:C:C2'	1:0:542:A:H5"	2.10	0.79
32:I:102:VAL:HG12	32:I:106:LYS:HE3	1.61	0.79
1:0:1160:G:H5'	1:0:1161:A:C5'	2.10	0.79
5:B:27:ASN:H	5:B:27:ASN:HD22	1.30	0.79
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.47	0.79
1:0:1165:G:H4'	1:0:1174:A:O2'	1.83	0.79
25:W:38:THR:HG22	25:W:39:ASP:H	1.47	0.79
16:N:12:ARG:HD3	16:N:18:THR:OG1	1.82	0.79
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.64	0.79
18:P:115:SER:OG	18:P:118:GLN:HG3	1.83	0.78
7:D:88:LEU:HB2	7:D:89:PRO:HD3	1.65	0.78
1:0:1450:C:H4'	1:0:1451:C:OP2	1.82	0.78
16:N:93:GLN:HE21	16:N:93:GLN:HA	1.47	0.78
6:C:236:THR:H	6:C:239:ALA:HB3	1.49	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:36:ASP:OD2	4:A:85:SER:HB2	1.84	0.77
12:J:45:VAL:HG23	12:J:130:VAL:O	1.83	0.77
1:0:2291:A:C8	1:0:2309:C:H5'	2.19	0.77
25:W:80:ASP:O	25:W:84:VAL:HG23	1.84	0.77
29:1:8:GLN:HE22	29:1:11:LYS:NZ	1.83	0.77
7:D:136:ARG:HD2	7:D:155:HIS:O	1.83	0.77
9:F:91:VAL:HG12	9:F:92:GLY:H	1.49	0.77
1:0:559:U:H5'	1:0:559:U:H6	1.49	0.77
27:Y:235:GLU:H	27:Y:235:GLU:CD	1.86	0.77
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.15	0.77
4:A:131:HIS:O	4:A:132:ASP:HB2	1.86	0.76
1:0:2748:G:H2'	38:0:7745:HOH:O	1.84	0.76
1:0:1244:U:OP1	12:J:18:ILE:HD13	1.85	0.76
1:0:877:G:H5'	1:0:878:G:OP1	1.85	0.76
5:B:238:ASN:HD22	5:B:240:GLY:H	1.33	0.76
6:C:115:LEU:HD21	6:C:243:VAL:HG13	1.64	0.76
1:0:871:G:H8	1:0:871:G:C5'	1.99	0.76
1:0:1162:G:H1'	32:I:117:LEU:HD11	1.67	0.76
1:0:870:G:C2'	1:0:871:G:H5''	2.16	0.76
7:D:135:VAL:HG22	7:D:136:ARG:H	1.51	0.76
1:0:56:G:H5''	24:V:50:ARG:HH12	1.49	0.76
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.67	0.75
21:S:57:THR:HG22	21:S:59:ASP:H	1.52	0.75
15:M:183:THR:HG22	15:M:194:ALA:HB1	1.67	0.75
25:W:122:ARG:HH11	25:W:122:ARG:HG2	1.51	0.75
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.50	0.75
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.66	0.75
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.69	0.75
6:C:139:VAL:HG13	38:C:9244:HOH:O	1.85	0.75
5:B:179:LEU:O	5:B:183:GLU:HG2	1.87	0.75
25:W:88:THR:HG22	25:W:89:ASP:H	1.49	0.75
1:0:1641:A:H2'	1:0:1642:A:H5'	1.69	0.75
1:0:1372:A:H3'	38:0:7407:HOH:O	1.87	0.74
11:H:166:SER:CB	11:H:167:PRO:HD3	2.13	0.74
1:0:2862:G:H4'	5:B:336:GLN:O	1.87	0.74
24:V:39:ALA:N	24:V:40:PRO:HD2	2.02	0.74
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.69	0.74
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.18	0.74
38:0:6419:HOH:O	4:A:223:ARG:HG3	1.86	0.74
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.70	0.74
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.68	0.74
2:9:3006:C:OP1	16:N:37:ARG:NH1	2.21	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
26:X:25:ARG:HD3	26:X:64:ALA:O	1.88	0.74
1:0:2908:A:H2'	1:0:2909:G:O4'	1.88	0.74
29:1:10:LYS:HG3	38:1:9236:HOH:O	1.87	0.74
1:0:2904:U:H4'	26:X:8:ARG:HH12	1.50	0.74
23:U:14:GLU:OE1	23:U:15:PRO:HD2	1.88	0.74
1:0:1116:U:HO2'	1:0:1118:A:H2	1.34	0.74
20:R:99:ALA:HB1	20:R:109:MET:CE	2.17	0.73
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.85	0.73
1:0:2756:U:H3	1:0:2896:A:H2	1.34	0.73
11:H:46:GLN:HB3	11:H:167:PRO:CD	2.15	0.73
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.68	0.73
1:0:1299:G:O6	14:L:6:ARG:HD3	1.89	0.73
16:N:17:ARG:NH1	16:N:17:ARG:HB3	2.03	0.73
9:F:91:VAL:HG12	9:F:92:GLY:N	2.03	0.73
2:9:3014:G:H8	2:9:3014:G:H5'	1.54	0.73
25:W:13:MET:HE1	25:W:17:ILE:HG22	1.71	0.73
16:N:151:ASP:O	16:N:154:LEU:HB2	1.88	0.73
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.70	0.73
2:9:3029:C:H2'	2:9:3030:C:H5'	1.70	0.73
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.70	0.73
12:J:131:THR:HG22	12:J:134:GLU:H	1.53	0.73
11:H:58:ARG:HG3	11:H:58:ARG:HH11	1.53	0.73
22:T:63:ILE:HD11	22:T:75:GLU:HB2	1.70	0.72
1:0:2716:G:H5''	5:B:206:THR:HG21	1.71	0.72
7:D:146:LYS:NZ	16:N:107:ASN:HD21	1.87	0.72
1:0:793:A:H5''	18:P:83:LYS:HG2	1.71	0.72
1:0:281:U:H2'	1:0:282:C:O4'	1.89	0.72
11:H:27:LYS:H	11:H:59:HIS:HD2	1.37	0.72
4:A:199:HIS:HD2	4:A:201:PHE:H	1.34	0.72
1:0:182:G:H5'	38:0:5431:HOH:O	1.90	0.72
14:L:133:VAL:HA	38:L:9371:HOH:O	1.88	0.72
1:0:1116:U:O2'	1:0:1118:A:H2	1.72	0.72
1:0:1119:G:N2	1:0:1246:A:C2	2.58	0.72
1:0:2270:G:H4'	4:A:223:ARG:HH12	1.54	0.72
1:0:506:G:H22	1:0:509:A:C5'	2.03	0.72
26:X:43:VAL:HG12	26:X:44:ASP:H	1.55	0.72
5:B:195:ARG:HG2	5:B:323:LEU:HD22	1.71	0.72
11:H:9:ILE:HD12	11:H:54:THR:HG22	1.71	0.71
2:9:3039:U:H1'	2:9:3044:A:H61	1.55	0.71
22:T:49:GLU:OE2	22:T:97:ARG:HD2	1.90	0.71
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.72	0.71
4:A:191:GLY:HA2	4:A:194:MET:HE2	1.72	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1701:A:H4'	1:0:1702:U:H5''	1.72	0.71
1:0:1184:C:H1'	38:0:7672:HOH:O	1.89	0.71
8:E:81:GLU:HG2	8:E:134:SER:HB3	1.72	0.71
30:2:41:HIS:H	30:2:45:ASN:ND2	1.82	0.71
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.06	0.71
27:Y:154:ARG:NH1	27:Y:155:ARG:HG3	2.06	0.71
1:0:1116:U:H3	1:0:1246:A:H62	1.35	0.71
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.25	0.71
12:J:74:ARG:CB	12:J:74:ARG:HH11	2.01	0.71
1:0:871:G:C8	1:0:871:G:C5'	2.74	0.71
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.73	0.71
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.20	0.71
5:B:168:GLY:H	5:B:174:ARG:HD3	1.56	0.71
1:0:380:A:H2'	38:0:7446:HOH:O	1.90	0.71
1:0:272:A:H5'	1:0:273:G:OP2	1.90	0.71
1:0:188:C:H5''	15:M:163:LEU:HD21	1.73	0.70
32:I:99:ASP:OD1	32:I:138:THR:HB	1.90	0.70
16:N:113:SER:HB2	38:N:9360:HOH:O	1.89	0.70
11:H:56:GLN:NE2	11:H:126:ARG:HE	1.89	0.70
15:M:187:LEU:CD2	15:M:194:ALA:HB3	2.21	0.70
26:X:43:VAL:HG12	26:X:44:ASP:N	2.05	0.70
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.72	0.70
16:N:47:LEU:HD11	16:N:127:LEU:HD21	1.74	0.70
12:J:93:ARG:HH11	12:J:93:ARG:HB3	1.55	0.70
4:A:191:GLY:HA2	4:A:194:MET:HE3	1.72	0.70
1:0:2533:C:C6	1:0:2533:C:H5'	2.25	0.70
1:0:2054:A:N3	20:R:128:ARG:NH2	2.39	0.70
7:D:99:ASP:HA	38:D:5675:HOH:O	1.92	0.70
16:N:169:PRO:O	16:N:172:PHE:HB3	1.91	0.70
28:Z:26:VAL:O	28:Z:30:GLU:HG3	1.91	0.70
4:A:33:GLU:O	4:A:34:ASP:HB2	1.90	0.70
6:C:115:LEU:HD13	6:C:223:LEU:HD21	1.72	0.70
6:C:246:ARG:HH11	6:C:246:ARG:HB3	1.56	0.70
6:C:162:VAL:HG12	6:C:192:ILE:HD11	1.72	0.70
5:B:62:ARG:HA	5:B:65:MET:CE	2.21	0.70
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.74	0.70
1:0:1118:A:H3'	1:0:1118:A:H8	1.56	0.70
4:A:153:ARG:NH1	4:A:153:ARG:HB2	2.07	0.70
20:R:17:MET:HE1	20:R:19:ARG:NH2	2.07	0.70
1:0:2256:G:H2'	1:0:2257:G:H5'	1.74	0.70
1:0:450:C:OP1	6:C:184:ARG:NH2	2.25	0.70
18:P:59:ARG:HH22	18:P:66:GLN:HE22	1.38	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:9:3006:C:H5''	16:N:37:ARG:HH12	1.57	0.69
27:Y:154:ARG:HH12	27:Y:155:ARG:HG3	1.55	0.69
7:D:99:ASP:HB3	7:D:103:ASN:H	1.55	0.69
22:T:32:ARG:NH1	22:T:38:ARG:HH12	1.90	0.69
18:P:103:THR:HA	18:P:106:ARG:NH1	2.06	0.69
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.75	0.69
8:E:3:VAL:HG22	8:E:49:ILE:HB	1.75	0.69
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.73	0.69
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.56	0.69
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.22	0.69
1:0:1118:A:H3'	1:0:1118:A:C8	2.28	0.69
1:0:1667:A:C8	1:0:1667:A:H5'	2.25	0.69
1:0:1559:A:H1'	38:0:6128:HOH:O	1.93	0.69
5:B:258:GLY:H	5:B:260:HIS:CE1	2.11	0.69
1:0:474:C:O3'	6:C:73:LEU:HD21	1.93	0.69
4:A:121:ALA:O	4:A:124:VAL:HG22	1.92	0.69
22:T:24:ARG:HH21	22:T:39:ASN:HD22	1.41	0.69
1:0:1209:C:H2'	1:0:1210:G:H8	1.56	0.69
23:U:52:THR:HG22	23:U:54:THR:H	1.58	0.68
1:0:1603:A:H5'	1:0:1605:G:O4'	1.93	0.68
15:M:24:GLN:NE2	15:M:27:ARG:HH11	1.90	0.68
1:0:2679:G:H2'	1:0:2681:A:OP2	1.93	0.68
17:O:32:ARG:HD3	17:O:32:ARG:O	1.92	0.68
4:A:153:ARG:CB	4:A:153:ARG:HH11	2.05	0.68
25:W:84:VAL:HG12	38:W:6679:HOH:O	1.93	0.68
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.75	0.68
1:0:1979:G:H2'	38:0:3601:HOH:O	1.92	0.68
8:E:97:VAL:HG12	38:E:4191:HOH:O	1.93	0.68
16:N:164:ASP:CG	16:N:167:ASP:HA	2.14	0.68
1:0:2851:G:O2'	1:0:2852:A:H5'	1.92	0.68
5:B:320:GLN:NE2	5:B:321:PRO:HD2	2.09	0.68
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.73	0.68
38:0:3542:HOH:O	32:I:92:PRO:HD2	1.93	0.68
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.75	0.68
1:0:603:A:H5''	1:0:604:G:OP1	1.94	0.68
5:B:141:ARG:HG2	5:B:165:ARG:HA	1.76	0.68
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.93	0.68
4:A:192:VAL:CG1	4:A:207:GLN:HB3	2.23	0.67
1:0:2426:G:H1'	38:0:6350:HOH:O	1.92	0.67
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.76	0.67
1:0:2769:C:C2'	1:0:2770:G:H5'	2.23	0.67
4:A:200:PRO:HG2	4:A:225:VAL:HG21	1.76	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:56:G:H5''	24:V:50:ARG:NH1	2.07	0.67
25:W:119:HIS:HD2	25:W:120:PRO:O	1.77	0.67
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.75	0.67
4:A:95:PRO:HG2	4:A:98:GLU:HG2	1.76	0.67
1:O:2840:A:OP1	5:B:211:THR:HG23	1.94	0.67
5:B:140:LEU:HA	38:B:9380:HOH:O	1.95	0.67
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.95	0.67
5:B:7:ARG:NH1	5:B:11:LEU:HD21	2.09	0.67
5:B:108:GLU:HB3	5:B:111:ARG:HD2	1.75	0.67
5:B:41:PHE:HB3	5:B:190:MET:HE1	1.75	0.67
1:O:1751:G:C2'	1:O:1752:G:H5''	2.24	0.67
7:D:95:THR:OG1	7:D:174:VAL:HG22	1.95	0.67
1:O:2827:A:H2'	1:O:2828:G:O4'	1.95	0.67
1:O:1474:C:C6	1:O:1474:C:H5'	2.23	0.66
2:9:3056:A:C2'	2:9:3057:A:H5''	2.24	0.66
7:D:25:MET:HE1	7:D:41:LEU:HG	1.77	0.66
12:J:54:VAL:HG11	12:J:138:THR:HG21	1.77	0.66
4:A:179:MET:HG2	4:A:186:TRP:CB	2.25	0.66
1:O:1441:G:H1'	38:O:7965:HOH:O	1.96	0.66
6:C:140:VAL:HB	38:C:9247:HOH:O	1.95	0.66
14:L:37:LYS:HG2	38:L:9335:HOH:O	1.95	0.66
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.25	0.66
13:K:62:PRO:HG3	13:K:65:ARG:NH2	2.09	0.66
1:O:1205:U:H2'	1:O:1206:U:H5''	1.78	0.66
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	1.77	0.66
1:O:1377:C:H6	1:O:1377:C:H5'	1.61	0.66
1:O:1328:A:OP1	27:Y:169:ARG:HD2	1.95	0.66
1:O:1189:A:H1'	1:O:1209:C:O4'	1.95	0.66
3:4:176:A:O4'	3:4:175:C:H2'	1.95	0.66
14:L:79:ASP:HB3	38:L:9356:HOH:O	1.95	0.66
1:O:560:C:H42	1:O:597:A:H61	1.41	0.66
21:S:57:THR:HG22	21:S:59:ASP:N	2.11	0.66
23:U:14:GLU:O	23:U:17:THR:HB	1.96	0.66
1:O:88:G:H5'	1:O:88:G:H8	1.61	0.66
15:M:164:THR:CG2	15:M:167:GLY:H	2.00	0.65
1:O:2578:G:H5'	1:O:2578:G:H8	1.60	0.65
1:O:21:G:H5''	20:R:1:GLY:O	1.96	0.65
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.25	0.65
25:W:38:THR:HG22	25:W:39:ASP:N	2.12	0.65
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.78	0.65
13:K:74:VAL:HG12	13:K:75:ARG:HG3	1.79	0.65
8:E:7:ILE:HG22	8:E:45:ASP:O	1.95	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
32:I:101:SER:H	32:I:104:GLN:NE2	1.94	0.65
8:E:22:VAL:HG12	8:E:76:VAL:HG11	1.78	0.65
29:1:25:LYS:HG3	30:2:49:GLU:H	1.60	0.65
12:J:19:MET:HE2	12:J:132:LEU:HD11	1.79	0.65
1:O:447:A:OP2	22:T:1:SER:HB2	1.96	0.65
24:V:12:THR:HG22	24:V:15:GLU:CG	2.17	0.65
9:F:58:GLU:HA	9:F:61:MET:HG3	1.78	0.65
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.61	0.65
26:X:78:GLU:HG2	26:X:79:GLU:H	1.60	0.65
1:O:2878:U:H2'	1:O:2879:A:O4'	1.95	0.65
1:O:545:G:C8	1:O:545:G:H5'	2.30	0.65
4:A:210:GLY:HA3	38:A:9379:HOH:O	1.97	0.65
7:D:44:ILE:HG12	7:D:83:PHE:HE1	1.62	0.65
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.36	0.65
5:B:275:GLY:O	5:B:291:ASP:HA	1.97	0.65
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.79	0.65
6:C:16:VAL:HG12	6:C:17:ASP:H	1.61	0.65
25:W:65:VAL:HA	25:W:68:THR:HG22	1.79	0.65
16:N:100:ALA:O	16:N:129:ILE:HG23	1.98	0.65
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.79	0.65
11:H:51:VAL:HG21	11:H:127:VAL:HG11	1.79	0.64
1:O:21:G:H4'	20:R:2:ILE:HG22	1.80	0.64
1:O:1667:A:H2'	1:O:1668:U:C6	2.32	0.64
4:A:192:VAL:HG13	38:A:9350:HOH:O	1.96	0.64
1:O:1666:C:O2'	1:O:1667:A:H5''	1.96	0.64
1:O:777:U:O2'	29:1:11:LYS:HG2	1.97	0.64
16:N:38:LYS:HE2	16:N:107:ASN:ND2	2.11	0.64
16:N:38:LYS:HE2	16:N:107:ASN:HD21	1.63	0.64
11:H:21:THR:O	11:H:120:ILE:HD12	1.98	0.64
1:O:544:G:H2'	1:O:545:G:H5''	1.78	0.64
25:W:106:THR:OG1	25:W:109:GLU:HG3	1.98	0.64
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.79	0.64
8:E:69:ILE:HA	8:E:72:MET:CE	2.27	0.64
1:O:1654:U:H2'	4:A:47:HIS:HD2	1.61	0.64
38:O:4899:HOH:O	17:O:39:THR:HB	1.97	0.64
18:P:64:GLU:HG2	38:P:169:HOH:O	1.98	0.64
6:C:16:VAL:HG12	6:C:17:ASP:N	2.12	0.64
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.31	0.64
4:A:57:ALA:HB1	4:A:65:ARG:HE	1.63	0.64
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.80	0.64
5:B:297:VAL:HB	38:B:9407:HOH:O	1.97	0.64
7:D:86:THR:C	7:D:89:PRO:HD2	2.17	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
32:I:125:ALA:O	32:I:129:VAL:HG23	1.97	0.64
1:O:2073:G:H5''	38:O:4124:HOH:O	1.98	0.64
1:O:2587:OMU:H2'	1:O:2589:U:H5''	1.79	0.64
1:O:2676:C:H4'	12:J:70:PHE:CE1	2.32	0.63
4:A:32:VAL:HG22	4:A:38:ILE:HG13	1.80	0.63
1:O:1189:A:H1'	1:O:1209:C:C1'	2.27	0.63
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.44	0.63
6:C:246:ARG:NH1	6:C:246:ARG:HB3	2.13	0.63
4:A:179:MET:HA	4:A:179:MET:CE	2.28	0.63
6:C:118:THR:HG22	6:C:137:PRO:HB3	1.81	0.63
10:G:16:LYS:O	10:G:20:VAL:HG23	1.98	0.63
2:9:3051:A:H5'	16:N:160:SER:HB3	1.81	0.63
24:V:64:GLY:O	24:V:65:ASP:HB2	1.96	0.63
14:L:143:THR:HG22	14:L:144:ASP:N	2.11	0.63
2:9:3039:U:H1'	2:9:3044:A:N6	2.13	0.63
5:B:81:ALA:O	5:B:186:GLY:HA3	1.99	0.63
9:F:53:ASP:OD1	9:F:80:GLN:HB2	1.97	0.63
1:O:338:C:H4'	6:C:174:ILE:CD1	2.29	0.63
1:O:1116:U:O2'	1:O:1118:A:C2	2.51	0.63
1:O:282:C:O2'	1:O:283:U:H5'	1.98	0.63
5:B:221:GLN:HE22	13:K:42:ASN:HD22	1.45	0.63
10:G:64:ASN:N	10:G:64:ASN:HD22	1.94	0.63
11:H:27:LYS:H	11:H:59:HIS:CD2	2.16	0.63
12:J:52:GLN:HG3	12:J:53:ILE:N	2.13	0.63
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.29	0.63
2:9:3041:C:H4'	7:D:48:MET:HB2	1.80	0.63
30:2:40:ARG:HA	30:2:45:ASN:ND2	2.14	0.63
1:O:1058:A:H2'	1:O:1060:C:H5''	1.79	0.63
1:O:542:A:H5'	1:O:542:A:C8	2.29	0.62
25:W:21:LEU:CD2	25:W:26:ILE:HD11	2.28	0.62
7:D:146:LYS:NZ	16:N:107:ASN:ND2	2.46	0.62
16:N:110:THR:HB	16:N:113:SER:OG	1.98	0.62
23:U:5:GLU:HG3	23:U:10:GLY:O	1.99	0.62
16:N:163:PHE:HZ	16:N:171:HIS:HD1	1.45	0.62
5:B:162:MET:HE3	5:B:308:LEU:HD21	1.81	0.62
30:2:40:ARG:HD2	30:2:47:THR:HG22	1.80	0.62
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.28	0.62
1:O:2256:G:C2'	1:O:2257:G:H5'	2.30	0.62
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.64	0.62
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.35	0.62
2:9:3054:A:O2'	2:9:3055:U:H5'	1.99	0.62
6:C:200:PRO:HB3	6:C:212:VAL:HG23	1.82	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
27:Y:103:THR:HG22	27:Y:104:GLU:OE2	1.98	0.62
1:0:111:C:O2'	29:1:20:ARG:HG2	1.99	0.62
9:F:2:VAL:HG22	9:F:57:GLU:OE1	2.00	0.62
1:0:1625:U:H4'	38:0:4948:HOH:O	1.97	0.62
27:Y:112:GLU:CD	27:Y:115:ARG:HH12	2.01	0.62
1:0:2534:C:H1'	38:0:3800:HOH:O	1.99	0.62
12:J:130:VAL:HG12	12:J:131:THR:N	2.15	0.62
1:0:1206:U:H5'	1:0:1206:U:H6	1.65	0.62
1:0:2251:G:H2'	1:0:2252:A:C8	2.34	0.62
5:B:145:HIS:HD2	5:B:146:THR:O	1.81	0.62
1:0:1634:G:H3'	38:0:4189:HOH:O	2.00	0.62
23:U:52:THR:HG22	23:U:54:THR:N	2.15	0.62
21:S:11:THR:H	21:S:14:ALA:HB3	1.65	0.62
1:0:299:U:H5'	38:0:7546:HOH:O	1.99	0.62
1:0:2780:C:H1'	8:E:143:GLN:HE21	1.65	0.62
1:0:31:C:H2'	38:0:7888:HOH:O	1.99	0.62
2:9:3001:U:H5''	2:9:3003:A:OP1	2.00	0.62
4:A:199:HIS:CD2	4:A:201:PHE:H	2.16	0.62
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.64	0.62
15:M:28:GLN:O	15:M:32:ARG:HG3	2.00	0.62
1:0:1819:G:H2'	1:0:1820:G:H4'	1.82	0.62
16:N:23:ARG:HH11	16:N:23:ARG:HG2	1.65	0.61
1:0:541:C:H2'	1:0:542:A:C5'	2.26	0.61
1:0:2256:G:H2'	1:0:2257:G:C5'	2.30	0.61
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.80	0.61
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.63	0.61
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.82	0.61
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.36	0.61
16:N:152:GLU:C	16:N:154:LEU:H	2.04	0.61
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.30	0.61
1:0:470:U:O2'	29:1:16:HIS:HD2	1.83	0.61
7:D:25:MET:HE3	7:D:37:ALA:CB	2.22	0.61
1:0:1166:A:H1'	1:0:1192:A:C2	2.36	0.61
5:B:84:LEU:HD23	5:B:142:LEU:HD23	1.82	0.61
1:0:119:A:H2'	1:0:120:A:H5''	1.81	0.61
32:I:76:ALA:O	32:I:80:LYS:HG3	2.01	0.61
21:S:33:SER:O	21:S:37:VAL:HG23	1.99	0.61
7:D:138:GLY:N	38:D:7597:HOH:O	2.33	0.61
2:9:3014:G:H5'	2:9:3014:G:C8	2.34	0.61
16:N:154:LEU:O	16:N:155:GLU:HB3	2.00	0.61
27:Y:144:ARG:CZ	38:Y:9407:HOH:O	2.48	0.61
1:0:20:G:H21	20:R:117:HIS:HD2	1.48	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2491:G:H1'	38:0:7098:HOH:O	1.99	0.61
16:N:80:SER:HB2	38:N:9335:HOH:O	2.01	0.61
1:0:656:G:OP2	17:O:37:ARG:HD2	2.01	0.61
38:0:4951:HOH:O	5:B:300:SER:HB3	1.99	0.61
5:B:144:THR:HB	38:B:9426:HOH:O	2.00	0.61
1:0:1527:A:H1'	1:0:1528:A:C8	2.35	0.61
18:P:16:VAL:CG1	18:P:20:ARG:HB2	2.31	0.61
5:B:254:GLN:HG2	5:B:255:GLY:N	2.14	0.61
15:M:187:LEU:HD23	15:M:194:ALA:HB3	1.81	0.61
8:E:81:GLU:HG2	8:E:134:SER:CB	2.30	0.61
32:I:92:PRO:C	32:I:94:GLU:H	2.02	0.61
1:0:969:G:H1	1:0:999:C:H42	1.49	0.61
1:0:1080:C:H4'	1:0:1081:A:OP1	2.00	0.61
1:0:2649:A:H5'	1:0:2649:A:H8	1.66	0.61
22:T:9:LYS:HE3	22:T:13:ARG:HH11	1.63	0.60
4:A:211:LYS:HB3	4:A:212:PRO:CD	2.27	0.60
1:0:538:C:OP2	27:Y:134:HIS:HE1	1.84	0.60
1:0:797:A:H4'	28:Z:10:ARG:N	2.16	0.60
1:0:1182:C:H1'	1:0:1192:A:H8	1.64	0.60
1:0:1180:U:H4'	32:I:91:GLU:HG2	1.82	0.60
5:B:305:ASP:O	5:B:306:LYS:HB2	2.01	0.60
1:0:247:A:H2'	38:0:4218:HOH:O	2.01	0.60
1:0:1535:G:H2'	1:0:1536:C:C6	2.36	0.60
1:0:902:G:N7	14:L:18:HIS:HD2	2.00	0.60
1:0:285:A:H2'	1:0:286:U:O4'	2.00	0.60
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.83	0.60
1:0:2346:C:O5'	1:0:2346:C:H6	1.84	0.60
8:E:93:MET:HE1	8:E:165:GLY:N	2.16	0.60
8:E:84:MET:HE1	8:E:148:ILE:HD12	1.81	0.60
23:U:39:ASN:ND2	23:U:44:ARG:HH11	1.98	0.60
38:0:5117:HOH:O	12:J:47:THR:HB	2.01	0.60
16:N:132:ASN:O	16:N:135:VAL:HG12	2.01	0.60
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.32	0.60
11:H:9:ILE:HG23	11:H:126:ARG:CZ	2.32	0.60
1:0:2896:A:H5''	38:0:6357:HOH:O	2.01	0.60
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.31	0.60
1:0:157:G:H4'	15:M:95:LYS:HE3	1.84	0.60
1:0:1118:A:H62	1:0:1244:U:H3	1.48	0.60
1:0:1741:U:H5'	1:0:1742:A:OP1	2.01	0.60
18:P:105:LEU:HD21	18:P:137:LEU:HD21	1.84	0.60
11:H:29:ALA:HB3	11:H:66:ARG:HH12	1.67	0.60
17:O:105:ASN:HD21	17:O:109:SER:H	1.49	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:74:ILE:HD13	5:B:309:VAL:HG21	1.84	0.60
25:W:35:VAL:HG23	25:W:41:TYR:CD2	2.36	0.60
6:C:27:ARG:HG3	6:C:29:ASP:OD1	2.02	0.60
8:E:13:ALA:HB2	8:E:22:VAL:HG22	1.84	0.60
27:Y:144:ARG:HH11	27:Y:144:ARG:CG	2.14	0.60
19:Q:26:PRO:O	19:Q:30:VAL:HG23	2.02	0.60
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.32	0.60
5:B:168:GLY:N	5:B:174:ARG:HD3	2.16	0.60
6:C:162:VAL:HG13	6:C:232:LEU:HD21	1.83	0.60
32:I:72:VAL:HG13	32:I:73:PRO:HD2	1.84	0.60
1:0:447:A:P	22:T:1:SER:HB2	2.42	0.60
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.37	0.60
1:0:2720:C:O2	13:K:87:ARG:NH2	2.35	0.59
7:D:23:VAL:O	7:D:23:VAL:HG23	2.02	0.59
27:Y:154:ARG:HH12	27:Y:155:ARG:CG	2.14	0.59
5:B:103:ASP:HB2	38:B:9394:HOH:O	2.02	0.59
1:0:2524:G:H21	1:0:2526:C:N4	2.00	0.59
1:0:1500:U:P	18:P:41:ARG:HH22	2.24	0.59
4:A:39:ALA:HB3	4:A:61:GLU:OE2	2.02	0.59
1:0:2505:G:O2'	1:0:2506:A:H5'	2.02	0.59
4:A:36:ASP:HA	4:A:83:GLY:HA3	1.84	0.59
5:B:36:PRO:CA	5:B:168:GLY:HA3	2.32	0.59
2:9:3013:A:O2'	2:9:3014:G:H5''	2.03	0.59
38:0:7663:HOH:O	5:B:211:THR:HG21	2.01	0.59
4:A:105:VAL:HG11	4:A:154:ALA:HB1	1.83	0.59
30:2:40:ARG:HG3	30:2:45:ASN:HB3	1.82	0.59
1:0:2769:C:H2'	1:0:2770:G:H5'	1.82	0.59
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.82	0.59
20:R:119:VAL:HG12	20:R:119:VAL:O	2.00	0.59
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.84	0.59
1:0:1972:U:H2'	1:0:1973:A:H5'	1.83	0.59
2:9:3114:G:O6	16:N:11:ARG:HD3	2.02	0.59
1:0:2851:G:C2'	1:0:2852:A:H5'	2.32	0.59
1:0:2414:A:H2'	1:0:2415:A:C8	2.37	0.59
1:0:820:G:H5''	38:0:3356:HOH:O	2.01	0.59
22:T:69:LYS:O	22:T:71:VAL:HG23	2.03	0.59
6:C:236:THR:HA	38:C:9247:HOH:O	2.03	0.59
32:I:102:VAL:CG1	32:I:106:LYS:HE3	2.30	0.59
1:0:558:C:C2'	1:0:559:U:H5''	2.33	0.59
7:D:146:LYS:HZ3	16:N:107:ASN:HD21	1.50	0.59
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.85	0.59
7:D:135:VAL:HG22	7:D:136:ARG:N	2.17	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:F:61:MET:HB3	15:M:19:GLN:OE1	2.01	0.59
28:Z:22:SER:O	28:Z:26:VAL:HG23	2.02	0.59
1:0:407:A:H2'	1:0:408:A:C8	2.38	0.59
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.84	0.59
12:J:107:ASN:HD22	12:J:108:PRO:N	2.01	0.59
1:0:2630:G:O6	4:A:206:ARG:NH2	2.36	0.59
2:9:3092:G:H2'	2:9:3093:A:C8	2.38	0.59
1:0:1187:U:O2'	1:0:1189:A:H2	1.86	0.58
1:0:2502:C:C2'	1:0:2503:A:H5'	2.33	0.58
1:0:2241:C:H2'	1:0:2242:U:C6	2.38	0.58
1:0:681:G:N3	1:0:681:G:H5'	2.18	0.58
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.38	0.58
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.85	0.58
14:L:143:THR:HG22	14:L:145:LEU:H	1.67	0.58
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.83	0.58
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.85	0.58
7:D:86:THR:O	7:D:90:LEU:HG	2.04	0.58
5:B:137:LEU:HD11	5:B:140:LEU:HD21	1.85	0.58
18:P:134:VAL:O	18:P:138:GLU:HG3	2.03	0.58
26:X:80:GLU:HB3	38:X:5564:HOH:O	2.02	0.58
1:0:952:G:OP1	19:Q:42:LYS:HE2	2.03	0.58
17:O:47:ARG:HG3	17:O:47:ARG:HH11	1.68	0.58
1:0:1594:C:OP2	18:P:120:ARG:HD2	2.02	0.58
5:B:154:VAL:HG12	5:B:156:LYS:HG2	1.85	0.58
14:L:54:PRO:HG2	14:L:57:VAL:HG21	1.85	0.58
24:V:11:MET:HB3	24:V:15:GLU:HB2	1.85	0.58
1:0:2812:A:C2	1:0:2814:A:N6	2.69	0.58
20:R:9:ASP:O	20:R:13:THR:HB	2.02	0.58
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.85	0.58
11:H:45:VAL:HA	11:H:167:PRO:O	2.03	0.58
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.85	0.58
11:H:56:GLN:HE21	11:H:126:ARG:NE	2.00	0.58
23:U:17:THR:HG22	23:U:18:GLY:N	2.18	0.58
8:E:69:ILE:HA	8:E:72:MET:HE3	1.84	0.58
4:A:76:VAL:HG23	28:Z:63:LYS:HB3	1.85	0.58
1:0:449:A:N7	6:C:43:LYS:HG2	2.19	0.58
1:0:1175:G:H1'	1:0:1193:A:H2'	1.85	0.58
5:B:307:ARG:CB	5:B:307:ARG:HH11	2.12	0.58
1:0:1835:U:C5	1:0:1840:A:N7	2.64	0.58
4:A:36:ASP:C	4:A:38:ILE:H	2.07	0.58
15:M:24:GLN:HE22	15:M:27:ARG:HH11	1.52	0.58
1:0:1060:C:H6	1:0:1060:C:H5'	1.69	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
27:Y:189:ASN:HD22	27:Y:189:ASN:C	2.07	0.58
23:U:46:ALA:HB1	23:U:52:THR:HG21	1.86	0.58
1:O:1593:C:OP1	18:P:117:SER:HB3	2.04	0.58
1:O:130:C:H2'	38:O:3467:HOH:O	2.02	0.58
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.34	0.58
16:N:170:GLU:O	16:N:174:GLU:HG3	2.03	0.58
13:K:98:VAL:HG13	13:K:99:ASP:N	2.18	0.58
23:U:13:ILE:HG12	23:U:32:CYS:HB3	1.84	0.58
1:O:280:C:H2'	1:O:281:U:O4'	2.03	0.58
17:O:14:LEU:HD23	17:O:102:ILE:HD11	1.86	0.58
13:K:32:ILE:HD11	13:K:56:SER:HB3	1.85	0.58
27:Y:98:GLN:HG3	27:Y:236:VAL:HB	1.84	0.58
26:X:31:ILE:O	26:X:35:GLU:HG3	2.03	0.58
15:M:60:VAL:C	15:M:61:ILE:HD12	2.23	0.58
12:J:107:ASN:HD21	12:J:109:TYR:HB2	1.68	0.57
12:J:19:MET:CE	12:J:132:LEU:HD11	2.34	0.57
5:B:314:ALA:HB3	5:B:317:PRO:HG3	1.86	0.57
24:V:58:THR:O	24:V:62:GLU:HG3	2.03	0.57
2:9:3029:C:C2'	2:9:3030:C:H5'	2.34	0.57
27:Y:144:ARG:HG3	27:Y:144:ARG:HH11	1.69	0.57
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.86	0.57
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.33	0.57
17:O:96:VAL:HA	38:O:4258:HOH:O	2.03	0.57
1:O:1342:C:C2'	1:O:1343:C:H5'	2.34	0.57
2:9:3076:G:C3'	2:9:3077:A:H5''	2.25	0.57
1:O:1377:C:H5'	1:O:1377:C:C6	2.39	0.57
1:O:95:A:H5''	1:O:97:G:O4'	2.03	0.57
17:O:42:GLU:HB2	38:O:2176:HOH:O	2.05	0.57
1:O:1010:C:H4'	16:N:4:PRO:HB2	1.84	0.57
1:O:1118:A:H8	1:O:1119:G:H5''	1.70	0.57
1:O:2541:U:H5'	38:O:9721:HOH:O	2.04	0.57
1:O:1189:A:H3'	38:O:7881:HOH:O	2.03	0.57
1:O:316:A:N3	1:O:336:G:O2'	2.37	0.57
5:B:58:PRO:HA	5:B:63:GLU:OE1	2.05	0.57
24:V:55:ARG:O	24:V:59:ILE:HG12	2.02	0.57
4:A:109:GLU:HG2	4:A:116:GLY:N	2.19	0.57
6:C:1:MET:HG2	6:C:2:GLN:N	2.12	0.57
1:O:558:C:H2'	1:O:559:U:C5'	2.34	0.57
8:E:8:PRO:HB2	8:E:11:VAL:HG23	1.87	0.57
1:O:2676:C:H4'	12:J:70:PHE:HE1	1.70	0.57
21:S:33:SER:OG	21:S:36:GLU:HG3	2.05	0.57
32:I:93:GLN:HA	32:I:96:PHE:CE2	2.40	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:O:87:THR:O	17:O:91:GLN:HG3	2.03	0.57
1:O:558:C:O2'	1:O:559:U:H5''	2.05	0.57
8:E:6:GLU:HA	8:E:46:THR:HG22	1.85	0.57
11:H:169:GLY:C	11:H:170:ASN:HD22	2.08	0.57
2:9:3028:U:H5''	16:N:40:ASN:ND2	2.20	0.57
21:S:57:THR:CG2	21:S:58:MET:N	2.67	0.57
1:O:2769:C:H2'	1:O:2770:G:C5'	2.35	0.57
28:Z:42:CYS:SG	28:Z:43:GLY:N	2.78	0.57
25:W:4:LEU:HD22	25:W:52:VAL:CG2	2.32	0.57
5:B:321:PRO:HA	38:B:9461:HOH:O	2.05	0.57
32:I:113:HIS:N	32:I:114:PRO:HD2	2.20	0.57
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.40	0.57
1:O:1185:U:H2'	1:O:1186:C:C6	2.40	0.57
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.68	0.57
20:R:132:ARG:HG2	20:R:133:ALA:N	2.20	0.57
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.19	0.56
24:V:39:ALA:N	24:V:40:PRO:CD	2.68	0.56
14:L:136:ALA:HB3	38:L:9371:HOH:O	2.05	0.56
1:O:1205:U:H2'	1:O:1206:U:C5'	2.35	0.56
7:D:65:GLU:HG3	38:D:6752:HOH:O	2.05	0.56
1:O:90:A:H2'	1:O:91:G:O4'	2.04	0.56
27:Y:132:ASP:OD1	27:Y:135:LYS:HD2	2.05	0.56
13:K:55:VAL:HG12	13:K:56:SER:N	2.20	0.56
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.33	0.56
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.05	0.56
29:1:45:ARG:HB3	38:1:9223:HOH:O	2.05	0.56
1:O:2420:G:O2'	1:O:2421:G:H5'	2.06	0.56
1:O:1352:A:H5''	1:O:1353:C:OP2	2.05	0.56
6:C:170:ASP:O	6:C:171:GLU:HG3	2.05	0.56
7:D:25:MET:CE	7:D:41:LEU:HG	2.35	0.56
1:O:1209:C:H2'	1:O:1210:G:C8	2.40	0.56
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.18	0.56
20:R:39:THR:HG23	20:R:107:GLU:O	2.05	0.56
18:P:103:THR:O	18:P:107:GLU:HG3	2.05	0.56
29:1:25:LYS:HD2	30:2:48:ASP:HA	1.87	0.56
1:O:2502:C:H2'	1:O:2503:A:H5'	1.85	0.56
10:G:12:ILE:N	10:G:13:PRO:HD3	2.20	0.56
1:O:328:U:O4'	6:C:202:THR:HG22	2.04	0.56
8:E:5:LEU:HD21	8:E:66:GLN:HG3	1.86	0.56
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.86	0.56
12:J:130:VAL:HG12	12:J:131:THR:H	1.71	0.56
10:G:20:VAL:O	10:G:24:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:138:U:H5''	1:0:139:C:OP2	2.05	0.56
11:H:58:ARG:HG3	11:H:58:ARG:NH1	2.20	0.56
32:I:129:VAL:HG13	32:I:139:ILE:HD11	1.88	0.56
1:0:200:U:H2'	38:0:3748:HOH:O	2.05	0.56
1:0:1687:C:O2	29:1:9:GLY:HA2	2.06	0.56
1:0:2468:A:H61	31:3:48:ASN:HD21	1.52	0.56
1:0:1242:A:OP2	12:J:60:ARG:NH2	2.36	0.56
2:9:3020:G:O2'	2:9:3021:G:H5'	2.06	0.56
1:0:2649:A:H5'	1:0:2649:A:C8	2.41	0.56
1:0:1679:C:H5'	38:0:9638:HOH:O	2.06	0.56
20:R:44:VAL:O	20:R:48:GLU:HG3	2.06	0.56
6:C:153:VAL:O	6:C:157:LEU:HG	2.06	0.56
30:2:41:HIS:O	30:2:45:ASN:HB2	2.06	0.56
1:0:1667:A:H2'	1:0:1668:U:H6	1.69	0.56
20:R:39:THR:HB	20:R:42:GLU:HG3	1.86	0.56
7:D:153:THR:O	7:D:156:ARG:HB2	2.06	0.56
16:N:37:ARG:NE	38:N:9333:HOH:O	2.35	0.56
1:0:65:C:O2'	1:0:66:G:H5'	2.05	0.56
1:0:2320:U:H4'	1:0:2321:A:O4'	2.05	0.56
1:0:1163:G:H5'	32:I:115:ASP:O	2.06	0.56
1:0:1086:A:N6	25:W:11:VAL:HG11	2.21	0.56
1:0:462:A:C2	30:2:37:HIS:HB3	2.41	0.56
25:W:122:ARG:HH21	25:W:154:ARG:HD2	1.70	0.56
5:B:62:ARG:HG2	5:B:65:MET:HE3	1.88	0.56
21:S:43:GLU:HB3	38:S:7106:HOH:O	2.05	0.56
5:B:30:PRO:HB2	5:B:39:GLN:NE2	2.21	0.56
14:L:93:VAL:HG21	14:L:122:ALA:HB2	1.88	0.56
1:0:1834:C:H2'	1:0:1840:A:N6	2.20	0.56
8:E:126:ILE:HB	8:E:131:LEU:HD23	1.88	0.56
38:0:7252:HOH:O	4:A:211:LYS:HG2	2.05	0.55
1:0:1167:G:H4'	32:I:135:LEU:HD22	1.88	0.55
4:A:192:VAL:HB	38:A:9388:HOH:O	2.06	0.55
1:0:2909:G:H2'	1:0:2910:A:H8	1.70	0.55
4:A:88:ILE:HG22	4:A:88:ILE:O	2.06	0.55
8:E:84:MET:HE1	8:E:148:ILE:CD1	2.36	0.55
1:0:1053:G:OP1	11:H:12:PRO:HG3	2.05	0.55
1:0:317:A:H5''	22:T:52:ARG:HD2	1.88	0.55
1:0:2690:U:O2'	8:E:111:LYS:HE3	2.06	0.55
25:W:26:ILE:O	25:W:26:ILE:HG13	2.06	0.55
32:I:138:THR:HG22	32:I:139:ILE:N	2.22	0.55
16:N:34:LEU:HA	16:N:47:LEU:HD23	1.86	0.55
1:0:2795:C:O2'	1:0:2796:U:H5'	2.05	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
38:O:5492:HOH:O	13:K:39:GLY:HA2	2.06	0.55
26:X:9:VAL:HG22	26:X:88:GLU:OE2	2.05	0.55
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.36	0.55
1:O:1441:G:O2'	1:O:1442:A:H5'	2.06	0.55
8:E:45:ASP:OD2	8:E:46:THR:HG23	2.06	0.55
1:O:1213:C:O2'	1:O:1214:G:H5'	2.07	0.55
31:3:17:HIS:O	31:3:18:GLN:HG3	2.07	0.55
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.21	0.55
4:A:105:VAL:CG1	4:A:154:ALA:HB1	2.37	0.55
19:Q:11:ARG:HD3	38:Q:5620:HOH:O	2.05	0.55
31:3:62:THR:HG23	31:3:86:GLY:HA2	1.88	0.55
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.21	0.55
1:O:2812:A:H2	1:O:2814:A:N6	1.97	0.55
14:L:133:VAL:HB	38:L:9355:HOH:O	2.07	0.55
5:B:57:GLU:O	5:B:63:GLU:HB2	2.06	0.55
38:O:4281:HOH:O	22:T:82:THR:HA	2.05	0.55
5:B:214:PRO:HD2	38:B:9320:HOH:O	2.06	0.55
25:W:5:VAL:HG22	25:W:32:CYS:HB2	1.87	0.55
1:O:1189:A:H1'	1:O:1209:C:H1'	1.87	0.55
1:O:2533:C:H6	1:O:2533:C:C5'	2.18	0.55
8:E:81:GLU:O	8:E:172:PRO:HD3	2.07	0.55
8:E:11:VAL:HG12	8:E:12:ASP:N	2.22	0.55
1:O:503:G:H2'	1:O:504:G:H8	1.72	0.55
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.62	0.55
1:O:2896:A:OP1	26:X:15:ARG:NH1	2.40	0.55
1:O:2526:C:O2'	1:O:2527:U:H5'	2.07	0.55
1:O:820:G:H3'	38:O:3356:HOH:O	2.05	0.55
1:O:1342:C:O2'	1:O:1343:C:H5'	2.05	0.55
6:C:25:PRO:HG2	38:C:9123:HOH:O	2.06	0.55
1:O:1506:U:H6	1:O:1506:U:H5'	1.71	0.55
25:W:88:THR:HG22	25:W:89:ASP:N	2.21	0.55
6:C:218:VAL:HG12	38:C:9220:HOH:O	2.04	0.55
1:O:2241:C:H2'	1:O:2242:U:H6	1.70	0.55
32:I:93:GLN:HA	32:I:96:PHE:HE2	1.72	0.55
38:O:6533:HOH:O	27:Y:158:LYS:HD3	2.06	0.55
1:O:2824:C:H5''	1:O:2825:C:H5'	1.88	0.55
1:O:2909:G:H2'	1:O:2910:A:C8	2.42	0.55
18:P:131:PHE:CD1	18:P:137:LEU:HD13	2.42	0.55
1:O:558:C:H2'	1:O:559:U:H5'	1.89	0.55
1:O:316:A:H5'	22:T:54:ASP:OD2	2.06	0.55
25:W:1:MET:N	25:W:37:GLU:HG3	2.22	0.55
1:O:816:G:H5'	1:O:1598:A:H4'	1.89	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2694:A:H4'	8:E:91:PHE:CE1	2.41	0.55
25:W:52:VAL:HG22	25:W:53:ALA:H	1.72	0.54
1:0:2781:U:H2'	1:0:2782:G:H5'	1.88	0.54
11:H:170:ASN:HD22	11:H:170:ASN:N	2.04	0.54
17:O:106:PRO:HG2	17:O:107:GLU:OE1	2.07	0.54
1:0:2890:A:H1'	23:U:56:ARG:NH2	2.22	0.54
1:0:1778:A:H2'	1:0:1779:A:H5'	1.89	0.54
1:0:159:G:OP1	15:M:74:LYS:HE3	2.07	0.54
25:W:82:GLU:O	25:W:86:GLU:HG3	2.07	0.54
2:9:3006:C:C5'	16:N:37:ARG:NH1	2.69	0.54
5:B:36:PRO:HA	5:B:168:GLY:CA	2.33	0.54
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.37	0.54
11:H:99:LYS:HD3	11:H:119:LYS:HD3	1.90	0.54
4:A:97:ALA:HB2	4:A:150:PRO:HB2	1.90	0.54
1:0:2506:A:O2'	1:0:2507:G:O5'	2.26	0.54
25:W:13:MET:HE2	25:W:18:GLN:CA	2.34	0.54
1:0:1120:U:H5'	1:0:1121:G:OP2	2.07	0.54
1:0:544:G:C2'	1:0:545:G:H5''	2.37	0.54
1:0:969:G:H1	1:0:999:C:N4	2.05	0.54
8:E:95:VAL:O	8:E:126:ILE:HD12	2.08	0.54
15:M:57:LYS:HE2	15:M:140:ALA:O	2.07	0.54
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.89	0.54
16:N:44:ARG:HG3	16:N:45:ALA:N	2.22	0.54
1:0:2504:A:H4'	11:H:71:ARG:HH11	1.72	0.54
1:0:1202:A:H2'	1:0:1203:G:H5'	1.88	0.54
24:V:39:ALA:O	24:V:41:GLU:N	2.36	0.54
1:0:2248:C:H3'	38:O:5709:HOH:O	2.07	0.54
7:D:51:ARG:HD3	38:D:7636:HOH:O	2.07	0.54
9:F:21:GLU:O	9:F:24:ARG:HG2	2.08	0.54
1:0:10:U:O4	1:0:532:A:OP2	2.25	0.54
26:X:78:GLU:HG2	26:X:79:GLU:N	2.22	0.54
5:B:71:VAL:HG11	5:B:296:LEU:HB3	1.89	0.54
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.43	0.54
6:C:35:VAL:HG21	6:C:227:GLY:HA2	1.90	0.54
8:E:77:THR:OG1	8:E:78:GLU:N	2.40	0.54
25:W:139:GLY:O	25:W:141:HIS:HD2	1.90	0.54
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.90	0.54
9:F:38:LYS:NZ	15:M:3:SER:HA	2.22	0.54
8:E:132:THR:HG23	8:E:132:THR:O	2.08	0.54
22:T:35:TYR:CG	22:T:112:LEU:HD22	2.43	0.54
13:K:62:PRO:CG	13:K:65:ARG:HH21	2.17	0.54
31:3:62:THR:HB	38:3:9351:HOH:O	2.08	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1596:U:H2'	1:0:1598:A:OP2	2.08	0.54
18:P:141:ILE:C	18:P:143:ALA:H	2.12	0.54
1:0:2755:G:H1'	38:0:4963:HOH:O	2.08	0.54
1:0:1666:C:H2'	1:0:1667:A:H5'	1.89	0.54
25:W:13:MET:CE	25:W:17:ILE:HG22	2.38	0.54
25:W:137:GLN:NE2	25:W:141:HIS:HE1	2.02	0.54
1:0:396:U:O2'	1:0:418:C:H4'	2.08	0.54
7:D:50:VAL:O	7:D:71:ALA:HA	2.08	0.54
21:S:77:VAL:O	21:S:80:ARG:HG2	2.07	0.54
1:0:2064:U:H5'	1:0:2652:U:O3'	2.08	0.54
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.25	0.53
32:I:116:LEU:HD22	32:I:127:GLU:OE1	2.09	0.53
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.36	0.53
2:9:3069:U:OP1	16:N:4:PRO:HG3	2.08	0.53
1:0:1787:C:H4'	1:0:2883:A:O4'	2.08	0.53
1:0:2385:G:H2'	1:0:2386:U:C6	2.43	0.53
1:0:1943:C:H4'	4:A:211:LYS:O	2.08	0.53
25:W:5:VAL:HG11	25:W:153:MET:HE3	1.90	0.53
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.90	0.53
2:9:3064:C:H2'	2:9:3065:A:H5'	1.90	0.53
5:B:112:THR:OG1	5:B:158:LYS:HG2	2.09	0.53
1:0:2443:C:O3'	14:L:56:LYS:HE3	2.08	0.53
1:0:625:U:H5''	1:0:1044:C:N4	2.22	0.53
1:0:1351:G:OP1	6:C:96:LYS:NZ	2.38	0.53
38:0:4905:HOH:O	4:A:6:GLY:HA3	2.08	0.53
24:V:1:THR:HG23	24:V:2:VAL:N	2.17	0.53
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.39	0.53
8:E:84:MET:HG2	8:E:168:ILE:HD13	1.90	0.53
1:0:1418:U:OP1	30:2:42:TRP:HB3	2.08	0.53
6:C:233:THR:HG22	6:C:234:VAL:N	2.24	0.53
15:M:122:GLN:OE1	15:M:127:LYS:HE2	2.09	0.53
1:0:960:G:N3	1:0:960:G:H2'	2.23	0.53
1:0:380:A:OP2	15:M:9:ARG:HD2	2.09	0.53
1:0:1166:A:H61	1:0:1180:U:H3	1.56	0.53
1:0:2768:A:H2'	1:0:2769:C:O4'	2.07	0.53
1:0:2241:C:O2'	1:0:2242:U:H5'	2.09	0.53
31:3:73:GLU:HB3	38:3:9363:HOH:O	2.07	0.53
17:O:73:ASP:HA	17:O:92:VAL:O	2.07	0.53
5:B:280:VAL:HG13	5:B:334:SER:HA	1.89	0.53
12:J:47:THR:HG22	12:J:48:GLY:H	1.74	0.53
4:A:32:VAL:HG12	4:A:34:ASP:H	1.72	0.53
4:A:36:ASP:O	4:A:38:ILE:N	2.40	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.39	0.53
18:P:143:ALA:HA	38:P:190:HOH:O	2.08	0.53
1:0:396:U:OP2	31:3:38:ARG:HD2	2.07	0.53
1:0:818:A:O2'	28:Z:13:ARG:HD3	2.08	0.53
13:K:125:ALA:C	13:K:127:ALA:H	2.12	0.53
5:B:175:LEU:C	5:B:175:LEU:HD23	2.28	0.53
38:0:5796:HOH:O	15:M:58:GLN:HG3	2.08	0.53
2:9:3044:A:O4'	7:D:76:ARG:NE	2.41	0.53
1:0:121:U:OP2	30:2:10:ARG:NH2	2.28	0.53
18:P:20:ARG:NH1	18:P:54:LYS:HD3	2.23	0.53
4:A:81:GLN:HB2	4:A:92:ASN:ND2	2.23	0.53
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.09	0.53
1:0:2265:U:H2'	1:0:2266:A:C8	2.44	0.53
9:F:48:VAL:HG23	9:F:74:PHE:CB	2.39	0.53
10:G:67:LEU:O	10:G:71:LEU:HG	2.08	0.53
25:W:149:LEU:HG	25:W:153:MET:HE2	1.90	0.53
1:0:588:G:O6	25:W:154:ARG:NH1	2.42	0.53
1:0:1766:U:O2	1:0:1778:A:H5'	2.09	0.53
5:B:175:LEU:O	5:B:175:LEU:HD23	2.07	0.53
9:F:96:ALA:HA	38:F:3111:HOH:O	2.08	0.53
5:B:248:ARG:O	5:B:251:VAL:HG13	2.08	0.53
7:D:25:MET:CE	7:D:37:ALA:HB1	2.23	0.53
23:U:9:CYS:CA	23:U:52:THR:HG23	2.36	0.53
4:A:132:ASP:OD1	4:A:133:ARG:N	2.42	0.53
20:R:34:GLU:HG2	20:R:46:TYR:OH	2.09	0.53
1:0:790:A:H2'	1:0:791:A:O4'	2.09	0.53
7:D:27:ILE:HD11	7:D:37:ALA:HB2	1.90	0.53
32:I:131:THR:HG22	32:I:131:THR:O	2.09	0.53
1:0:1299:G:N7	14:L:6:ARG:NH1	2.56	0.53
7:D:167:GLU:OE2	7:D:173:GLU:HG2	2.09	0.53
8:E:13:ALA:CB	8:E:22:VAL:HG22	2.39	0.53
1:0:2073:G:OP2	1:0:2490:A:H5'	2.09	0.53
1:0:1477:C:H5'	1:0:1868:G:C5'	2.39	0.53
3:4:74:DCZ:C2'	3:4:75:DC:H5'	2.38	0.53
22:T:50:VAL:HG12	22:T:56:ALA:HA	1.91	0.53
1:0:644:G:N3	1:0:644:G:H5'	2.23	0.53
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.08	0.53
1:0:797:A:C4'	28:Z:10:ARG:N	2.71	0.52
1:0:244:C:OP2	9:F:38:LYS:HE3	2.09	0.52
1:0:1406:A:H4'	1:0:1407:A:H5''	1.90	0.52
25:W:108:ARG:HE	25:W:114:PRO:CG	2.23	0.52
16:N:62:HIS:HB3	16:N:65:ASP:OD1	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:185:G:O3'	1:0:186:A:H4'	2.09	0.52
22:T:38:ARG:HG3	22:T:38:ARG:NH1	2.24	0.52
1:0:1741:U:O2'	1:0:2723:G:H4'	2.09	0.52
1:0:1477:C:H5'	1:0:1868:G:H5'	1.90	0.52
24:V:42:ASN:HB3	38:V:7247:HOH:O	2.09	0.52
1:0:2423:C:H5''	38:0:7262:HOH:O	2.08	0.52
32:I:139:ILE:C	32:I:140:GLU:HG3	2.28	0.52
1:0:2781:U:C2'	1:0:2782:G:H5'	2.40	0.52
7:D:170:TYR:O	7:D:171:ASP:HB3	2.10	0.52
27:Y:133:HIS:HD2	38:Y:9379:HOH:O	1.93	0.52
25:W:88:THR:CG2	25:W:110:GLN:NE2	2.73	0.52
14:L:114:VAL:HG11	38:L:9371:HOH:O	2.08	0.52
16:N:179:LEU:HD23	16:N:184:ILE:CD1	2.39	0.52
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.40	0.52
9:F:19:ALA:O	9:F:22:VAL:HG22	2.09	0.52
5:B:87:TYR:CE2	5:B:96:PRO:HG3	2.44	0.52
1:0:1632:A:H2'	1:0:1633:C:H5'	1.91	0.52
1:0:468:U:H3'	38:0:7773:HOH:O	2.10	0.52
1:0:2072:G:C6	1:0:2533:C:H1'	2.45	0.52
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.92	0.52
1:0:2769:C:O2'	1:0:2770:G:H5'	2.08	0.52
2:9:3051:A:H5'	16:N:160:SER:CB	2.39	0.52
17:O:77:ALA:HB1	17:O:98:LEU:HD12	1.89	0.52
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.44	0.52
1:0:1130:U:H2'	1:0:1131:G:O4'	2.09	0.52
7:D:85:GLN:O	7:D:86:THR:HG23	2.09	0.52
5:B:190:MET:HE2	5:B:194:PHE:CD1	2.44	0.52
5:B:71:VAL:HG11	5:B:296:LEU:HD22	1.92	0.52
4:A:94:LEU:HG	4:A:99:ILE:HD11	1.92	0.52
21:S:56:ASN:O	30:2:8:LYS:NZ	2.35	0.52
8:E:137:ASP:O	8:E:141:VAL:HG23	2.09	0.52
6:C:140:VAL:HG12	6:C:141:SER:N	2.24	0.52
25:W:4:LEU:O	25:W:32:CYS:HA	2.10	0.52
32:I:75:THR:N	32:I:112:LYS:HZ1	2.08	0.52
12:J:45:VAL:HG22	12:J:46:ILE:N	2.24	0.52
29:1:8:GLN:HE22	29:1:11:LYS:HZ1	1.57	0.52
24:V:39:ALA:C	24:V:41:GLU:H	2.13	0.52
23:U:17:THR:CG2	23:U:18:GLY:N	2.72	0.52
27:Y:155:ARG:NH1	38:Y:9358:HOH:O	2.42	0.52
31:3:14:CYS:HB3	31:3:16:GLU:HG2	1.90	0.52
14:L:21:ARG:N	38:L:9329:HOH:O	2.43	0.52
5:B:177:HIS:O	5:B:181:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:1:GLY:HA2	4:A:197:VAL:HG23	1.91	0.52
16:N:72:GLU:HG2	16:N:72:GLU:O	2.10	0.52
7:D:146:LYS:HZ1	16:N:107:ASN:HD21	1.58	0.52
5:B:320:GLN:HE21	5:B:321:PRO:HD2	1.75	0.52
24:V:64:GLY:O	24:V:65:ASP:CB	2.57	0.52
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.25	0.52
1:O:958:G:H2'	1:O:959:C:C6	2.45	0.52
7:D:163:VAL:HA	38:D:6326:HOH:O	2.10	0.52
7:D:67:ASP:O	7:D:69:ILE:HG13	2.10	0.52
1:O:1701:A:H5'	38:O:6532:HOH:O	2.10	0.52
18:P:105:LEU:CD2	18:P:137:LEU:HD21	2.39	0.52
1:O:1669:A:H2'	1:O:1670:G:C8	2.45	0.52
30:2:39:ARG:HG2	38:2:3143:HOH:O	2.09	0.52
8:E:107:PHE:CE2	8:E:108:LEU:HD13	2.44	0.52
7:D:88:LEU:C	7:D:90:LEU:H	2.13	0.52
1:O:447:A:O2'	1:O:448:G:H5'	2.10	0.52
1:O:447:A:OP1	22:T:2:LYS:HG2	2.10	0.52
5:B:148:PRO:HB2	5:B:156:LYS:O	2.10	0.52
24:V:16:ARG:NH2	24:V:63:GLU:HG3	2.25	0.52
4:A:86:ALA:HB3	4:A:94:LEU:HD13	1.92	0.52
1:O:1234:U:N3	5:B:244:PRO:HB3	2.25	0.52
12:J:26:VAL:HG13	12:J:36:VAL:HG11	1.92	0.52
9:F:113:ASP:O	9:F:117:GLU:HG3	2.10	0.52
12:J:74:ARG:O	12:J:78:ILE:HG12	2.11	0.51
1:O:2054:A:H2	20:R:128:ARG:HH22	1.51	0.51
1:O:2769:C:H2'	1:O:2770:G:O4'	2.10	0.51
31:3:3:MET:O	31:3:90:PHE:HA	2.09	0.51
5:B:217:ARG:CG	5:B:257:THR:HG22	2.37	0.51
22:T:48:VAL:HG23	22:T:98:VAL:HA	1.93	0.51
1:O:524:A:H5''	20:R:29:LYS:HD3	1.93	0.51
16:N:47:LEU:HD12	16:N:92:ALA:HB1	1.92	0.51
5:B:52:VAL:C	5:B:53:LEU:HD12	2.30	0.51
4:A:76:VAL:CG2	28:Z:63:LYS:HB3	2.40	0.51
3:4:74:DCZ:H2'1	3:4:75:DC:O4'	2.10	0.51
1:O:848:C:H5'	38:O:7491:HOH:O	2.09	0.51
21:S:81:ILE:HG12	38:S:4527:HOH:O	2.10	0.51
26:X:43:VAL:HG12	26:X:47:ALA:HB3	1.91	0.51
1:O:2252:A:C6	1:O:2253:G:H1'	2.45	0.51
1:O:2717:C:O2'	1:O:2718:C:H5''	2.11	0.51
26:X:30:MET:CE	26:X:55:ASN:HA	2.37	0.51
26:X:78:GLU:CG	26:X:79:GLU:H	2.23	0.51
2:9:3049:G:O2'	2:9:3050:G:H5'	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:C:129:HIS:HE1	6:C:231:ARG:HA	1.76	0.51
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.92	0.51
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.26	0.51
16:N:32:PRO:HD2	16:N:99:GLU:O	2.10	0.51
12:J:108:PRO:HG2	12:J:109:TYR:CD1	2.45	0.51
22:T:41:ARG:NH1	22:T:41:ARG:HG2	2.25	0.51
8:E:126:ILE:HB	8:E:131:LEU:CD2	2.41	0.51
8:E:95:VAL:HG22	8:E:104:ILE:HG12	1.92	0.51
1:O:669:G:O2'	1:O:670:G:H5'	2.10	0.51
1:O:2597:U:H2'	1:O:2598:U:H5'	1.93	0.51
1:O:1375:A:H2'	1:O:1376:G:H5'	1.93	0.51
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.46	0.51
32:I:134:SER:O	32:I:135:LEU:HD23	2.11	0.51
1:O:1641:A:C2'	1:O:1642:A:H5'	2.39	0.51
16:N:149:GLU:O	16:N:152:GLU:HB2	2.10	0.51
5:B:108:GLU:HA	5:B:110:ASP:OD1	2.11	0.51
11:H:170:ASN:N	11:H:170:ASN:ND2	2.59	0.51
1:O:512:G:O3'	1:O:513:A:H8	1.94	0.51
5:B:265:LEU:HD21	5:B:316:ARG:HD3	1.92	0.51
25:W:126:ASP:HB3	25:W:135:GLY:O	2.10	0.51
1:O:1119:G:H22	1:O:1246:A:H2	1.50	0.51
32:I:131:THR:O	32:I:135:LEU:HG	2.10	0.51
2:9:3057:A:C8	7:D:141:VAL:HG21	2.46	0.51
2:9:3039:U:HO2'	2:9:3042:C:H5	1.55	0.51
1:O:474:C:O3'	6:C:73:LEU:CD2	2.59	0.51
5:B:42:ALA:HB1	5:B:308:LEU:HD11	1.92	0.51
1:O:1787:C:H2'	1:O:1788:U:H6	1.75	0.51
12:J:51:GLU:O	12:J:55:GLU:HG3	2.10	0.51
1:O:553:G:OP2	27:Y:204:ARG:NH2	2.37	0.51
11:H:167:PRO:O	11:H:168:ALA:HB2	2.11	0.51
26:X:43:VAL:CG1	26:X:47:ALA:HB3	2.40	0.51
1:O:1559:A:OP2	1:O:1559:A:H8	1.94	0.51
1:O:2338:G:OP1	7:D:97:GLN:HG2	2.10	0.51
1:O:517:U:H1'	38:O:7782:HOH:O	2.10	0.51
4:A:43:VAL:HG21	4:A:59:GLU:HG3	1.93	0.51
23:U:6:CYS:C	23:U:8:TYR:H	2.14	0.51
9:F:79:GLN:HG3	9:F:82:ASP:OD2	2.11	0.51
24:V:4:HIS:HB3	38:V:6622:HOH:O	2.10	0.51
4:A:179:MET:HE3	4:A:179:MET:HA	1.93	0.51
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.26	0.51
8:E:166:VAL:HG12	38:E:3134:HOH:O	2.10	0.51
13:K:118:ALA:HA	13:K:125:ALA:HB2	1.93	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:834:G:H4'	1:0:835:U:OP2	2.11	0.51
1:0:920:C:H4'	1:0:921:G:C2	2.45	0.51
1:0:1123:A:C6	1:0:1238:C:H5'	2.46	0.51
25:W:46:ALA:O	25:W:49:ASN:HB2	2.10	0.51
20:R:33:ARG:NH1	38:R:9345:HOH:O	2.44	0.51
5:B:150:ALA:O	5:B:152:PRO:HD3	2.10	0.51
4:A:212:PRO:HB2	38:A:9353:HOH:O	2.10	0.51
7:D:84:LEU:C	7:D:86:THR:H	2.13	0.51
1:0:1086:A:C6	25:W:11:VAL:HG11	2.45	0.51
8:E:131:LEU:HD12	8:E:166:VAL:HG11	1.92	0.51
1:0:2591:C:OP1	5:B:1:PRO:HG3	2.11	0.51
6:C:79:ARG:O	6:C:87:ARG:HG2	2.10	0.51
38:0:7104:HOH:O	15:M:178:LYS:HB2	2.09	0.51
19:Q:77:ASP:HB3	19:Q:82:LYS:HE3	1.91	0.51
1:0:289:G:H22	1:0:363:A:H2	1.57	0.51
12:J:93:ARG:NH1	12:J:93:ARG:HB3	2.23	0.50
1:0:1181:A:H5'	32:I:94:GLU:OE2	2.10	0.50
1:0:1123:A:C2	1:0:1129:C:H4'	2.46	0.50
19:Q:32:GLU:O	19:Q:93:ARG:NH2	2.44	0.50
1:0:1236:A:H2'	1:0:1237:U:O4'	2.12	0.50
4:A:37:VAL:HG22	38:A:9391:HOH:O	2.11	0.50
21:S:6:LYS:O	21:S:7:HIS:HB3	2.11	0.50
1:0:1289:C:H3'	38:0:6650:HOH:O	2.10	0.50
1:0:2717:C:H2'	1:0:2718:C:C5'	2.29	0.50
4:A:88:ILE:HD13	4:A:100:PRO:CD	2.38	0.50
1:0:1044:C:H3'	1:0:1045:G:H5''	1.93	0.50
1:0:1940:C:H4'	38:0:7555:HOH:O	2.11	0.50
22:T:73:HIS:CD2	22:T:88:PRO:HG3	2.46	0.50
26:X:74:ALA:HB2	26:X:85:VAL:HG13	1.92	0.50
6:C:236:THR:HG21	38:C:9171:HOH:O	2.11	0.50
9:F:91:VAL:CG1	9:F:92:GLY:H	2.21	0.50
4:A:131:HIS:O	4:A:132:ASP:CB	2.59	0.50
2:9:3002:U:OP2	2:9:3003:A:H5'	2.12	0.50
11:H:28:ILE:HG23	38:H:9179:HOH:O	2.11	0.50
29:1:28:HIS:CD2	29:1:30:LYS:HB2	2.46	0.50
8:E:137:ASP:OD1	8:E:139:GLU:HB2	2.11	0.50
1:0:702:G:O2'	1:0:703:G:H5'	2.11	0.50
14:L:73:VAL:HG11	14:L:118:LEU:HD21	1.93	0.50
15:M:164:THR:HG23	15:M:165:GLY:N	2.25	0.50
25:W:141:HIS:HB2	25:W:146:ILE:HG12	1.93	0.50
7:D:64:ARG:NE	7:D:67:ASP:HB3	2.27	0.50
18:P:134:VAL:O	18:P:137:LEU:HB3	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1132:A:N6	1:0:1229:C:H2'	2.27	0.50
9:F:37:THR:O	9:F:41:GLU:HG3	2.10	0.50
1:0:1423:C:O2'	1:0:1424:A:H5'	2.11	0.50
1:0:343:C:O2'	1:0:344:C:H5'	2.11	0.50
11:H:148:GLU:HA	11:H:148:GLU:OE1	2.12	0.50
25:W:21:LEU:CD1	25:W:26:ILE:HD11	2.40	0.50
38:9:7568:HOH:O	16:N:107:ASN:HB3	2.11	0.50
14:L:143:THR:CG2	14:L:144:ASP:N	2.74	0.50
8:E:84:MET:HE3	8:E:148:ILE:HG21	1.94	0.50
27:Y:107:PRO:HB3	27:Y:182:PHE:CD2	2.47	0.50
18:P:120:ARG:NH2	18:P:123:TYR:CD2	2.79	0.50
30:2:40:ARG:CD	30:2:47:THR:HG22	2.42	0.50
5:B:7:ARG:HG2	5:B:7:ARG:HH11	1.77	0.50
29:1:28:HIS:O	29:1:32:LYS:N	2.44	0.50
1:0:2898:G:H4'	5:B:288:GLY:HA2	1.94	0.50
8:E:101:GLU:HB2	8:E:116:THR:O	2.11	0.50
15:M:46:LEU:HG	38:M:9416:HOH:O	2.10	0.50
1:0:441:A:H1'	1:0:442:A:N7	2.27	0.50
38:0:3205:HOH:O	12:J:46:ILE:HA	2.12	0.50
27:Y:235:GLU:CD	27:Y:235:GLU:N	2.62	0.50
21:S:57:THR:HG22	21:S:58:MET:N	2.26	0.50
24:V:38:GLY:C	24:V:40:PRO:HD2	2.32	0.50
16:N:47:LEU:HD13	16:N:97:VAL:HG11	1.93	0.50
16:N:143:ARG:HA	16:N:172:PHE:CD2	2.47	0.50
1:0:920:C:H5'	1:0:921:G:C4	2.46	0.50
1:0:2668:G:H2'	1:0:2669:U:C6	2.47	0.50
27:Y:187:VAL:CG2	27:Y:192:ASP:HB2	2.28	0.50
1:0:1201:C:H5''	38:0:6487:HOH:O	2.12	0.50
16:N:143:ARG:NH1	16:N:173:ASP:OD1	2.45	0.50
1:0:475:G:C5'	6:C:73:LEU:HD23	2.42	0.50
2:9:3049:G:H2'	2:9:3050:G:O4'	2.12	0.50
10:G:64:ASN:N	10:G:64:ASN:ND2	2.59	0.50
1:0:1375:A:C2'	1:0:1376:G:H5'	2.41	0.50
11:H:83:TYR:C	11:H:83:TYR:CD1	2.85	0.50
5:B:279:THR:OG1	5:B:290:VAL:HB	2.12	0.50
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.25	0.50
7:D:146:LYS:HZ3	16:N:107:ASN:ND2	2.07	0.50
5:B:132:HIS:HB2	5:B:137:LEU:HD22	1.94	0.50
1:0:2064:U:H4'	1:0:2653:A:OP1	2.11	0.50
20:R:27:HIS:O	20:R:31:ILE:HG13	2.12	0.50
25:W:63:GLU:HG2	25:W:93:ILE:HG22	1.93	0.50
9:F:58:GLU:OE1	15:M:27:ARG:NH2	2.33	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:F:46:GLU:OE2	9:F:100:ASP:HA	2.12	0.49
1:0:2036:C:O4'	13:K:44:LEU:HG	2.12	0.49
4:A:36:ASP:HB2	4:A:85:SER:H	1.77	0.49
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.93	0.49
26:X:43:VAL:HG22	26:X:76:ARG:NH1	2.27	0.49
7:D:94:ALA:HB3	7:D:97:GLN:HG3	1.94	0.49
30:2:5:LYS:O	30:2:9:LYS:HG3	2.12	0.49
8:E:119:HIS:O	8:E:140:ALA:HB1	2.12	0.49
5:B:66:GLU:OE1	5:B:328:ARG:HD2	2.12	0.49
5:B:294:TYR:HE2	38:B:9454:HOH:O	1.95	0.49
25:W:5:VAL:HG11	25:W:153:MET:CE	2.41	0.49
7:D:23:VAL:HG21	7:D:45:THR:HG21	1.94	0.49
1:0:2521:A:OP2	11:H:3:ALA:HB3	2.12	0.49
18:P:13:VAL:HG21	18:P:41:ARG:HG2	1.94	0.49
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.12	0.49
6:C:61:PHE:HB3	38:C:9242:HOH:O	2.13	0.49
1:0:2710:U:H1'	38:0:7824:HOH:O	2.12	0.49
19:Q:16:ASN:HB2	38:Q:6597:HOH:O	2.11	0.49
14:L:67:ARG:HB2	14:L:112:GLY:HA3	1.94	0.49
2:9:3023:U:O2'	2:9:3024:U:H4'	2.12	0.49
1:0:1014:A:H2'	1:0:1015:C:H5'	1.93	0.49
30:2:40:ARG:HG2	30:2:40:ARG:HH11	1.77	0.49
38:0:3592:HOH:O	13:K:9:THR:HA	2.11	0.49
27:Y:234:VAL:HG12	27:Y:235:GLU:N	2.27	0.49
16:N:34:LEU:HD22	16:N:129:ILE:HD13	1.94	0.49
4:A:179:MET:HG2	4:A:186:TRP:CG	2.47	0.49
8:E:24:GLY:HA3	8:E:76:VAL:HB	1.94	0.49
27:Y:106:THR:CG2	27:Y:107:PRO:HD2	2.43	0.49
6:C:133:ARG:NE	6:C:138:VAL:HG22	2.27	0.49
4:A:94:LEU:N	4:A:94:LEU:HD23	2.27	0.49
1:0:1503:U:H2'	1:0:1504:A:O4'	2.12	0.49
16:N:47:LEU:CD1	16:N:97:VAL:HG11	2.42	0.49
27:Y:200:THR:HG22	27:Y:201:GLU:CG	2.42	0.49
26:X:9:VAL:HG13	26:X:88:GLU:OE1	2.12	0.49
27:Y:184:GLU:OE1	27:Y:204:ARG:NH1	2.45	0.49
14:L:73:VAL:HG23	14:L:74:THR:N	2.28	0.49
7:D:154:LYS:H	7:D:154:LYS:CD	2.19	0.49
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.95	0.49
1:0:1820:G:C6	1:0:2030:A:C2	3.00	0.49
11:H:63:GLU:HA	38:H:9179:HOH:O	2.12	0.49
26:X:71:ARG:HD3	38:X:2171:HOH:O	2.12	0.49
1:0:1787:C:OP1	18:P:68:LYS:HE2	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:F:101:ALA:HA	38:F:5413:HOH:O	2.13	0.49
1:0:263:U:O4'	9:F:59:ILE:HD13	2.12	0.49
9:F:16:ALA:HA	9:F:111:ILE:HD13	1.94	0.49
1:0:2392:C:H4'	38:Q:2875:HOH:O	2.13	0.49
1:0:1462:C:H2'	1:0:1463:A:C8	2.48	0.49
14:L:35:ARG:HD3	14:L:35:ARG:C	2.33	0.49
1:0:1733:A:H4'	5:B:212:GLN:HA	1.94	0.49
1:0:1845:A:O3'	4:A:187:PRO:HB2	2.12	0.49
1:0:705:C:H2'	1:0:705:C:O2	2.13	0.49
32:I:118:SER:HB2	32:I:123:ASN:HB2	1.94	0.49
31:3:55:VAL:HB	31:3:56:PRO:HD2	1.94	0.49
1:0:256:C:H2'	1:0:257:G:O4'	2.12	0.49
25:W:26:ILE:HG22	38:W:5420:HOH:O	2.12	0.49
22:T:48:VAL:HG22	22:T:97:ARG:O	2.13	0.49
5:B:221:GLN:HE22	13:K:42:ASN:ND2	2.10	0.49
1:0:661:G:C5	1:0:686:A:C2	3.01	0.49
5:B:82:VAL:HG12	5:B:82:VAL:O	2.13	0.49
2:9:3057:A:O2'	7:D:152:PRO:HD2	2.13	0.49
25:W:139:GLY:O	25:W:141:HIS:CD2	2.66	0.49
1:0:1202:A:H2'	1:0:1203:G:C5'	2.43	0.49
4:A:220:PRO:HD2	4:A:223:ARG:HD3	1.95	0.49
29:1:28:HIS:HD2	29:1:30:LYS:H	1.60	0.49
1:0:2694:A:H4'	8:E:91:PHE:HE1	1.78	0.49
2:9:3064:C:C2'	2:9:3065:A:H5'	2.42	0.49
6:C:7:ASP:OD2	6:C:9:ASP:HB2	2.12	0.49
1:0:2894:C:O2'	1:0:2895:C:H5'	2.12	0.49
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.48	0.49
38:0:9532:HOH:O	4:A:11:ARG:HD3	2.12	0.49
1:0:1118:A:C8	1:0:1118:A:C3'	2.91	0.49
13:K:81:ARG:HB2	13:K:87:ARG:NH1	2.24	0.49
1:0:2252:A:C5	1:0:2253:G:H1'	2.47	0.49
5:B:314:ALA:CB	5:B:317:PRO:HG3	2.43	0.49
1:0:585:C:H5''	38:0:5151:HOH:O	2.13	0.49
38:0:5676:HOH:O	4:A:164:ARG:CZ	2.60	0.49
22:T:71:VAL:HG12	22:T:72:ILE:N	2.27	0.48
17:O:26:TRP:HA	17:O:26:TRP:HE3	1.76	0.48
9:F:107:ASP:O	9:F:111:ILE:HG13	2.12	0.48
9:F:111:ILE:O	9:F:115:VAL:HG23	2.13	0.48
17:O:113:VAL:O	17:O:114:ILE:HD13	2.13	0.48
1:0:1878:G:H1'	38:0:6378:HOH:O	2.11	0.48
15:M:78:LYS:HD3	38:M:9434:HOH:O	2.13	0.48
25:W:22:GLU:HG2	25:W:27:HIS:CD2	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:32:VAL:HG12	4:A:34:ASP:N	2.27	0.48
15:M:166:ALA:HA	15:M:169:ARG:HH12	1.73	0.48
32:I:75:THR:OG1	32:I:112:LYS:NZ	2.45	0.48
1:O:1701:A:H4'	1:O:1702:U:C5'	2.42	0.48
17:O:77:ALA:HA	17:O:96:VAL:O	2.13	0.48
1:O:926:A:H5'	14:L:39:GLU:OE2	2.13	0.48
1:O:221:G:H2'	1:O:222:A:C8	2.48	0.48
8:E:9:GLU:HG3	8:E:10:ASP:N	2.28	0.48
4:A:215:ILE:HG13	4:A:216:SER:N	2.28	0.48
14:L:104:ASP:O	14:L:105:TYR:HB3	2.12	0.48
1:O:1427:A:H61	1:O:1440:U:C1'	2.25	0.48
25:W:21:LEU:HB3	25:W:26:ILE:CG1	2.43	0.48
1:O:282:C:H1'	1:O:368:C:H42	1.74	0.48
20:R:39:THR:HB	20:R:42:GLU:CG	2.43	0.48
22:T:41:ARG:NH1	22:T:42:VAL:O	2.46	0.48
8:E:15:GLN:HG2	8:E:19:ASP:O	2.13	0.48
11:H:28:ILE:HA	11:H:63:GLU:OE1	2.12	0.48
1:O:941:G:C5	1:O:942:U:C4	3.01	0.48
1:O:74:A:H2'	1:O:75:U:C6	2.48	0.48
1:O:1135:G:H5'	38:O:6188:HOH:O	2.12	0.48
21:S:23:LYS:HE2	38:S:3430:HOH:O	2.12	0.48
1:O:800:G:H4'	38:O:7283:HOH:O	2.13	0.48
1:O:1904:A:H2'	1:O:1905:U:O4'	2.13	0.48
1:O:2762:C:H3'	38:O:3673:HOH:O	2.13	0.48
32:I:75:THR:CA	32:I:112:LYS:HZ1	2.27	0.48
1:O:1165:G:H1'	1:O:1174:A:H1'	1.96	0.48
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.48	0.48
32:I:96:PHE:HA	32:I:136:GLY:CA	2.44	0.48
1:O:1352:A:N1	6:C:48:SER:HB3	2.27	0.48
9:F:14:ASP:O	9:F:18:GLU:HG3	2.13	0.48
24:V:56:ILE:O	24:V:60:GLN:HG3	2.14	0.48
8:E:2:ARG:HH21	8:E:48:VAL:HG21	1.77	0.48
19:Q:14:LEU:HD21	19:Q:43:ILE:HD12	1.95	0.48
1:O:2730:G:O2'	1:O:2731:G:H5'	2.13	0.48
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.79	0.48
26:X:30:MET:CE	26:X:58:ALA:HB3	2.44	0.48
5:B:254:GLN:NE2	38:B:9390:HOH:O	2.46	0.48
22:T:75:GLU:O	22:T:76:ASP:HB2	2.12	0.48
8:E:15:GLN:NE2	8:E:40:VAL:O	2.46	0.48
1:O:1717:A:H5''	18:P:54:LYS:HB2	1.96	0.48
1:O:2356:A:H2'	1:O:2357:G:O4'	2.13	0.48
1:O:602:A:O2'	1:O:605:C:H4'	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:536:A:H3'	38:O:5327:HOH:O	2.12	0.48
28:Z:60:CYS:O	28:Z:61:ASP:HB2	2.13	0.48
8:E:154:ILE:HD11	8:E:157:LYS:HB2	1.94	0.48
1:O:1666:C:H2'	1:O:1667:A:C5'	2.44	0.48
12:J:133:GLY:O	12:J:137:GLU:HG3	2.14	0.48
8:E:69:ILE:HA	8:E:72:MET:HE2	1.95	0.48
5:B:84:LEU:HD23	5:B:142:LEU:CD2	2.42	0.48
14:L:54:PRO:HG2	14:L:57:VAL:CG2	2.42	0.48
1:O:317:A:OP1	22:T:52:ARG:O	2.30	0.48
11:H:88:ARG:NH1	11:H:135:THR:OG1	2.40	0.48
1:O:1363:G:OP1	6:C:76:ARG:NH2	2.45	0.48
1:O:827:A:H2'	1:O:828:G:O4'	2.14	0.48
7:D:27:ILE:HD11	7:D:37:ALA:CB	2.44	0.48
32:I:87:THR:HG22	32:I:88:GLY:N	2.28	0.48
1:O:1201:C:H2'	1:O:1202:A:H5'	1.95	0.48
8:E:31:ARG:HH12	8:E:68:HIS:CG	2.32	0.48
21:S:37:VAL:O	21:S:41:VAL:HG23	2.13	0.48
27:Y:144:ARG:CG	27:Y:144:ARG:NH1	2.76	0.48
4:A:105:VAL:HG12	4:A:106:CYS:N	2.28	0.48
32:I:96:PHE:HD2	32:I:136:GLY:HA2	1.79	0.48
5:B:75:GLU:C	5:B:77:PRO:HD3	2.34	0.48
1:O:1829:A:H2'	1:O:1830:C:H5'	1.96	0.48
11:H:154:TYR:CD1	11:H:154:TYR:C	2.87	0.48
6:C:138:VAL:O	6:C:234:VAL:HA	2.13	0.48
9:F:48:VAL:CG2	9:F:74:PHE:HB3	2.43	0.48
1:O:1785:G:OP1	18:P:76:GLY:HA3	2.13	0.48
19:Q:3:SER:HB3	38:Q:5998:HOH:O	2.13	0.48
17:O:38:ARG:NH1	38:O:7674:HOH:O	2.47	0.48
1:O:2718:C:H6	1:O:2718:C:H5'	1.78	0.48
12:J:39:VAL:HG12	12:J:40:ASN:ND2	2.29	0.48
14:L:6:ARG:NH2	38:L:9347:HOH:O	2.45	0.48
6:C:136:VAL:HG22	6:C:137:PRO:HA	1.95	0.48
14:L:80:ASP:HB2	14:L:90:ARG:O	2.14	0.48
1:O:2685:C:H1'	38:O:3745:HOH:O	2.13	0.48
1:O:1380:U:O4	1:O:2043:U:H4'	2.13	0.48
26:X:49:ARG:HG3	26:X:49:ARG:O	2.09	0.48
1:O:1790:C:H2'	1:O:1791:U:H6	1.79	0.48
1:O:1333:U:H2'	1:O:1334:C:C6	2.49	0.48
1:O:1087:G:H4'	1:O:1088:A:OP1	2.14	0.48
1:O:1544:U:H2'	1:O:1545:C:H6	1.79	0.48
1:O:1029:U:O2'	1:O:1273:C:OP1	2.27	0.48
1:O:1130:U:H5'	38:O:7873:HOH:O	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:V:49:LEU:O	24:V:53:ILE:HG13	2.14	0.48
1:0:1300:G:H1'	38:0:4964:HOH:O	2.14	0.48
38:0:6937:HOH:O	27:Y:165:GLU:HB3	2.13	0.48
1:0:2613:G:O2'	1:0:2614:C:H5'	2.14	0.48
7:D:10:PHE:CD1	7:D:11:HIS:N	2.82	0.48
1:0:1202:A:C2'	1:0:1203:G:H5'	2.43	0.47
1:0:2255:A:O2'	1:0:2256:G:H5'	2.14	0.47
1:0:2256:G:O2'	1:0:2257:G:H5'	2.14	0.47
8:E:100:ASP:HB2	38:E:2789:HOH:O	2.13	0.47
1:0:170:U:H2'	1:0:171:C:H5'	1.95	0.47
6:C:236:THR:CG2	6:C:239:ALA:H	2.12	0.47
25:W:4:LEU:HD11	25:W:45:VAL:HG12	1.96	0.47
9:F:91:VAL:CG1	9:F:92:GLY:N	2.74	0.47
2:9:3039:U:H3'	2:9:3040:C:H5''	1.96	0.47
1:0:378:A:OP1	15:M:9:ARG:NH2	2.45	0.47
6:C:118:THR:CG2	6:C:137:PRO:HB3	2.44	0.47
1:0:1681:G:H5''	1:0:1682:A:H5'	1.95	0.47
12:J:135:ILE:O	12:J:139:LEU:HG	2.13	0.47
5:B:195:ARG:CZ	5:B:323:LEU:HD13	2.44	0.47
1:0:2361:A:H2'	1:0:2362:A:C8	2.49	0.47
5:B:310:ARG:HD2	38:B:9452:HOH:O	2.14	0.47
12:J:46:ILE:O	12:J:46:ILE:HG12	2.13	0.47
18:P:83:LYS:O	18:P:86:ALA:HB3	2.13	0.47
1:0:1180:U:H2'	1:0:1181:A:C8	2.49	0.47
19:Q:18:PRO:O	19:Q:21:ARG:HB2	2.15	0.47
1:0:2782:G:O6	1:0:2790:C:H5''	2.14	0.47
4:A:105:VAL:HG11	4:A:154:ALA:CB	2.44	0.47
14:L:125:PHE:CE1	14:L:140:VAL:HG13	2.49	0.47
5:B:128:ILE:O	5:B:131:ALA:HB3	2.14	0.47
1:0:415:A:O2'	1:0:416:G:H5'	2.15	0.47
6:C:37:ALA:O	6:C:41:ASN:ND2	2.48	0.47
1:0:1097:A:H5''	25:W:125:HIS:NE2	2.30	0.47
6:C:2:GLN:HB3	38:C:9181:HOH:O	2.14	0.47
1:0:2507:G:H2'	1:0:2510:C:H42	1.78	0.47
16:N:73:ALA:HB1	16:N:74:PRO:HD2	1.97	0.47
1:0:821:U:H2'	1:0:822:C:H6	1.79	0.47
1:0:2541:U:H4'	1:0:2542:C:OP1	2.13	0.47
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.96	0.47
38:0:9672:HOH:O	29:1:1:THR:HA	2.13	0.47
1:0:2403:C:H3'	38:0:5482:HOH:O	2.15	0.47
1:0:1919:A:H4'	38:0:5131:HOH:O	2.13	0.47
16:N:27:LEU:HD22	16:N:50:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:N:37:ARG:NH2	38:N:9333:HOH:O	2.47	0.47
20:R:39:THR:HB	20:R:42:GLU:CD	2.35	0.47
7:D:173:GLU:HG3	7:D:174:VAL:N	2.30	0.47
18:P:10:ALA:O	18:P:13:VAL:HG12	2.14	0.47
16:N:22:GLN:HG2	16:N:26:LEU:HD22	1.97	0.47
21:S:39:ASP:HB3	21:S:43:GLU:OE2	2.15	0.47
6:C:234:VAL:HG22	6:C:234:VAL:O	2.14	0.47
1:0:2897:C:H2'	1:0:2898:G:H8	1.79	0.47
9:F:101:ALA:HB3	9:F:105:ASP:OD1	2.15	0.47
1:0:1878:G:O2'	1:0:1879:U:P	2.72	0.47
7:D:39:ASP:HB2	38:D:5583:HOH:O	2.15	0.47
1:0:1666:C:C2'	1:0:1667:A:H5''	2.45	0.47
32:I:113:HIS:NE2	32:I:121:LEU:HD22	2.29	0.47
16:N:164:ASP:OD1	16:N:167:ASP:HA	2.15	0.47
1:0:1654:U:H2'	4:A:47:HIS:CD2	2.46	0.47
5:B:162:MET:CE	5:B:308:LEU:HD21	2.44	0.47
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.45	0.47
15:M:61:ILE:N	15:M:61:ILE:HD12	2.29	0.47
3:4:74:DCZ:H2'1	3:4:75:DC:H5'	1.96	0.47
1:0:1406:A:H4'	1:0:1407:A:C5'	2.44	0.47
28:Z:25:ARG:O	28:Z:29:ILE:HG13	2.15	0.47
1:0:37:A:H2'	1:0:38:G:C8	2.49	0.47
1:0:587:A:H5''	38:0:7501:HOH:O	2.15	0.47
8:E:79:GLY:HA3	38:E:7046:HOH:O	2.15	0.47
8:E:86:VAL:CG1	8:E:129:GLU:HA	2.44	0.47
1:0:177:A:H2'	1:0:178:U:O4'	2.14	0.47
5:B:238:ASN:HD22	5:B:240:GLY:N	2.07	0.47
1:0:475:G:OP1	6:C:73:LEU:HD22	2.15	0.47
24:V:42:ASN:O	24:V:44:GLY:N	2.48	0.47
1:0:660:A:H4'	1:0:661:G:O5'	2.15	0.47
1:0:1495:C:H2'	1:0:1496:G:C8	2.50	0.47
19:Q:66:LYS:HB2	19:Q:70:ALA:O	2.15	0.47
5:B:16:ARG:NH1	38:B:9418:HOH:O	2.47	0.47
2:9:3055:U:H4'	2:9:3056:A:C8	2.50	0.47
12:J:75:PRO:HD3	12:J:136:SER:OG	2.15	0.47
1:0:1972:U:H2'	1:0:1973:A:C5'	2.45	0.47
12:J:22:VAL:O	12:J:26:VAL:HG23	2.15	0.47
6:C:55:ARG:NH2	29:1:56:GLU:OE2	2.39	0.47
31:3:57:GLY:HA2	38:3:9327:HOH:O	2.15	0.47
1:0:12:U:H2'	1:0:13:G:H5'	1.96	0.47
5:B:277:GLU:N	5:B:278:PRO:HD2	2.29	0.47
9:F:13:GLU:OE2	9:F:78:GLU:HG2	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
38:O:5785:HOH:O	5:B:298:LYS:HD3	2.14	0.47
2:9:3055:U:H4'	2:9:3056:A:H8	1.79	0.47
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.96	0.47
1:0:2428:G:N7	31:3:60:LYS:NZ	2.63	0.47
1:0:1183:C:N4	1:0:1184:C:H41	2.13	0.47
18:P:103:THR:HB	38:P:180:HOH:O	2.15	0.47
9:F:38:LYS:HZ3	15:M:3:SER:HA	1.80	0.47
1:0:2361:A:H5''	38:O:9323:HOH:O	2.15	0.47
1:0:1118:A:C8	1:0:1119:G:H5''	2.49	0.46
1:0:558:C:C2'	1:0:559:U:C5'	2.92	0.46
18:P:59:ARG:HH22	18:P:66:GLN:NE2	2.09	0.46
32:I:138:THR:HG22	32:I:139:ILE:H	1.79	0.46
16:N:34:LEU:HD13	16:N:47:LEU:HD21	1.97	0.46
5:B:258:GLY:H	5:B:260:HIS:HE1	1.56	0.46
8:E:73:PHE:O	8:E:76:VAL:HG22	2.14	0.46
25:W:11:VAL:O	25:W:12:ASN:HB2	2.14	0.46
1:0:553:G:P	27:Y:204:ARG:HH22	2.38	0.46
5:B:25:ARG:HA	5:B:310:ARG:HH21	1.80	0.46
7:D:35:ALA:N	38:D:5576:HOH:O	2.47	0.46
2:9:3048:C:H4'	16:N:141:ARG:HH21	1.79	0.46
9:F:26:THR:HG21	9:F:103:GLU:HG3	1.97	0.46
1:0:2011:A:H4'	1:0:2012:U:O5'	2.15	0.46
6:C:185:LYS:HD3	6:C:186:TYR:CE1	2.50	0.46
6:C:130:GLU:HA	6:C:130:GLU:OE1	2.15	0.46
4:A:35:GLY:O	4:A:36:ASP:CB	2.56	0.46
12:J:39:VAL:HG13	12:J:106:GLY:O	2.15	0.46
26:X:15:ARG:HB3	26:X:15:ARG:HH11	1.80	0.46
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.46	0.46
16:N:69:TYR:CE2	16:N:184:ILE:HD11	2.50	0.46
18:P:13:VAL:HG13	18:P:14:LEU:N	2.31	0.46
1:0:2846:C:H4'	5:B:156:LYS:HB3	1.98	0.46
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.15	0.46
1:0:1427:A:H61	1:0:1440:U:H1'	1.80	0.46
1:0:485:A:N3	1:0:487:G:H5''	2.30	0.46
25:W:130:HIS:O	25:W:136:GLY:HA3	2.14	0.46
1:0:1172:G:H1'	38:O:5254:HOH:O	2.15	0.46
1:0:2548:C:OP2	5:B:5:ARG:NH2	2.48	0.46
32:I:106:LYS:O	32:I:110:GLU:HG3	2.15	0.46
1:0:2748:G:H1'	38:O:8206:HOH:O	2.14	0.46
2:9:3050:G:H2'	2:9:3051:A:C8	2.50	0.46
38:O:3949:HOH:O	17:O:3:THR:HG21	2.15	0.46
8:E:87:PHE:O	8:E:93:MET:HE3	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:2694:A:H5''	8:E:90:HIS:CE1	2.51	0.46
25:W:108:ARG:HE	25:W:114:PRO:HG2	1.80	0.46
31:3:3:MET:HG3	31:3:4:PRO:HD2	1.97	0.46
8:E:114:ARG:HB3	8:E:151:LEU:HD11	1.97	0.46
11:H:9:ILE:HG12	11:H:56:GLN:CG	2.46	0.46
32:I:75:THR:HA	32:I:112:LYS:HZ1	1.79	0.46
38:O:9868:HOH:O	25:W:119:HIS:HE1	1.97	0.46
10:G:64:ASN:O	10:G:68:GLU:HG3	2.16	0.46
1:O:776:A:OP1	29:1:28:HIS:HE1	1.99	0.46
1:O:2301:A:H5''	1:O:2302:A:H5'	1.98	0.46
1:O:1385:G:O3'	26:X:49:ARG:NH1	2.48	0.46
28:Z:81:ARG:O	28:Z:82:SER:C	2.53	0.46
1:O:2866:U:H4'	1:O:2867:G:H5'	1.97	0.46
1:O:424:C:H2'	1:O:425:U:C6	2.50	0.46
6:C:242:GLU:HG3	38:C:9178:HOH:O	2.15	0.46
1:O:29:C:O2'	1:O:30:U:H5'	2.16	0.46
1:O:1119:G:H8	12:J:52:GLN:NE2	2.13	0.46
25:W:149:LEU:HG	25:W:153:MET:CE	2.46	0.46
23:U:9:CYS:HA	23:U:52:THR:CG2	2.39	0.46
16:N:110:THR:HB	16:N:113:SER:HG	1.79	0.46
6:C:200:PRO:HB3	6:C:212:VAL:CG2	2.45	0.46
1:O:775:G:OP1	29:1:16:HIS:HE1	1.99	0.46
17:O:21:SER:HB3	17:O:107:GLU:HA	1.96	0.46
1:O:2708:G:N2	13:K:1:MET:O	2.47	0.46
1:O:236:A:H4'	1:O:237:G:H5'	1.97	0.46
9:F:39:SER:HB3	9:F:45:ALA:HB2	1.98	0.46
1:O:2487:C:H5	38:O:5168:HOH:O	1.98	0.46
24:V:1:THR:O	24:V:4:HIS:CE1	2.69	0.46
20:R:113:HIS:O	20:R:145:LEU:HD12	2.15	0.46
14:L:145:LEU:O	14:L:148:GLU:HG3	2.15	0.46
1:O:2064:U:H5'	1:O:2652:U:H4'	1.98	0.46
24:V:57:LYS:HA	24:V:60:GLN:HE21	1.81	0.46
18:P:40:VAL:O	18:P:44:VAL:HG23	2.15	0.46
1:O:482:G:H4'	1:O:508:A:N1	2.31	0.46
21:S:8:PRO:HD2	24:V:32:ALA:HA	1.98	0.46
1:O:1278:A:H4'	1:O:1279:U:C4	2.50	0.46
6:C:142:ASP:OD1	6:C:236:THR:HG23	2.16	0.46
1:O:558:C:H2'	1:O:559:U:H5''	1.97	0.46
1:O:2269:C:C2'	1:O:2270:G:H5'	2.46	0.46
1:O:1205:U:C2'	1:O:1206:U:H5''	2.45	0.46
5:B:145:HIS:HA	5:B:160:ASP:O	2.15	0.46
1:O:2415:A:N3	16:N:26:LEU:HD13	2.31	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:154:VAL:CG1	5:B:156:LYS:HG2	2.45	0.46
1:0:1427:A:N6	1:0:1440:U:H1'	2.31	0.46
11:H:154:TYR:HD1	11:H:154:TYR:C	2.18	0.46
13:K:22:ASP:HB2	38:K:5264:HOH:O	2.14	0.46
1:0:2324:G:H4'	1:0:2418:G:O2'	2.15	0.46
1:0:87:C:H2'	30:2:28:LYS:O	2.16	0.46
1:0:21:G:H5''	20:R:2:ILE:HA	1.96	0.46
16:N:154:LEU:C	16:N:156:GLU:H	2.19	0.46
1:0:1086:A:OP1	25:W:9:GLY:N	2.43	0.46
1:0:1236:A:C8	12:J:63:ILE:HD11	2.51	0.46
1:0:2445:U:H2'	1:0:2446:G:C8	2.51	0.46
15:M:64:ARG:HD2	38:M:9383:HOH:O	2.15	0.46
28:Z:39:CYS:HA	28:Z:47:VAL:HG21	1.97	0.46
1:0:2670:G:O2'	1:0:2671:U:H5'	2.16	0.46
12:J:52:GLN:HG3	12:J:53:ILE:H	1.80	0.46
6:C:162:VAL:CG1	6:C:192:ILE:HD11	2.44	0.46
1:0:88:G:H2'	1:0:89:G:C8	2.51	0.46
29:1:25:LYS:HD2	30:2:49:GLU:N	2.30	0.46
9:F:57:GLU:HB2	15:M:23:LEU:HD11	1.97	0.46
9:F:48:VAL:HG23	9:F:74:PHE:HB2	1.97	0.46
1:0:1878:G:O2'	1:0:1879:U:C6	2.67	0.46
36:0:9303:CL:CL	30:2:2:LYS:HE3	2.52	0.46
4:A:123:GLY:HA3	4:A:162:GLY:HA2	1.98	0.46
1:0:2832:C:H5	38:0:7432:HOH:O	1.98	0.46
4:A:165:THR:O	4:A:165:THR:HG22	2.15	0.46
30:2:40:ARG:HG3	30:2:45:ASN:CB	2.44	0.46
25:W:21:LEU:HD21	25:W:48:VAL:HG13	1.98	0.46
22:T:35:TYR:CD2	22:T:112:LEU:HD22	2.51	0.46
1:0:2365:G:H4'	19:Q:45:PRO:O	2.16	0.46
12:J:107:ASN:HD22	12:J:107:ASN:C	2.16	0.46
1:0:793:A:C5'	18:P:83:LYS:HG2	2.41	0.46
20:R:119:VAL:O	20:R:119:VAL:CG1	2.63	0.46
1:0:960:G:N3	1:0:960:G:C2'	2.79	0.46
9:F:33:THR:HG21	9:F:59:ILE:O	2.16	0.46
1:0:1613:C:H2'	1:0:1614:G:O4'	2.15	0.46
7:D:140:ARG:O	7:D:144:ARG:HG2	2.16	0.46
38:0:4054:HOH:O	22:T:9:LYS:HD3	2.16	0.45
25:W:65:VAL:HA	25:W:68:THR:CG2	2.45	0.45
20:R:17:MET:CE	20:R:19:ARG:CZ	2.94	0.45
32:I:96:PHE:HA	32:I:136:GLY:HA3	1.97	0.45
1:0:2472:C:O2'	1:0:2634:G:H4'	2.16	0.45
15:M:72:ALA:HB2	15:M:93:ARG:HG2	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:36:ASP:C	4:A:38:ILE:N	2.69	0.45
32:I:102:VAL:O	32:I:106:LYS:HG3	2.17	0.45
7:D:166:ILE:HB	38:D:6326:HOH:O	2.15	0.45
7:D:81:GLU:C	7:D:83:PHE:H	2.20	0.45
26:X:43:VAL:CG1	26:X:44:ASP:H	2.24	0.45
13:K:75:ARG:CZ	38:K:4172:HOH:O	2.63	0.45
16:N:34:LEU:HD22	16:N:129:ILE:CD1	2.45	0.45
8:E:102:VAL:HG11	8:E:148:ILE:HG12	1.98	0.45
15:M:69:LYS:HG2	15:M:127:LYS:HG3	1.98	0.45
1:O:289:G:N2	1:O:363:A:H2	2.15	0.45
1:O:1168:C:H4'	38:I:5128:HOH:O	2.15	0.45
20:R:17:MET:HE1	20:R:19:ARG:CZ	2.47	0.45
22:T:32:ARG:CZ	22:T:38:ARG:NH1	2.80	0.45
1:O:1120:U:H5''	1:O:1120:U:C6	2.51	0.45
1:O:894:A:C2	6:C:87:ARG:NH2	2.84	0.45
8:E:154:ILE:HD11	8:E:157:LYS:HE2	1.97	0.45
5:B:97:LEU:HD21	38:B:9444:HOH:O	2.17	0.45
1:O:2372:A:H2'	1:O:2373:U:C6	2.52	0.45
21:S:52:VAL:C	21:S:53:ASN:HD22	2.20	0.45
1:O:500:G:H21	20:R:98:ASN:HD21	1.62	0.45
1:O:156:C:H5''	15:M:171:ARG:CD	2.24	0.45
32:I:112:LYS:O	32:I:116:LEU:HG	2.16	0.45
22:T:49:GLU:HG3	22:T:97:ARG:HB3	1.97	0.45
13:K:75:ARG:O	13:K:93:ASN:HA	2.16	0.45
1:O:2415:A:C2	16:N:25:ARG:HB3	2.52	0.45
1:O:2300:A:H4'	1:O:2301:A:O5'	2.16	0.45
20:R:132:ARG:CZ	38:R:9383:HOH:O	2.65	0.45
5:B:202:VAL:HG11	5:B:301:VAL:HG13	1.99	0.45
1:O:1309:U:O2'	1:O:1310:U:H5'	2.15	0.45
14:L:34:GLY:C	14:L:36:ASP:H	2.20	0.45
26:X:7:GLU:HA	26:X:74:ALA:O	2.16	0.45
12:J:47:THR:O	12:J:53:ILE:HD11	2.17	0.45
4:A:36:ASP:CG	4:A:85:SER:HB2	2.36	0.45
7:D:159:PRO:O	7:D:163:VAL:HG23	2.16	0.45
1:O:1095:U:O2	25:W:120:PRO:HG2	2.16	0.45
1:O:952:G:N3	1:O:2302:A:H2'	2.31	0.45
1:O:2467:A:H1'	38:O:5014:HOH:O	2.17	0.45
1:O:2563:U:H2'	1:O:2565:C:O5'	2.16	0.45
1:O:270:U:H1'	38:O:4020:HOH:O	2.16	0.45
15:M:98:GLN:O	15:M:102:GLU:HG3	2.17	0.45
6:C:165:ASP:O	6:C:168:ARG:HB3	2.17	0.45
1:O:2385:G:H2'	1:O:2386:U:H6	1.80	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:F:46:GLU:O	9:F:73:PRO:HD2	2.17	0.45
1:0:678:G:OP2	6:C:107:ARG:NH2	2.50	0.45
1:0:290:C:O2'	1:0:291:C:H5'	2.15	0.45
26:X:75:ALA:O	26:X:83:ALA:HA	2.16	0.45
1:0:2619:UR3:H6	1:0:2619:UR3:O5'	2.17	0.45
15:M:167:GLY:O	15:M:171:ARG:HG3	2.17	0.45
4:A:192:VAL:HG12	4:A:192:VAL:O	2.17	0.45
5:B:51:VAL:HG21	5:B:327:VAL:HG13	1.99	0.45
38:0:3990:HOH:O	8:E:143:GLN:HG2	2.16	0.45
1:0:136:C:H2'	1:0:137:U:O4'	2.17	0.45
9:F:72:VAL:HA	9:F:73:PRO:HD3	1.86	0.45
1:0:2729:C:O2'	1:0:2730:G:H5'	2.17	0.45
1:0:1314:U:H2'	38:0:6137:HOH:O	2.15	0.45
6:C:214:THR:HG23	38:C:9234:HOH:O	2.15	0.45
1:0:2816:A:H5''	1:0:2817:G:H5'	1.99	0.45
1:0:2004:U:H4'	38:0:5579:HOH:O	2.16	0.45
1:0:1711:A:O2'	1:0:1712:A:H5'	2.17	0.45
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.52	0.45
26:X:74:ALA:CB	26:X:85:VAL:HG22	2.46	0.45
16:N:93:GLN:NE2	16:N:93:GLN:HA	2.23	0.45
1:0:559:U:H2'	1:0:560:C:O4'	2.17	0.45
16:N:140:GLN:HA	16:N:143:ARG:HD3	1.99	0.45
5:B:86:ALA:HA	38:B:9380:HOH:O	2.16	0.45
5:B:51:VAL:HG13	5:B:51:VAL:O	2.16	0.45
8:E:43:ASP:O	8:E:45:ASP:N	2.47	0.45
8:E:118:ILE:HG23	8:E:144:THR:HG21	1.99	0.45
17:O:47:ARG:HG3	17:O:47:ARG:NH1	2.31	0.45
38:0:7005:HOH:O	16:N:4:PRO:HD2	2.16	0.45
1:0:703:G:O2'	1:0:704:C:H5'	2.17	0.45
14:L:66:VAL:HG23	14:L:67:ARG:N	2.32	0.45
1:0:2281:C:C2'	1:0:2282:U:H5'	2.46	0.45
26:X:66:THR:HG22	26:X:67:PRO:O	2.17	0.45
1:0:907:A:H2'	1:0:908:A:H8	1.81	0.45
6:C:172:THR:HG22	6:C:188:ARG:CZ	2.47	0.45
12:J:47:THR:HG22	12:J:48:GLY:N	2.31	0.45
13:K:30:LYS:O	13:K:55:VAL:HG13	2.17	0.45
12:J:107:ASN:HD22	12:J:108:PRO:CD	2.29	0.45
5:B:276:ASP:HB3	5:B:291:ASP:OD1	2.17	0.45
1:0:1163:G:H2'	1:0:1164:U:C5	2.52	0.45
18:P:142:ASP:O	18:P:143:ALA:O	2.35	0.45
24:V:46:ILE:HA	24:V:49:LEU:HD12	1.99	0.45
1:0:1007:A:H2'	11:H:19:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:243:A:H61	1:0:269:G:H1'	1.81	0.45
1:0:23:G:H1'	1:0:520:A:N6	2.32	0.45
7:D:23:VAL:HG21	7:D:45:THR:CG2	2.46	0.45
7:D:81:GLU:O	7:D:85:GLN:HG3	2.17	0.45
38:0:5725:HOH:O	10:G:12:ILE:HA	2.16	0.45
6:C:133:ARG:HG2	6:C:135:GLU:O	2.17	0.45
1:0:920:C:H5''	1:0:921:G:O5'	2.17	0.45
1:0:2698:G:H2'	1:0:2699:A:O4'	2.16	0.45
9:F:49:PHE:HE1	9:F:98:VAL:HG23	1.82	0.45
8:E:34:TRP:HA	38:E:4572:HOH:O	2.17	0.45
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.32	0.45
14:L:64:ILE:HG13	14:L:68:GLU:OE1	2.15	0.45
1:0:451:C:O2'	1:0:452:G:H5'	2.17	0.45
2:9:3106:C:O2'	2:9:3107:C:H5'	2.16	0.45
32:I:132:CYS:C	32:I:134:SER:H	2.19	0.44
8:E:15:GLN:CG	8:E:20:ILE:HG12	2.47	0.44
19:Q:25:PRO:HB2	38:Q:4350:HOH:O	2.16	0.44
16:N:39:SER:HB3	16:N:42:HIS:H	1.82	0.44
1:0:1289:C:O2'	1:0:1290:G:H5'	2.16	0.44
16:N:63:SER:HB2	16:N:75:THR:HB	1.99	0.44
14:L:12:THR:HG21	14:L:16:GLY:O	2.17	0.44
1:0:1304:U:H2'	1:0:1305:C:C6	2.52	0.44
1:0:249:G:O2'	1:0:250:C:H5'	2.16	0.44
31:3:65:THR:CG2	31:3:67:LEU:HG	2.47	0.44
1:0:432:G:O2'	1:0:433:C:H5'	2.17	0.44
12:J:99:GLU:HA	38:J:9371:HOH:O	2.17	0.44
1:0:1942:A:O2'	1:0:1943:C:H5'	2.17	0.44
25:W:38:THR:O	25:W:42:ARG:HB2	2.17	0.44
5:B:198:GLU:HA	38:B:9461:HOH:O	2.15	0.44
8:E:43:ASP:HA	38:E:5864:HOH:O	2.16	0.44
29:1:37:CYS:SG	29:1:39:PHE:HB2	2.57	0.44
1:0:2781:U:H2'	1:0:2782:G:C5'	2.47	0.44
1:0:816:G:C6	1:0:817:G:N1	2.85	0.44
38:0:9937:HOH:O	9:F:38:LYS:HE2	2.17	0.44
1:0:1200:A:H4'	38:0:7550:HOH:O	2.17	0.44
38:0:9851:HOH:O	18:P:81:LYS:HG2	2.18	0.44
4:A:135:VAL:HG21	4:A:147:ARG:HG2	2.00	0.44
1:0:1657:A:H2'	1:0:1658:A:C8	2.52	0.44
1:0:1056:U:H2'	1:0:1057:A:O4'	2.16	0.44
7:D:24:HIS:HB2	7:D:72:LYS:HB3	1.99	0.44
1:0:1943:C:O4'	4:A:212:PRO:HA	2.17	0.44
1:0:2715:G:O2'	5:B:262:ARG:HD2	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:100:PRO:HG2	4:A:103:VAL:CG2	2.45	0.44
8:E:31:ARG:NH1	8:E:68:HIS:CG	2.86	0.44
1:O:35:U:H5'	6:C:47:GLY:O	2.17	0.44
14:L:121:ILE:HG12	14:L:141:GLU:HB2	1.99	0.44
6:C:133:ARG:NE	6:C:135:GLU:O	2.50	0.44
22:T:64:ASN:HB3	22:T:73:HIS:HB2	1.98	0.44
1:O:2061:C:C2'	1:O:2062:A:H5'	2.48	0.44
1:O:2438:G:H2'	1:O:2439:C:O4'	2.17	0.44
4:A:53:ALA:HB3	38:A:9400:HOH:O	2.17	0.44
11:H:46:GLN:NE2	11:H:137:TYR:HE2	2.15	0.44
1:O:2036:C:C4'	13:K:44:LEU:HG	2.47	0.44
1:O:1167:G:H2'	1:O:1168:C:O4'	2.17	0.44
12:J:39:VAL:HG11	12:J:107:ASN:HB2	1.99	0.44
1:O:1174:A:C5	1:O:1201:C:H4'	2.52	0.44
16:N:18:THR:HG21	38:N:9348:HOH:O	2.17	0.44
32:I:92:PRO:O	32:I:94:GLU:HG3	2.16	0.44
27:Y:112:GLU:OE1	27:Y:115:ARG:NH1	2.50	0.44
5:B:301:VAL:HG13	5:B:302:PRO:HD2	1.98	0.44
11:H:38:LYS:HE2	11:H:42:ASP:HB2	1.98	0.44
38:O:7568:HOH:O	4:A:177:HIS:HE1	2.01	0.44
1:O:1249:U:H2'	1:O:1250:C:C6	2.52	0.44
7:D:158:ASN:HB2	7:D:161:ASP:OD2	2.16	0.44
22:T:53:GLY:HA3	38:T:6384:HOH:O	2.16	0.44
13:K:90:PHE:CD1	13:K:90:PHE:N	2.86	0.44
16:N:15:GLU:HB3	16:N:17:ARG:HG3	1.99	0.44
25:W:88:THR:CG2	25:W:110:GLN:HE21	2.22	0.44
32:I:110:GLU:HA	32:I:113:HIS:CD2	2.52	0.44
16:N:154:LEU:HD12	16:N:156:GLU:O	2.17	0.44
6:C:246:ARG:NE	38:C:9220:HOH:O	2.51	0.44
9:F:50:VAL:HG11	9:F:60:VAL:HG11	1.99	0.44
32:I:101:SER:OG	32:I:104:GLN:HG3	2.18	0.44
18:P:141:ILE:O	18:P:143:ALA:N	2.41	0.44
11:H:77:LEU:HD12	11:H:83:TYR:CD2	2.52	0.44
1:O:1544:U:H2'	1:O:1545:C:C6	2.53	0.44
1:O:2403:C:H2'	1:O:2404:G:O5'	2.17	0.44
1:O:2061:C:H2'	1:O:2062:A:H5'	2.00	0.44
1:O:113:A:OP2	1:O:114:A:H2'	2.18	0.44
8:E:21:THR:HG23	8:E:30:THR:OG1	2.17	0.44
14:L:77:ALA:HB3	38:L:9328:HOH:O	2.18	0.44
20:R:114:VAL:HG13	20:R:114:VAL:O	2.18	0.44
26:X:70:ILE:HG23	26:X:70:ILE:O	2.17	0.44
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.16	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:C:16:VAL:CG1	6:C:17:ASP:N	2.80	0.44
7:D:64:ARG:CD	7:D:67:ASP:HB3	2.47	0.44
22:T:48:VAL:HG22	22:T:97:ARG:C	2.38	0.44
1:O:656:G:H5'	17:O:3:THR:CG2	2.48	0.44
1:O:968:G:H1'	11:H:32:LYS:HD2	2.00	0.44
1:O:968:G:O2'	1:O:969:G:H5'	2.17	0.44
16:N:11:ARG:NH2	38:N:9316:HOH:O	2.51	0.44
20:R:40:ALA:O	20:R:44:VAL:HG23	2.18	0.44
1:O:1632:A:C2'	1:O:1633:C:H5'	2.47	0.44
11:H:38:LYS:HE2	11:H:42:ASP:CB	2.47	0.44
1:O:1067:A:H5'	38:O:4638:HOH:O	2.18	0.44
24:V:12:THR:CG2	24:V:15:GLU:HG3	2.22	0.44
25:W:122:ARG:NH1	25:W:122:ARG:HG2	2.25	0.44
5:B:212:GLN:HG2	5:B:257:THR:OG1	2.17	0.44
7:D:44:ILE:HG12	7:D:83:PHE:CE1	2.49	0.44
4:A:130:THR:HG22	4:A:131:HIS:N	2.32	0.44
7:D:76:ARG:O	7:D:77:ASP:HB2	2.16	0.44
13:K:114:ALA:HB3	13:K:117:VAL:HG23	2.00	0.44
7:D:173:GLU:O	7:D:174:VAL:C	2.56	0.44
30:2:10:ARG:HH11	30:2:49:GLU:CD	2.21	0.44
6:C:129:HIS:HD2	6:C:165:ASP:OD2	2.01	0.44
9:F:12:LEU:HD21	9:F:111:ILE:HG23	1.99	0.44
1:O:926:A:O2'	14:L:41:HIS:CD2	2.70	0.44
6:C:102:LEU:HD12	38:C:9117:HOH:O	2.16	0.44
6:C:65:ARG:HG3	6:C:67:GLN:HB2	2.00	0.44
1:O:1307:A:H2'	1:O:1308:A:C8	2.53	0.44
1:O:2015:A:H2'	1:O:2016:U:O4'	2.17	0.44
1:O:1811:A:C2	1:O:2752:C:H1'	2.52	0.44
16:N:15:GLU:OE1	16:N:17:ARG:HD2	2.17	0.44
23:U:52:THR:CG2	23:U:54:THR:HB	2.48	0.44
2:9:3042:C:O2	7:D:76:ARG:NH1	2.50	0.44
6:C:233:THR:HG22	6:C:234:VAL:H	1.83	0.44
1:O:1829:A:H5''	38:O:3389:HOH:O	2.16	0.44
5:B:14:GLY:HA3	38:B:9410:HOH:O	2.17	0.44
1:O:425:U:H4'	38:O:7160:HOH:O	2.17	0.44
16:N:63:SER:O	16:N:66:LEU:HB2	2.17	0.44
16:N:64:SER:C	16:N:66:LEU:H	2.21	0.44
1:O:1587:U:H2'	1:O:1588:G:O4'	2.18	0.44
25:W:73:LEU:O	25:W:74:GLU:HG2	2.18	0.44
6:C:19:PRO:HD2	6:C:240:LEU:HD21	2.00	0.44
28:Z:56:GLN:HA	28:Z:62:TYR:O	2.17	0.44
16:N:108:SER:HA	16:N:109:PRO:HD3	1.75	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:N:37:ARG:HA	16:N:37:ARG:HD3	1.75	0.44
5:B:312:ARG:HD3	5:B:315:VAL:HG13	2.00	0.44
26:X:76:ARG:NH1	26:X:76:ARG:HG3	2.31	0.44
5:B:7:ARG:HD3	5:B:9:GLY:O	2.18	0.44
1:O:248:A:H5'	1:O:249:G:OP2	2.18	0.44
1:O:1204:C:H1'	38:O:5023:HOH:O	2.18	0.44
1:O:2511:A:H2'	1:O:2512:U:O4'	2.18	0.44
1:O:2329:C:O2'	1:O:2330:U:H5'	2.17	0.44
18:P:91:LYS:O	18:P:95:GLU:HG3	2.18	0.44
5:B:268:ARG:NH2	5:B:325:PRO:HG3	2.33	0.44
8:E:71:ASN:HD22	8:E:138:ILE:HD13	1.83	0.44
22:T:43:ASN:HD22	22:T:108:ARG:NH2	2.15	0.44
25:W:143:THR:N	38:W:3520:HOH:O	2.51	0.44
5:B:304:PRO:HD2	5:B:307:ARG:NH1	2.32	0.43
13:K:14:LYS:HG3	13:K:32:ILE:O	2.18	0.43
6:C:5:ILE:CD1	6:C:16:VAL:HG23	2.40	0.43
7:D:44:ILE:HG23	7:D:45:THR:HG23	2.00	0.43
25:W:64:THR:O	25:W:68:THR:HG22	2.18	0.43
16:N:154:LEU:HD11	16:N:157:PRO:HA	1.99	0.43
25:W:105:THR:HG23	25:W:106:THR:N	2.31	0.43
6:C:136:VAL:HA	6:C:137:PRO:C	2.39	0.43
1:O:999:C:H2'	1:O:1000:C:O4'	2.18	0.43
17:O:96:VAL:HG12	17:O:100:GLN:HB2	1.99	0.43
1:O:958:G:H2'	1:O:959:C:H6	1.82	0.43
1:O:2684:A:H2'	1:O:2685:C:C6	2.53	0.43
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.53	0.43
6:C:72:LYS:HG2	6:C:77:ALA:HA	1.99	0.43
1:O:1224:G:H2'	1:O:1225:C:C6	2.52	0.43
5:B:24:PRO:HA	5:B:261:GLN:OE1	2.18	0.43
1:O:1926:G:H2'	1:O:1927:A:C8	2.53	0.43
1:O:1666:C:C2'	1:O:1667:A:C5'	2.96	0.43
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.48	0.43
16:N:154:LEU:O	16:N:155:GLU:CB	2.65	0.43
2:9:3049:G:C2'	2:9:3050:G:H5'	2.48	0.43
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.81	0.43
5:B:175:LEU:O	5:B:178:ALA:HB3	2.18	0.43
16:N:42:HIS:CB	16:N:62:HIS:HE1	2.31	0.43
4:A:43:VAL:HG21	4:A:59:GLU:OE2	2.18	0.43
22:T:81:LYS:HD2	22:T:87:VAL:HG11	1.99	0.43
1:O:162:C:H2'	1:O:163:U:H5'	2.01	0.43
1:O:806:A:H2'	1:O:807:A:O4'	2.18	0.43
9:F:110:ASP:O	9:F:114:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1168:C:H5''	32:I:87:THR:HG23	2.00	0.43
32:I:92:PRO:C	32:I:94:GLU:N	2.70	0.43
5:B:51:VAL:HG13	5:B:53:LEU:CD1	2.48	0.43
6:C:168:ARG:NH2	6:C:190:ALA:O	2.51	0.43
7:D:58:VAL:HG12	7:D:60:GLU:HG2	2.00	0.43
1:0:1015:C:H2'	1:0:1016:U:C6	2.53	0.43
1:0:1504:A:H5'	38:0:4704:HOH:O	2.17	0.43
1:0:2684:A:H1'	38:0:3235:HOH:O	2.18	0.43
1:0:1682:A:H2'	38:0:3108:HOH:O	2.18	0.43
1:0:1849:G:H1'	1:0:2011:A:N1	2.33	0.43
20:R:114:VAL:HA	20:R:144:GLU:O	2.18	0.43
1:0:1398:G:H2'	1:0:1399:A:C8	2.53	0.43
1:0:946:C:H2'	1:0:947:U:C6	2.53	0.43
1:0:2724:U:H2'	1:0:2725:G:O4'	2.18	0.43
1:0:333:G:O2'	1:0:334:G:H5'	2.18	0.43
14:L:130:ARG:O	14:L:134:GLU:HG3	2.18	0.43
24:V:12:THR:HG23	24:V:14:ALA:N	2.21	0.43
1:0:2717:C:OP1	5:B:207:LYS:HG3	2.18	0.43
13:K:55:VAL:CG1	13:K:56:SER:N	2.81	0.43
20:R:99:ALA:CB	20:R:109:MET:HE1	2.39	0.43
1:0:1450:C:O2'	1:0:1494:A:H5'	2.17	0.43
1:0:2756:U:N3	1:0:2896:A:H2	2.08	0.43
5:B:51:VAL:HG13	5:B:53:LEU:HD11	2.00	0.43
27:Y:112:GLU:CD	27:Y:115:ARG:NH1	2.70	0.43
16:N:23:ARG:NH1	16:N:23:ARG:HG2	2.33	0.43
1:0:1528:A:H2'	1:0:1529:G:O4'	2.18	0.43
1:0:1973:A:H8	1:0:1973:A:H5'	1.83	0.43
1:0:1595:G:O2'	1:0:1596:U:H5'	2.19	0.43
1:0:2338:G:H1'	7:D:105:SER:OG	2.18	0.43
14:L:73:VAL:HG21	14:L:116:HIS:CD2	2.54	0.43
1:0:1250:C:O2'	1:0:1251:C:H5'	2.18	0.43
1:0:574:C:H2'	1:0:575:G:O4'	2.19	0.43
1:0:2455:A:H2'	1:0:2456:A:O4'	2.18	0.43
1:0:2504:A:H2'	1:0:2505:G:O4'	2.18	0.43
6:C:7:ASP:OD1	6:C:11:ASN:O	2.37	0.43
1:0:926:A:O2'	14:L:41:HIS:HD2	2.01	0.43
14:L:59:GLU:HG2	14:L:104:ASP:CG	2.39	0.43
20:R:47:LEU:O	20:R:51:ILE:HG13	2.18	0.43
1:0:2365:G:P	19:Q:15:LYS:HG3	2.59	0.43
29:1:8:GLN:NE2	29:1:11:LYS:NZ	2.59	0.43
38:0:7762:HOH:O	31:3:60:LYS:HG3	2.17	0.43
22:T:32:ARG:NH1	22:T:38:ARG:NH1	2.63	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:79:MET:O	5:B:80:ARG:HG3	2.19	0.43
8:E:145:ALA:HB1	8:E:168:ILE:HD11	2.01	0.43
20:R:4:TYR:HA	20:R:144:GLU:OE2	2.19	0.43
11:H:87:LEU:HD13	11:H:134:PHE:CE2	2.53	0.43
4:A:51:ARG:NH1	4:A:120:ARG:O	2.51	0.43
5:B:27:ASN:N	5:B:27:ASN:HD22	2.01	0.43
15:M:182:LYS:HD2	15:M:193:LYS:HB2	1.99	0.43
1:0:475:G:H5'	6:C:73:LEU:HD23	2.00	0.43
8:E:31:ARG:HH12	8:E:68:HIS:CD2	2.37	0.43
1:0:120:A:H2'	1:0:120:A:N3	2.34	0.43
1:0:1878:G:O2'	1:0:1879:U:OP2	2.35	0.43
24:V:20:LEU:HD22	24:V:60:GLN:HE22	1.84	0.43
1:0:2456:A:H2'	1:0:2457:U:C6	2.54	0.43
1:0:622:G:O2'	1:0:623:U:H5'	2.19	0.43
8:E:156:ASP:N	8:E:156:ASP:OD1	2.51	0.43
7:D:152:PRO:O	7:D:156:ARG:HG2	2.18	0.43
1:0:1189:A:O2'	1:0:1208:C:H2'	2.18	0.43
1:0:392:U:O2'	15:M:182:LYS:HE2	2.18	0.43
5:B:52:VAL:O	5:B:53:LEU:HD12	2.19	0.43
1:0:2587:OMU:HM23	1:0:2589:U:C6	2.54	0.43
18:P:38:GLU:HA	18:P:41:ARG:HH11	1.83	0.43
14:L:93:VAL:CG2	14:L:122:ALA:HB2	2.48	0.43
1:0:644:G:H1'	38:0:6645:HOH:O	2.19	0.43
5:B:69:VAL:HA	5:B:70:PRO:HD3	1.86	0.43
1:0:1419:U:H5'	1:0:1420:C:OP2	2.18	0.43
6:C:150:THR:HA	6:C:203:ALA:O	2.18	0.43
1:0:2379:G:H5'	1:0:2381:C:O4'	2.18	0.43
1:0:1636:G:O2'	1:0:1637:A:H5'	2.18	0.43
1:0:1930:A:H2'	1:0:1931:A:C8	2.53	0.43
10:G:23:ILE:O	10:G:27:ILE:HG13	2.19	0.43
4:A:114:ASP:C	4:A:114:ASP:OD1	2.56	0.43
6:C:236:THR:O	6:C:239:ALA:N	2.51	0.43
38:0:7650:HOH:O	4:A:211:LYS:NZ	2.51	0.43
15:M:182:LYS:O	15:M:194:ALA:HB2	2.18	0.43
13:K:113:ILE:HG22	13:K:114:ALA:O	2.19	0.43
15:M:59:GLY:C	15:M:141:ILE:HD11	2.39	0.43
2:9:3003:A:H2	2:9:3021:G:N3	2.17	0.43
16:N:49:THR:CG2	16:N:56:ASP:HB2	2.47	0.43
7:D:170:TYR:CD1	7:D:170:TYR:N	2.86	0.43
1:0:245:C:H2'	1:0:246:G:H5'	2.01	0.43
1:0:154:C:P	15:M:188:ARG:HH12	2.41	0.43
1:0:2715:G:N2	5:B:264:GLU:OE1	2.52	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.59	0.43
26:X:76:ARG:O	26:X:77:PHE:HB3	2.18	0.43
13:K:113:ILE:HD12	13:K:128:ALA:HB2	2.01	0.43
5:B:17:LYS:O	5:B:260:HIS:HD2	2.02	0.43
15:M:31:TRP:HA	15:M:34:GLU:HG3	2.01	0.43
1:O:2780:C:H2'	1:O:2781:U:C6	2.54	0.43
18:P:38:GLU:HA	18:P:41:ARG:NH1	2.34	0.43
1:O:222:A:H2'	1:O:223:G:O4'	2.18	0.43
5:B:14:GLY:HA2	5:B:15:PRO:C	2.40	0.43
11:H:80:GLU:HA	38:H:9183:HOH:O	2.18	0.43
1:O:303:C:H2'	1:O:304:G:O4'	2.19	0.43
38:O:9991:HOH:O	27:Y:163:THR:HG23	2.19	0.43
1:O:912:A:C4	1:O:1294:A:C2	3.07	0.43
1:O:709:G:O2'	17:O:25:VAL:CG1	2.67	0.43
1:O:2134:G:C6	1:O:2258:A:C8	3.07	0.43
18:P:22:TRP:CH2	18:P:24:ASN:HA	2.54	0.43
32:I:132:CYS:CB	32:I:137:VAL:HB	2.35	0.42
32:I:92:PRO:HG3	38:I:6825:HOH:O	2.18	0.42
5:B:79:MET:C	5:B:80:ARG:HG3	2.39	0.42
16:N:61:ALA:CB	16:N:88:ALA:HB2	2.48	0.42
8:E:145:ALA:O	8:E:148:ILE:HB	2.19	0.42
4:A:94:LEU:HG	4:A:99:ILE:CD1	2.49	0.42
9:F:28:ALA:HB3	9:F:99:THR:HG23	2.01	0.42
1:O:1675:C:H5''	30:2:5:LYS:HD2	2.01	0.42
14:L:24:ALA:HB2	14:L:30:ARG:HD2	2.01	0.42
32:I:124:ALA:O	32:I:128:VAL:HG23	2.19	0.42
6:C:91:PRO:O	6:C:93:LYS:HG3	2.19	0.42
1:O:1008:C:H5''	11:H:16:ARG:HH12	1.84	0.42
1:O:737:A:H2'	1:O:738:G:O4'	2.19	0.42
24:V:12:THR:OG1	24:V:13:PRO:HD2	2.19	0.42
24:V:7:GLU:O	24:V:11:MET:HG3	2.18	0.42
7:D:23:VAL:CG2	7:D:23:VAL:O	2.66	0.42
8:E:3:VAL:CG2	8:E:49:ILE:HB	2.47	0.42
1:O:2251:G:H2'	1:O:2252:A:H8	1.81	0.42
1:O:795:G:N3	1:O:817:G:C2	2.87	0.42
1:O:1309:U:H2'	1:O:1310:U:O4'	2.19	0.42
4:A:107:ASN:OD1	4:A:120:ARG:HD2	2.20	0.42
1:O:2820:A:H2'	1:O:2821:C:O4'	2.18	0.42
1:O:2067:A:H2'	1:O:2068:G:O4'	2.19	0.42
38:E:2512:HOH:O	12:J:127:ILE:HD11	2.18	0.42
1:O:2815:G:N7	12:J:80:LYS:NZ	2.65	0.42
15:M:43:PRO:HG3	15:M:62:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:638:C:H2'	1:0:639:A:C8	2.54	0.42
5:B:207:LYS:HG2	5:B:304:PRO:HB3	2.01	0.42
12:J:130:VAL:CG1	12:J:131:THR:N	2.82	0.42
16:N:34:LEU:HA	16:N:47:LEU:CD2	2.49	0.42
11:H:20:ILE:HG23	11:H:120:ILE:HD11	2.00	0.42
1:0:2467:A:O2'	1:0:2468:A:H2'	2.19	0.42
1:0:920:C:H4'	1:0:921:G:N2	2.33	0.42
14:L:59:GLU:HG2	14:L:104:ASP:OD2	2.19	0.42
8:E:35:TYR:CD2	8:E:36:PRO:HD2	2.54	0.42
19:Q:64:GLU:HA	19:Q:64:GLU:OE1	2.19	0.42
27:Y:108:ASP:N	27:Y:108:ASP:OD1	2.53	0.42
6:C:236:THR:O	6:C:237:GLU:C	2.58	0.42
1:0:2255:A:C6	1:0:2256:G:C5	3.08	0.42
15:M:24:GLN:O	15:M:28:GLN:HG3	2.19	0.42
5:B:305:ASP:O	5:B:306:LYS:CB	2.66	0.42
13:K:22:ASP:O	13:K:110:LYS:HE3	2.20	0.42
1:0:2564:G:OP2	1:0:2565:C:H5''	2.19	0.42
2:9:3034:A:H2'	2:9:3035:C:O4'	2.19	0.42
7:D:104:PHE:CE2	7:D:132:VAL:HB	2.55	0.42
1:0:2314:G:C2'	1:0:2315:C:H5'	2.49	0.42
20:R:72:VAL:CG1	20:R:75:TRP:HB3	2.49	0.42
23:U:37:GLU:O	23:U:40:ALA:HB3	2.20	0.42
6:C:16:VAL:CG1	6:C:17:ASP:H	2.30	0.42
25:W:38:THR:CG2	25:W:39:ASP:N	2.82	0.42
7:D:81:GLU:C	7:D:83:PHE:N	2.73	0.42
4:A:88:ILE:CD1	4:A:100:PRO:HD3	2.45	0.42
7:D:95:THR:HG1	7:D:174:VAL:HG22	1.81	0.42
1:0:2346:C:O2'	7:D:52:THR:HG21	2.19	0.42
5:B:277:GLU:N	5:B:278:PRO:CD	2.83	0.42
1:0:764:C:H2'	1:0:765:G:O4'	2.20	0.42
20:R:125:ARG:HG2	38:R:9344:HOH:O	2.19	0.42
11:H:43:TYR:HA	11:H:44:PRO:HD3	1.79	0.42
18:P:7:LYS:HD3	18:P:21:VAL:CG2	2.49	0.42
6:C:13:ASP:OD1	6:C:13:ASP:O	2.37	0.42
22:T:71:VAL:CG1	22:T:72:ILE:N	2.82	0.42
7:D:66:GLY:O	7:D:67:ASP:HB3	2.18	0.42
7:D:99:ASP:CB	7:D:103:ASN:HB2	2.50	0.42
20:R:17:MET:HE3	20:R:19:ARG:NE	2.34	0.42
27:Y:144:ARG:NH2	38:Y:9407:HOH:O	2.51	0.42
1:0:2524:G:H21	1:0:2526:C:H41	1.68	0.42
5:B:55:ASN:HB3	5:B:63:GLU:HA	2.01	0.42
8:E:108:LEU:HD11	8:E:164:ASP:HB2	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
19:Q:93:ARG:NH1	19:Q:93:ARG:HG3	2.35	0.42
1:0:37:A:H2'	1:0:38:G:H8	1.84	0.42
28:Z:39:CYS:HA	28:Z:47:VAL:CG2	2.50	0.42
1:0:67:A:H5''	1:0:69:A:C8	2.55	0.42
1:0:2044:G:OP1	26:X:23:HIS:HE1	2.03	0.42
2:9:3052:A:O2'	2:9:3053:G:H5'	2.20	0.42
1:0:1151:G:OP1	10:G:63:ARG:NH1	2.53	0.42
11:H:69:ALA:HB2	11:H:153:ALA:HB2	2.00	0.42
1:0:2761:A:H2'	38:0:5903:HOH:O	2.18	0.42
1:0:514:G:OP1	1:0:514:G:H2'	2.20	0.42
1:0:1160:G:O2'	1:0:1190:G:H1'	2.19	0.42
27:Y:187:VAL:HB	27:Y:203:VAL:CG2	2.49	0.42
5:B:307:ARG:CG	5:B:307:ARG:HH11	2.33	0.42
26:X:30:MET:HE2	26:X:58:ALA:HB3	2.02	0.42
12:J:39:VAL:CG1	12:J:107:ASN:HB2	2.50	0.42
7:D:88:LEU:O	7:D:90:LEU:N	2.53	0.42
26:X:15:ARG:HB3	26:X:15:ARG:NH1	2.34	0.42
1:0:1206:U:H2'	1:0:1207:A:O4'	2.19	0.42
1:0:820:G:O2'	1:0:856:G:H4'	2.19	0.42
16:N:42:HIS:CG	16:N:62:HIS:HE1	2.37	0.42
9:F:99:THR:O	9:F:100:ASP:HB2	2.19	0.42
1:0:1380:U:H5'	38:0:9533:HOH:O	2.20	0.42
1:0:1483:C:O2'	1:0:1484:G:H5'	2.19	0.42
1:0:347:A:O2'	6:C:205:ARG:NH2	2.53	0.42
1:0:1771:U:O2	28:Z:19:GLY:HA2	2.19	0.42
1:0:1409:G:H5'	38:0:4024:HOH:O	2.19	0.42
1:0:783:C:OP1	4:A:180:LYS:HE3	2.19	0.42
1:0:371:U:H2'	1:0:372:A:H8	1.84	0.42
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.85	0.42
6:C:237:GLU:HB2	38:C:9226:HOH:O	2.18	0.42
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.45	0.42
4:A:130:THR:HG22	4:A:131:HIS:O	2.19	0.42
1:0:1881:A:OP1	4:A:199:HIS:HE1	2.02	0.42
32:I:99:ASP:O	32:I:100:LEU:HD23	2.20	0.42
1:0:1058:A:H2'	1:0:1060:C:C5'	2.48	0.42
1:0:1634:G:H2'	1:0:1635:U:C6	2.54	0.42
11:H:66:ARG:HD3	38:H:9179:HOH:O	2.19	0.42
4:A:109:GLU:HG2	4:A:116:GLY:H	1.83	0.42
26:X:36:HIS:CE1	26:X:40:HIS:CD2	3.08	0.42
1:0:236:A:H8	1:0:236:A:OP1	2.03	0.42
10:G:27:ILE:HD12	10:G:70:ALA:HB1	2.01	0.42
1:0:1525:G:H5'	1:0:1526:A:OP2	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:270:ILE:O	5:B:271:ASP:HB2	2.19	0.42
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.84	0.42
32:I:112:LYS:C	32:I:114:PRO:HD2	2.40	0.42
12:J:42:GLU:O	12:J:131:THR:HG23	2.20	0.42
5:B:329:TYR:HE2	23:U:15:PRO:HG2	1.81	0.42
14:L:120:LEU:HD12	14:L:133:VAL:HG21	2.01	0.42
32:I:129:VAL:HG13	32:I:139:ILE:CD1	2.49	0.42
1:O:475:G:OP1	6:C:73:LEU:CD2	2.68	0.42
6:C:27:ARG:CG	6:C:27:ARG:HH11	2.32	0.42
1:O:2266:A:H2'	1:O:2267:G:C8	2.55	0.42
1:O:164:G:O3'	14:L:30:ARG:HB2	2.20	0.42
4:A:87:GLU:HB3	38:A:9415:HOH:O	2.20	0.42
1:O:125:U:H2'	38:O:4064:HOH:O	2.18	0.42
1:O:1697:G:O2'	1:O:1698:U:H5'	2.20	0.42
1:O:1331:A:OP2	27:Y:142:SER:OG	2.34	0.42
1:O:1335:C:H2'	1:O:1336:U:C6	2.55	0.42
1:O:2105:C:H2'	1:O:2106:C:C6	2.54	0.42
1:O:645:U:O2	1:O:761:A:H2	2.03	0.42
1:O:42:C:H1'	38:O:4957:HOH:O	2.19	0.42
1:O:2837:U:H1'	5:B:307:ARG:HH12	1.85	0.42
32:I:132:CYS:C	32:I:134:SER:N	2.73	0.42
25:W:21:LEU:O	25:W:26:ILE:HG12	2.20	0.42
12:J:107:ASN:HD22	12:J:108:PRO:HD2	1.85	0.42
11:H:3:ALA:HA	11:H:58:ARG:HH12	1.85	0.42
1:O:1184:C:O2'	1:O:1185:U:OP2	2.31	0.42
26:X:78:GLU:CG	26:X:79:GLU:N	2.82	0.42
1:O:621:C:H5'	27:Y:132:ASP:OD2	2.20	0.42
5:B:280:VAL:HG22	5:B:333:GLU:O	2.19	0.42
9:F:99:THR:HA	38:F:3461:HOH:O	2.19	0.42
1:O:700:A:C2	14:L:71:GLU:HG2	2.55	0.42
27:Y:153:GLN:HG3	27:Y:160:LYS:O	2.20	0.42
1:O:813:C:H2'	1:O:814:G:O4'	2.20	0.42
11:H:166:SER:HB3	38:H:9143:HOH:O	2.20	0.41
1:O:2269:C:H2'	1:O:2270:G:C5'	2.50	0.41
1:O:1181:A:N1	1:O:1192:A:O2'	2.50	0.41
16:N:73:ALA:HB2	16:N:163:PHE:CE2	2.55	0.41
5:B:243:ASN:HA	5:B:244:PRO:C	2.39	0.41
1:O:704:C:H2'	1:O:705:C:H6	1.85	0.41
8:E:4:GLU:HG2	8:E:48:VAL:HG22	2.02	0.41
1:O:2330:U:H4'	1:O:2331:C:OP1	2.20	0.41
30:2:19:SER:HB3	38:2:4479:HOH:O	2.20	0.41
1:O:1252:A:H2'	1:O:1253:C:O4'	2.19	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:R:82:GLU:O	20:R:86:LYS:HG3	2.20	0.41
11:H:46:GLN:HE21	11:H:137:TYR:HE2	1.68	0.41
6:C:140:VAL:CG1	6:C:141:SER:N	2.83	0.41
7:D:23:VAL:HG22	7:D:73:VAL:HB	2.02	0.41
16:N:157:PRO:HA	38:N:9323:HOH:O	2.21	0.41
16:N:67:ALA:C	16:N:69:TYR:N	2.74	0.41
18:P:16:VAL:HG12	18:P:17:GLY:N	2.35	0.41
6:C:27:ARG:CG	6:C:27:ARG:NH1	2.83	0.41
20:R:119:VAL:HG21	20:R:142:ASP:CG	2.40	0.41
6:C:54:LEU:HD23	6:C:79:ARG:HG3	2.01	0.41
1:0:1453:G:N2	1:0:1675:C:C2	2.87	0.41
14:L:67:ARG:O	14:L:71:GLU:HG3	2.20	0.41
1:0:2821:C:O2'	5:B:114:ASP:O	2.36	0.41
1:0:1948:G:O2'	1:0:1949:G:H5'	2.21	0.41
1:0:2604:A:H5'	38:0:6052:HOH:O	2.19	0.41
1:0:401:C:H2'	1:0:402:U:C6	2.55	0.41
4:A:161:GLY:O	28:Z:68:SER:OG	2.34	0.41
1:0:1921:A:C6	1:0:1922:A:C2	3.08	0.41
1:0:419:A:H1'	1:0:1921:A:C2	2.55	0.41
21:S:29:ASP:OD1	21:S:31:ARG:HG3	2.21	0.41
11:H:17:ARG:HD3	11:H:23:ILE:CD1	2.50	0.41
4:A:48:ASP:HA	4:A:49:PRO:HD3	1.83	0.41
1:0:1046:G:N3	1:0:1082:A:H2	2.18	0.41
1:0:629:A:H2'	1:0:630:A:O4'	2.20	0.41
1:0:2028:U:H2'	1:0:2029:C:C6	2.55	0.41
1:0:39:G:H2'	1:0:40:C:O4'	2.20	0.41
20:R:9:ASP:HA	20:R:10:PRO:HD2	1.92	0.41
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.35	0.41
1:0:1701:A:H5''	1:0:1702:U:H3'	2.01	0.41
5:B:258:GLY:N	5:B:260:HIS:CE1	2.85	0.41
1:0:1377:C:C5'	1:0:1377:C:H6	2.32	0.41
6:C:27:ARG:HG2	6:C:27:ARG:NH1	2.34	0.41
1:0:138:U:OP2	1:0:139:C:H5	2.03	0.41
1:0:2363:G:O3'	19:Q:11:ARG:NH1	2.53	0.41
18:P:141:ILE:C	18:P:143:ALA:N	2.73	0.41
22:T:43:ASN:ND2	22:T:108:ARG:CZ	2.83	0.41
1:0:1398:G:O2'	1:0:1399:A:H5'	2.20	0.41
4:A:82:VAL:HG13	4:A:93:THR:HB	2.01	0.41
1:0:128:A:O2'	1:0:129:A:H5'	2.20	0.41
29:1:53:LYS:HD3	29:1:53:LYS:HA	1.92	0.41
15:M:181:GLU:N	15:M:181:GLU:OE1	2.48	0.41
13:K:9:THR:O	13:K:10:GLN:C	2.58	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:D:151:ILE:HA	7:D:152:PRO:HD3	1.95	0.41
25:W:115:THR:HG23	38:W:5420:HOH:O	2.21	0.41
1:0:1641:A:H2'	1:0:1642:A:C5'	2.45	0.41
1:0:2270:G:H4'	4:A:223:ARG:NH1	2.29	0.41
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.27	0.41
17:O:21:SER:OG	17:O:106:PRO:HB2	2.20	0.41
1:0:1333:U:H2'	1:0:1334:C:H6	1.85	0.41
25:W:125:HIS:CD2	25:W:127:GLY:H	2.38	0.41
5:B:119:HIS:O	5:B:121:PRO:HD3	2.20	0.41
30:2:30:ASP:O	30:2:31:ARG:HB2	2.20	0.41
1:0:1023:C:O2'	1:0:1024:G:H5'	2.20	0.41
1:0:671:A:O2'	1:0:672:G:H2'	2.20	0.41
4:A:217:ARG:HG3	38:A:9325:HOH:O	2.20	0.41
1:0:932:U:H2'	1:0:933:C:C6	2.56	0.41
1:0:870:G:C3'	1:0:871:G:H5''	2.50	0.41
25:W:122:ARG:CG	25:W:122:ARG:NH1	2.82	0.41
1:0:2269:C:H2'	1:0:2270:G:H5'	2.01	0.41
13:K:113:ILE:HG22	13:K:114:ALA:N	2.34	0.41
13:K:75:ARG:HE	13:K:94:ALA:HB3	1.85	0.41
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.50	0.41
8:E:11:VAL:HG13	8:E:76:VAL:HG21	2.03	0.41
16:N:183:ASP:O	16:N:184:ILE:O	2.38	0.41
1:0:538:C:H5''	1:0:539:G:C8	2.55	0.41
1:0:2821:C:H4'	5:B:116:PRO:HG3	2.01	0.41
1:0:426:G:H2'	1:0:427:C:O4'	2.21	0.41
1:0:2401:A:H2'	1:0:2402:A:C8	2.55	0.41
1:0:1734:C:OP1	5:B:234:ARG:NH1	2.50	0.41
6:C:236:THR:HG22	6:C:239:ALA:CB	2.50	0.41
25:W:48:VAL:CG1	25:W:48:VAL:O	2.68	0.41
5:B:255:GLY:O	5:B:257:THR:HG23	2.21	0.41
12:J:42:GLU:HG2	12:J:43:ARG:HG3	2.03	0.41
1:0:2768:A:O2'	1:0:2769:C:H5'	2.21	0.41
8:E:68:HIS:O	8:E:72:MET:HG3	2.20	0.41
1:0:470:U:O2'	29:1:16:HIS:CD2	2.69	0.41
1:0:1528:A:H62	1:0:1663:G:H21	1.67	0.41
1:0:1080:C:H6	1:0:1080:C:O5'	2.04	0.41
1:0:820:G:H5'	1:0:821:U:H5'	2.03	0.41
1:0:137:U:H2'	1:0:139:C:C5	2.56	0.41
9:F:26:THR:HB	9:F:102:GLY:HA3	2.03	0.41
1:0:485:A:O2'	1:0:487:G:H5'	2.21	0.41
1:0:946:C:H2'	1:0:947:U:H6	1.84	0.41
1:0:2078:U:O2'	1:0:2079:G:H5'	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2783:A:H2'	1:0:2784:A:C8	2.56	0.41
16:N:101:VAL:HG12	38:N:9328:HOH:O	2.19	0.41
6:C:78:ARG:HH11	6:C:78:ARG:HG3	1.85	0.41
6:C:114:ALA:HB1	6:C:223:LEU:HB3	2.03	0.41
1:0:1185:U:H2'	1:0:1186:C:H6	1.84	0.41
1:0:2754:G:O2'	1:0:2755:G:H5'	2.21	0.41
5:B:16:ARG:HD3	38:B:9410:HOH:O	2.19	0.41
1:0:736:A:H2'	1:0:737:A:O4'	2.21	0.41
1:0:1391:G:H2'	1:0:1392:A:H5'	2.02	0.41
1:0:1744:G:H2'	1:0:1745:G:H5'	2.02	0.41
19:Q:53:HIS:ND1	19:Q:55:ARG:HB2	2.36	0.41
1:0:1269:G:H2'	1:0:1270:U:C6	2.56	0.41
1:0:2377:U:O5'	1:0:2377:U:H6	2.03	0.41
11:H:9:ILE:O	11:H:9:ILE:HG22	2.20	0.41
1:0:1268:C:O2'	27:Y:169:ARG:HB2	2.20	0.41
5:B:51:VAL:O	5:B:53:LEU:HD13	2.21	0.41
18:P:16:VAL:CG1	18:P:17:GLY:N	2.84	0.41
1:0:1500:U:OP2	18:P:41:ARG:NH2	2.54	0.41
1:0:2413:A:H2'	1:0:2414:A:O4'	2.20	0.41
1:0:821:U:H2'	1:0:822:C:C6	2.56	0.41
31:3:48:ASN:ND2	31:3:50:GLY:H	2.17	0.41
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.86	0.41
1:0:958:G:O2'	1:0:959:C:H5'	2.20	0.41
16:N:29:SER:OG	16:N:101:VAL:HG21	2.20	0.41
11:H:95:LEU:HD11	11:H:124:ALA:HB2	2.03	0.41
1:0:2353:A:H4'	1:0:2354:A:O5'	2.20	0.41
7:D:92:GLU:HB2	38:D:3862:HOH:O	2.19	0.41
1:0:189:A:OP1	15:M:171:ARG:NH2	2.53	0.41
27:Y:187:VAL:CG1	27:Y:205:ILE:HA	2.51	0.41
1:0:2718:C:P	5:B:45:LYS:HZ1	2.44	0.41
1:0:542:A:H2'	1:0:543:G:O4'	2.21	0.41
25:W:21:LEU:CD2	25:W:48:VAL:HG11	2.50	0.41
4:A:33:GLU:O	4:A:34:ASP:CB	2.61	0.41
25:W:3:ALA:O	25:W:54:PHE:HA	2.21	0.41
1:0:281:U:O2'	1:0:282:C:H5'	2.20	0.41
32:I:113:HIS:N	32:I:114:PRO:CD	2.83	0.41
12:J:131:THR:HG22	12:J:133:GLY:N	2.35	0.41
6:C:223:LEU:HA	6:C:223:LEU:HD12	1.94	0.41
22:T:40:VAL:HG22	22:T:41:ARG:N	2.36	0.41
17:O:32:ARG:HH11	17:O:115:ARG:HH21	1.69	0.41
1:0:1180:U:H4'	32:I:91:GLU:OE2	2.21	0.41
15:M:59:GLY:HA3	15:M:141:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:9:3114:G:H2'	2:9:3115:C:C6	2.56	0.41
6:C:46:TYR:CE1	6:C:92:PRO:HB3	2.56	0.41
6:C:133:ARG:HD2	38:C:9206:HOH:O	2.20	0.41
5:B:175:LEU:C	5:B:175:LEU:CD2	2.89	0.41
7:D:105:SER:HB2	7:D:131:THR:HG23	2.01	0.41
1:0:926:A:C4'	14:L:39:GLU:HG2	2.51	0.41
5:B:5:ARG:HH11	5:B:8:LYS:HE2	1.86	0.41
1:0:907:A:H2'	1:0:908:A:C8	2.54	0.41
2:9:3107:C:H5	38:9:3167:HOH:O	2.03	0.41
11:H:38:LYS:O	11:H:84:LYS:HE2	2.21	0.41
5:B:199:TYR:CE2	5:B:268:ARG:HB2	2.56	0.41
11:H:146:VAL:HG22	38:H:9176:HOH:O	2.21	0.41
2:9:3060:C:O2'	2:9:3061:C:H5'	2.20	0.41
22:T:23:VAL:C	22:T:93:THR:HG21	2.41	0.41
1:0:2387:U:H2'	1:0:2388:C:C6	2.56	0.41
17:O:24:ALA:O	17:O:28:ASP:HB2	2.20	0.41
22:T:47:THR:HB	22:T:100:ASP:HB3	2.01	0.41
1:0:1194:A:O2'	1:0:1195:G:H5'	2.21	0.41
1:0:1755:A:H2'	1:0:1756:G:O4'	2.20	0.41
17:O:41:ALA:HA	38:O:5104:HOH:O	2.21	0.41
28:Z:67:GLY:N	28:Z:70:LYS:O	2.53	0.41
23:U:45:GLU:HB2	23:U:48:ASN:ND2	2.36	0.41
5:B:224:LYS:HA	5:B:224:LYS:HD3	1.94	0.41
6:C:123:LEU:HA	6:C:123:LEU:HD23	1.94	0.41
1:0:2365:G:OP1	19:Q:15:LYS:HG3	2.21	0.41
25:W:153:MET:O	25:W:154:ARG:C	2.59	0.41
1:0:1173:A:H4'	1:0:1174:A:C8	2.56	0.41
28:Z:13:ARG:NH1	38:Z:9218:HOH:O	2.53	0.41
1:0:2265:U:H2'	1:0:2266:A:H8	1.86	0.41
1:0:1477:C:O2'	1:0:1478:U:H5'	2.21	0.41
21:S:17:ASP:HB3	21:S:23:LYS:HB2	2.02	0.41
7:D:10:PHE:CG	7:D:11:HIS:N	2.89	0.41
1:0:1419:U:H2'	1:0:1685:A:C2	2.55	0.41
1:0:155:C:OP2	15:M:188:ARG:HD3	2.20	0.41
32:I:78:LEU:HD13	32:I:108:ILE:HG23	2.03	0.41
1:0:1773:G:N2	1:0:1774:G:C8	2.88	0.41
1:0:1976:G:O2'	1:0:1977:U:H5'	2.21	0.41
4:A:211:LYS:HB2	38:A:9413:HOH:O	2.21	0.40
13:K:44:LEU:HA	13:K:45:PRO:HD2	1.96	0.40
25:W:72:PRO:CG	25:W:77:ALA:HB3	2.39	0.40
7:D:57:THR:HG23	7:D:63:ILE:CA	2.42	0.40
1:0:1158:G:O2'	1:0:1159:G:H5'	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:380:A:C2	15:M:13:GLU:HB3	2.56	0.40
15:M:9:ARG:HB2	15:M:47:ASP:OD2	2.20	0.40
15:M:134:ILE:O	15:M:136:PRO:HD3	2.21	0.40
16:N:181:ASP:O	16:N:184:ILE:HG22	2.21	0.40
7:D:55:LYS:HA	38:D:6752:HOH:O	2.21	0.40
4:A:165:THR:O	4:A:165:THR:CG2	2.69	0.40
38:O:9988:HOH:O	6:C:214:THR:HB	2.20	0.40
1:O:1761:U:H5'	18:P:81:LYS:O	2.22	0.40
22:T:47:THR:HG22	22:T:99:THR:OG1	2.21	0.40
2:9:3059:C:H5'	38:9:5233:HOH:O	2.21	0.40
1:O:228:C:H2'	1:O:229:G:H5'	2.03	0.40
1:O:1789:G:O6	18:P:73:HIS:HE1	2.04	0.40
1:O:1714:C:O2'	1:O:1715:C:H5'	2.21	0.40
13:K:89:LYS:HA	38:K:7064:HOH:O	2.21	0.40
1:O:1933:G:O2'	1:O:1934:A:H5'	2.20	0.40
1:O:732:C:O2'	1:O:733:U:H5'	2.21	0.40
1:O:571:C:H6	1:O:571:C:O5'	2.03	0.40
1:O:1943:C:H5''	4:A:209:PRO:HG3	2.03	0.40
1:O:1562:C:N4	38:O:6128:HOH:O	2.55	0.40
5:B:80:ARG:HA	5:B:186:GLY:O	2.21	0.40
1:O:1741:U:H3'	38:O:3074:HOH:O	2.21	0.40
1:O:1311:G:O6	6:C:173:LYS:HE3	2.22	0.40
1:O:2619:UR3:H5'	3:4:76:5AA:H103	2.03	0.40
1:O:1855:G:H4'	1:O:1856:C:O5'	2.21	0.40
26:X:26:ALA:HB1	26:X:59:TRP:CE2	2.56	0.40
1:O:1513:C:O2'	1:O:1514:C:H5'	2.21	0.40
1:O:1996:U:O2'	1:O:1997:A:H5'	2.21	0.40
5:B:171:VAL:HG23	5:B:172:SER:N	2.35	0.40
1:O:2740:G:H2'	1:O:2741:A:O4'	2.21	0.40
1:O:1643:C:O2'	1:O:1644:C:H5'	2.22	0.40
6:C:187:ARG:NH2	38:C:9162:HOH:O	2.51	0.40
38:O:7751:HOH:O	5:B:2:GLN:HG3	2.21	0.40
32:I:119:TYR:CD1	32:I:119:TYR:N	2.89	0.40
14:L:89:PHE:CD1	14:L:89:PHE:N	2.89	0.40
5:B:205:VAL:O	5:B:307:ARG:NE	2.54	0.40
1:O:1167:G:H4'	32:I:135:LEU:CD2	2.51	0.40
25:W:48:VAL:HG12	25:W:48:VAL:O	2.21	0.40
11:H:54:THR:HA	11:H:127:VAL:O	2.22	0.40
2:9:3029:C:H2'	2:9:3030:C:C5'	2.45	0.40
11:H:26:SER:HA	11:H:59:HIS:HD2	1.85	0.40
6:C:118:THR:O	6:C:136:VAL:HG13	2.21	0.40
8:E:144:THR:O	8:E:148:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:U:39:ASN:HD22	23:U:44:ARG:HH11	1.68	0.40
14:L:122:ALA:HB3	14:L:125:PHE:CZ	2.56	0.40
14:L:125:PHE:CZ	14:L:140:VAL:HG13	2.57	0.40
1:O:2266:A:OP2	15:M:90:ARG:NH2	2.52	0.40
1:O:790:A:H1'	1:O:1710:A:O2'	2.22	0.40
1:O:1631:A:H2'	1:O:1632:A:C8	2.56	0.40
9:F:99:THR:O	9:F:99:THR:HG23	2.21	0.40
25:W:125:HIS:HE1	38:W:3071:HOH:O	2.05	0.40
13:K:22:ASP:OD1	13:K:22:ASP:C	2.60	0.40
1:O:291:C:H2'	1:O:292:G:O4'	2.21	0.40
1:O:2379:G:N7	1:O:2408:A:N1	2.70	0.40
1:O:949:U:O2'	19:Q:40:HIS:HE1	2.03	0.40
7:D:75:LEU:HD22	7:D:79:MET:HB3	2.02	0.40
13:K:78:LYS:HA	13:K:79:PRO:HD3	1.95	0.40
1:O:1434:A:H2'	1:O:1436:C:C5	2.56	0.40
1:O:2050:G:OP1	20:R:79:ARG:HB3	2.21	0.40
1:O:2115:U:H2'	1:O:2116:U:C6	2.56	0.40
1:O:646:G:H2'	1:O:647:U:C6	2.56	0.40
1:O:1167:G:H3'	38:O:7702:HOH:O	2.20	0.40
25:W:137:GLN:HG3	25:W:137:GLN:O	2.21	0.40
7:D:64:ARG:HG2	7:D:67:ASP:HB3	2.04	0.40
5:B:183:GLU:OE1	5:B:183:GLU:HA	2.21	0.40
7:D:99:ASP:HB2	7:D:103:ASN:HB2	2.04	0.40
4:A:186:TRP:CD1	4:A:187:PRO:HA	2.56	0.40
16:N:183:ASP:O	16:N:184:ILE:C	2.59	0.40
14:L:53:ARG:NH2	14:L:57:VAL:CG1	2.84	0.40
24:V:59:ILE:O	24:V:63:GLU:HG2	2.21	0.40
20:R:132:ARG:NH1	38:R:9383:HOH:O	2.54	0.40
14:L:68:GLU:HG3	38:L:9342:HOH:O	2.22	0.40
25:W:73:LEU:HA	25:W:73:LEU:HD12	1.74	0.40
1:O:2314:G:O2'	1:O:2315:C:H5'	2.22	0.40
1:O:1744:G:C2'	1:O:1745:G:H5'	2.51	0.40
1:O:2776:A:H2'	1:O:2777:G:O4'	2.20	0.40
2:9:3012:C:H5'	2:9:3070:U:O4'	2.21	0.40
20:R:69:LYS:HE2	20:R:78:GLY:O	2.21	0.40
1:O:1805:G:O2'	1:O:1806:G:H5'	2.21	0.40
22:T:37:GLN:OE1	22:T:118:SER:HA	2.21	0.40
1:O:1624:A:H4'	1:O:1626:A:H5''	2.03	0.40
5:B:33:ASP:HB3	5:B:34:GLY:H	1.57	0.40
1:O:549:A:O2'	1:O:550:C:H5'	2.21	0.40
7:D:19:GLU:HG3	38:D:6165:HOH:O	2.21	0.40
30:2:40:ARG:HG2	30:2:40:ARG:NH1	2.37	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.18	0.40
12:J:107:ASN:HD22	12:J:109:TYR:H	1.64	0.40
12:J:11:ILE:HD11	12:J:109:TYR:CD2	2.57	0.40
1:O:56:G:C5'	24:V:50:ARG:HH12	2.27	0.40
22:T:24:ARG:HH21	22:T:39:ASN:ND2	2.14	0.40
8:E:20:ILE:HD11	8:E:40:VAL:CG1	2.51	0.40
27:Y:144:ARG:NH1	38:Y:9373:HOH:O	2.54	0.40
29:1:28:HIS:CD2	29:1:31:LYS:H	2.39	0.40
15:M:69:LYS:HG3	15:M:126:GLN:CA	2.52	0.40
6:C:173:LYS:O	6:C:186:TYR:HA	2.22	0.40
15:M:40:ILE:HG21	15:M:64:ARG:NH2	2.36	0.40
5:B:115:VAL:HA	5:B:116:PRO:HD3	1.88	0.40
38:O:9429:HOH:O	6:C:103:ASN:HB3	2.20	0.40
1:O:2515:C:H2'	1:O:2516:G:O4'	2.21	0.40
6:C:80:VAL:HA	6:C:81:PRO:HD3	1.95	0.40
1:O:2093:G:H5''	38:B:9327:HOH:O	2.21	0.40
15:M:184:ARG:HG3	15:M:185:PRO:HA	2.04	0.40
1:O:2659:U:H4'	20:R:76:ASP:HB3	2.03	0.40
11:H:114:ARG:O	11:H:115:ALA:C	2.60	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:9:3020:G:OP1	5:B:195:ARG:NH2[7_545]	1.98	0.22
1:O:1171:A:N3	1:O:1964:U:O5'[3.655]	2.13	0.07
13:K:63:GLU:CB	13:K:63:GLU:CB[3.655]	2.13	0.07

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	235/240 (98%)	206 (88%)	24 (10%)	5 (2%)	11	19
5	B	335/338 (99%)	294 (88%)	35 (10%)	6 (2%)	13	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	C	244/246 (99%)	217 (89%)	26 (11%)	1 (0%)	43	72
7	D	134/177 (76%)	97 (72%)	25 (19%)	12 (9%)	1	1
8	E	170/178 (96%)	156 (92%)	13 (8%)	1 (1%)	33	63
9	F	117/120 (98%)	106 (91%)	7 (6%)	4 (3%)	6	8
10	G	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
11	H	156/171 (91%)	142 (91%)	11 (7%)	3 (2%)	12	23
12	J	140/145 (97%)	130 (93%)	8 (6%)	2 (1%)	16	32
13	K	130/132 (98%)	119 (92%)	8 (6%)	3 (2%)	10	17
14	L	141/165 (86%)	120 (85%)	19 (14%)	2 (1%)	16	32
15	M	192/194 (99%)	178 (93%)	14 (7%)	0	100	100
16	N	184/187 (98%)	167 (91%)	11 (6%)	6 (3%)	6	9
17	O	113/116 (97%)	104 (92%)	8 (7%)	1 (1%)	25	49
18	P	141/149 (95%)	135 (96%)	6 (4%)	0	100	100
19	Q	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
20	R	148/155 (96%)	138 (93%)	8 (5%)	2 (1%)	16	32
21	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
22	T	117/120 (98%)	107 (92%)	10 (8%)	0	100	100
23	U	51/66 (77%)	47 (92%)	3 (6%)	1 (2%)	11	21
24	V	63/71 (89%)	55 (87%)	6 (10%)	2 (3%)	6	9
25	W	152/154 (99%)	146 (96%)	5 (3%)	1 (1%)	30	58
26	X	80/92 (87%)	70 (88%)	8 (10%)	2 (2%)	9	14
27	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
28	Z	71/83 (86%)	60 (84%)	7 (10%)	4 (6%)	3	3
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
31	3	90/92 (98%)	88 (98%)	0	2 (2%)	10	18
32	I	68/162 (42%)	51 (75%)	17 (25%)	0	100	100
All	All	3705/4430 (84%)	3350 (90%)	295 (8%)	60 (2%)	14	28

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	34	ASP

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Mol	Chain	Res	Type
4	A	132	ASP
9	F	101	ALA
11	H	168	ALA
12	J	5	GLU
16	N	154	LEU
16	N	184	ILE
28	Z	81	ARG
4	A	37	VAL
5	B	34	GLY
5	B	169	GLY
6	C	8	LEU
7	D	65	GLU
7	D	137	PRO
7	D	173	GLU
9	F	44	SER
11	H	166	SER
24	V	43	PRO
5	B	107	SER
7	D	86	THR
11	H	140	VAL
13	K	126	SER
14	L	80	ASP
14	L	143	THR
16	N	113	SER
16	N	164	ASP
23	U	7	ASP
26	X	78	GLU
28	Z	42	CYS
5	B	185	GLY
7	D	171	ASP
8	E	44	GLY
9	F	61	MET
9	F	64	PRO
12	J	143	LYS
16	N	167	ASP
26	X	70	ILE
31	3	56	PRO
5	B	2	GLN
7	D	89	PRO
16	N	160	SER
25	W	49	ASN
28	Z	20	ARG

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Mol	Chain	Res	Type
31	3	57	GLY
7	D	16	PRO
7	D	97	GLN
28	Z	43	GLY
4	A	211	LYS
4	A	236	GLY
7	D	28	GLY
24	V	40	PRO
7	D	27	ILE
17	O	108	GLY
20	R	106	GLY
7	D	69	ILE
7	D	135	VAL
13	K	39	GLY
20	R	81	PRO
5	B	30	PRO
13	K	111	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	179/182 (98%)	169 (94%)	10 (6%)	30	55
5	B	282/283 (100%)	265 (94%)	17 (6%)	27	51
6	C	193/193 (100%)	176 (91%)	17 (9%)	14	27
7	D	117/148 (79%)	112 (96%)	5 (4%)	40	69
8	E	152/156 (97%)	148 (97%)	4 (3%)	59	85
9	F	93/94 (99%)	92 (99%)	1 (1%)	84	96
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	126 (96%)	6 (4%)	38	67
12	J	118/121 (98%)	109 (92%)	9 (8%)	19	36
13	K	106/106 (100%)	101 (95%)	5 (5%)	36	65
14	L	113/127 (89%)	107 (95%)	6 (5%)	32	58
15	M	158/158 (100%)	151 (96%)	7 (4%)	39	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	N	149/150 (99%)	144 (97%)	5 (3%)	49	78
17	O	93/94 (99%)	90 (97%)	3 (3%)	51	80
18	P	113/117 (97%)	109 (96%)	4 (4%)	48	77
19	Q	79/80 (99%)	76 (96%)	3 (4%)	44	74
20	R	117/122 (96%)	114 (97%)	3 (3%)	59	85
21	S	71/74 (96%)	69 (97%)	2 (3%)	56	84
22	T	105/106 (99%)	101 (96%)	4 (4%)	44	74
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	50 (98%)	1 (2%)	68	90
25	W	130/130 (100%)	124 (95%)	6 (5%)	37	66
26	X	66/74 (89%)	61 (92%)	5 (8%)	19	36
27	Y	120/196 (61%)	111 (92%)	9 (8%)	19	36
28	Z	60/68 (88%)	60 (100%)	0	100	100
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	41 (98%)	1 (2%)	61	87
31	3	79/79 (100%)	76 (96%)	3 (4%)	44	74
32	I	58/130 (45%)	57 (98%)	1 (2%)	73	92
All	All	3093/3611 (86%)	2956 (96%)	137 (4%)	39	68

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	ARG
4	A	33	GLU
4	A	36	ASP
4	A	69	LEU
4	A	78	ASP
4	A	94	LEU
4	A	120	ARG
4	A	125	ASN
4	A	179	MET
4	A	217	ARG
5	B	5	ARG
5	B	7	ARG
5	B	11	LEU
5	B	27	ASN

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Mol	Chain	Res	Type
5	B	33	ASP
5	B	49	THR
5	B	63	GLU
5	B	98	THR
5	B	149	ASP
5	B	162	MET
5	B	195	ARG
5	B	251	VAL
5	B	254	GLN
5	B	280	VAL
5	B	304	PRO
5	B	307	ARG
5	B	312	ARG
6	C	2	GLN
6	C	27	ARG
6	C	67	GLN
6	C	76	ARG
6	C	91	PRO
6	C	94	THR
6	C	106	GLU
6	C	115	LEU
6	C	136	VAL
6	C	187	ARG
6	C	214	THR
6	C	222	ASP
6	C	223	LEU
6	C	234	VAL
6	C	236	THR
6	C	240	LEU
6	C	246	ARG
7	D	24	HIS
7	D	61	PHE
7	D	86	THR
7	D	133	ASN
7	D	136	ARG
8	E	15	GLN
8	E	102	VAL
8	E	126	ILE
8	E	164	ASP
9	F	105	ASP
11	H	30	GLN
11	H	84	LYS

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Mol	Chain	Res	Type
11	H	88	ARG
11	H	96	ARG
11	H	111	ASP
11	H	154	TYR
12	J	16	ASP
12	J	46	ILE
12	J	52	GLN
12	J	74	ARG
12	J	76	ASP
12	J	79	PHE
12	J	107	ASN
12	J	112	ASP
12	J	131	THR
13	K	7	ASP
13	K	10	GLN
13	K	49	LEU
13	K	98	VAL
13	K	129	THR
14	L	4	LYS
14	L	30	ARG
14	L	35	ARG
14	L	99	GLU
14	L	102	ASP
14	L	104	ASP
15	M	23	LEU
15	M	46	LEU
15	M	68	ARG
15	M	93	ARG
15	M	99	ARG
15	M	116	ASN
15	M	164	THR
16	N	17	ARG
16	N	26	LEU
16	N	93	GLN
16	N	139	TRP
16	N	152	GLU
17	O	3	THR
17	O	43	VAL
17	O	115	ARG
18	P	21	VAL
18	P	52	LYS
18	P	91	LYS

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Mol	Chain	Res	Type
18	P	98	ILE
19	Q	11	ARG
19	Q	57	ASP
19	Q	95	GLU
20	R	13	THR
20	R	39	THR
20	R	82	GLU
21	S	10	VAL
21	S	53	ASN
22	T	39	ASN
22	T	48	VAL
22	T	112	LEU
22	T	115	GLU
24	V	65	ASP
25	W	35	VAL
25	W	52	VAL
25	W	73	LEU
25	W	122	ARG
25	W	146	ILE
25	W	154	ARG
26	X	15	ARG
26	X	27	ASP
26	X	49	ARG
26	X	72	VAL
26	X	79	GLU
27	Y	141	THR
27	Y	144	ARG
27	Y	163	THR
27	Y	174	VAL
27	Y	186	ARG
27	Y	189	ASN
27	Y	203	VAL
27	Y	204	ARG
27	Y	235	GLU
30	2	18	ASN
31	3	11	CYS
31	3	42	ARG
31	3	56	PRO
32	I	86	GLU

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

Mol	Chain	Res	Type
4	A	29	HIS
4	A	92	ASN
4	A	176	HIS
4	A	199	HIS
5	B	27	ASN
5	B	145	HIS
5	B	221	GLN
5	B	238	ASN
5	B	260	HIS
5	B	320	GLN
5	B	332	ASN
6	C	2	GLN
6	C	39	GLN
6	C	129	HIS
7	D	47	GLN
7	D	97	GLN
7	D	103	ASN
7	D	133	ASN
8	E	71	ASN
8	E	90	HIS
8	E	106	ASN
8	E	143	GLN
10	G	64	ASN
11	H	31	HIS
11	H	56	GLN
11	H	59	HIS
11	H	70	ASN
11	H	170	ASN
12	J	52	GLN
12	J	107	ASN
13	K	10	GLN
14	L	18	HIS
14	L	41	HIS
14	L	42	ASN
15	M	24	GLN
15	M	26	GLN
15	M	58	GLN
15	M	143	ASN
15	M	170	ASN
16	N	40	ASN
16	N	93	GLN
16	N	107	ASN
18	P	50	GLN

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Mol	Chain	Res	Type
18	P	66	GLN
18	P	73	HIS
18	P	88	GLN
18	P	118	GLN
19	Q	16	ASN
19	Q	40	HIS
20	R	61	GLN
20	R	94	ASN
20	R	98	ASN
20	R	113	HIS
20	R	117	HIS
21	S	25	GLN
21	S	53	ASN
22	T	39	ASN
22	T	43	ASN
22	T	73	HIS
23	U	39	ASN
23	U	48	ASN
24	V	29	ASN
24	V	60	GLN
25	W	2	HIS
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	23	HIS
27	Y	133	HIS
27	Y	134	HIS
27	Y	149	GLN
27	Y	189	ASN
29	1	8	GLN
29	1	16	HIS
29	1	28	HIS
30	2	16	ASN
30	2	18	ASN
30	2	41	HIS
30	2	45	ASN
31	3	2	GLN
31	3	15	ASN
31	3	30	GLN
31	3	48	ASN
32	I	104	GLN

## 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	235 (8%)	32 (1%)
2	9	121/122 (99%)	15 (12%)	1 (0%)
3	4	0/8	-	-
All	All	2866/3052 (93%)	250 (8%)	33 (1%)

All (250) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	60	A
1	0	67	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	139	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	185	G
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	285	A
1	0	308	U
1	0	309	C
1	0	318	C
1	0	331	A
1	0	336	G
1	0	337	A

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Mol	Chain	Res	Type
1	0	345	G
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
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	701	U
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	872	U
1	0	875	A
1	0	877	G

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Mol	Chain	Res	Type
1	0	878	G
1	0	885	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1131	G
1	0	1137	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1216	G
1	0	1234	U
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

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Mol	Chain	Res	Type
1	0	1360	C
1	0	1377	C
1	0	1407	A
1	0	1409	G
1	0	1451	C
1	0	1474	C
1	0	1485	A
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1559	A
1	0	1564	C
1	0	1592	G
1	0	1603	A
1	0	1625	U
1	0	1626	A
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1710	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C
1	0	1732	A
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

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Mol	Chain	Res	Type
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1978	A
1	0	1979	G
1	0	1996	U
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	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	2110	G
1	0	2238	A
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2422	U
1	0	2462	G
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

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Mol	Chain	Res	Type
1	0	2541	U
1	0	2542	C
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2637	A
1	0	2645	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	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2825	C
1	0	2850	C
1	0	2864	U
1	0	2867	G
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3041	C
2	9	3043	G

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Mol	Chain	Res	Type
2	9	3044	A
2	9	3052	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	129	A
1	0	169	A
1	0	338	C
1	0	603	A
1	0	699	C
1	0	834	G
1	0	857	A
1	0	869	G
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1563	G
1	0	1667	A
1	0	1692	C
1	0	1856	C
1	0	1942	A
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2541	U
1	0	2637	A
1	0	2649	A
1	0	2718	C
1	0	2726	U

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Mol	Chain	Res	Type
1	0	2791	U
2	9	3065	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
1	OMU	0	2587	1,35	20,22,23	0.71	1 (5%)	24,31,34	0.72	0
1	OMG	0	2588	1,3	24,26,27	0.93	2 (8%)	32,38,41	5.31	3 (9%)
1	UR3	0	2619	1	20,22,23	0.79	0	23,32,35	0.81	0
1	PSU	0	2621	1	19,21,22	1.23	2 (10%)	23,30,33	1.06	1 (4%)
1	1MA	0	628	1	23,25,26	0.86	0	32,37,40	1.00	1 (3%)
3	5AA	4	76	1,3	24,26,27	0.76	1 (4%)	35,38,41	0.90	1 (2%)

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	OMU	0	2587	1,35	-	0/8/27/28	0/2/2/2
1	OMG	0	2588	1,3	-	0/10/27/28	0/1/3/3
1	UR3	0	2619	1	-	0/6/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/8/25/26	0/2/2/2
1	1MA	0	628	1	-	1/8/25/26	0/1/3/3
3	5AA	4	76	1,3	-	0/12/29/30	0/1/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	3.15	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2588	OMG	P-OP1	2.83	1.49	1.46
1	0	2621	PSU	C6-N1	2.79	1.34	1.32
1	0	2587	OMU	P-OP1	2.25	1.49	1.46
3	4	76	5AA	P-OP1	2.03	1.49	1.46
1	0	2588	OMG	C8-N7	-2.00	1.30	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2588	OMG	C6-C5-N7	-29.46	130.17	134.14
3	4	76	5AA	C2-N1-C6	3.37	118.83	111.53
1	0	2588	OMG	C6-N1-C2	3.19	125.09	119.51
1	0	628	1MA	C2-N3-C4	-3.12	110.89	116.23
1	0	2621	PSU	C5-C4-N3	-2.34	114.59	118.86
1	0	2588	OMG	C2-N3-C4	-2.23	111.96	115.09

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	628	1MA	C2'-C1'-N9-C8

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 234 ligands modelled in this entry, 234 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.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	0	2754/2922 (94%)	0.36	96 (3%) 42 38	24, 51, 98, 161	0
2	9	122/122 (100%)	0.51	5 (4%) 35 32	46, 68, 96, 153	0
3	4	8/8 (100%)	0.45	0 100 100	42, 45, 47, 54	0
4	A	237/240 (98%)	0.43	17 (7%) 15 12	31, 55, 94, 120	0
5	B	337/338 (99%)	0.99	32 (9%) 8 6	33, 65, 94, 103	0
6	C	246/246 (100%)	0.01	5 (2%) 62 60	26, 51, 75, 86	0
7	D	140/177 (79%)	2.06	58 (41%) 1 0	64, 110, 134, 141	0
8	E	172/178 (96%)	1.65	53 (30%) 1 1	50, 81, 105, 115	0
9	F	119/120 (99%)	0.75	17 (14%) 3 2	57, 81, 107, 122	0
10	G	29/348 (8%)	2.79	18 (62%) 0 0	74, 95, 105, 107	0
11	H	160/171 (93%)	0.92	17 (10%) 7 5	42, 63, 94, 101	0
12	J	142/145 (97%)	0.71	5 (3%) 42 38	42, 59, 82, 97	0
13	K	132/132 (100%)	0.76	10 (7%) 14 11	37, 62, 86, 90	0
14	L	145/165 (87%)	0.74	19 (13%) 4 3	28, 74, 118, 131	0
15	M	194/194 (100%)	0.04	0 100 100	33, 48, 64, 72	0
16	N	186/187 (99%)	0.82	26 (13%) 3 2	43, 69, 118, 124	0
17	O	115/116 (99%)	0.24	2 (1%) 67 66	43, 61, 79, 89	0
18	P	143/149 (95%)	0.57	4 (2%) 50 48	46, 62, 75, 81	0
19	Q	95/96 (98%)	0.37	3 (3%) 45 42	40, 50, 66, 77	0
20	R	150/155 (96%)	0.22	2 (1%) 74 75	36, 51, 72, 82	0
21	S	81/85 (95%)	0.37	6 (7%) 14 12	48, 65, 85, 94	0
22	T	119/120 (99%)	0.44	7 (5%) 22 18	44, 61, 90, 111	0
23	U	53/66 (80%)	0.92	5 (9%) 9 6	48, 63, 80, 88	0
24	V	65/71 (91%)	1.21	14 (21%) 1 1	59, 83, 117, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	154/154 (100%)	0.41	0 100 100	41, 57, 78, 88	0
26	X	82/92 (89%)	0.81	9 (10%) 6 4	49, 66, 89, 106	0
27	Y	142/241 (58%)	0.52	11 (7%) 13 10	32, 51, 74, 95	0
28	Z	73/83 (87%)	0.29	4 (5%) 24 20	45, 64, 78, 96	0
29	1	56/57 (98%)	-0.15	0 100 100	31, 38, 46, 61	0
30	2	46/50 (92%)	1.68	16 (34%) 1 1	40, 70, 123, 128	0
31	3	92/92 (100%)	0.37	4 (4%) 34 30	37, 60, 74, 89	0
32	I	70/162 (43%)	3.64	54 (77%) 0 0	108, 129, 152, 155	0
All	All	6659/7482 (89%)	0.57	519 (7%) 14 10	24, 58, 109, 161	0

All (519) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	93	GLN	11.8
32	I	133	THR	8.9
32	I	71	GLY	7.6
32	I	137	VAL	7.4
10	G	27	ILE	7.2
7	D	88	LEU	7.2
32	I	81	ASP	6.9
2	9	3001	U	6.9
24	V	1	THR	6.9
32	I	111	GLN	6.9
30	2	44	ARG	6.7
30	2	48	ASP	6.5
30	2	36	ASN	6.4
7	D	44	ILE	6.3
24	V	39	ALA	6.3
7	D	58	VAL	6.3
7	D	69	ILE	6.2
30	2	38	LYS	6.1
24	V	43	PRO	6.1
30	2	49	GLU	6.1
7	D	90	LEU	6.1
7	D	84	LEU	6.0
30	2	37	HIS	6.0
32	I	114	PRO	6.0
1	0	1173	A	5.9
24	V	40	PRO	5.8

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Mol	Chain	Res	Type	RSRZ
32	I	78	LEU	5.8
32	I	96	PHE	5.8
7	D	63	ILE	5.8
4	A	37	VAL	5.8
8	E	100	ASP	5.8
32	I	121	LEU	5.8
7	D	89	PRO	5.7
32	I	72	VAL	5.6
10	G	23	ILE	5.6
1	0	282	C	5.5
32	I	110	GLU	5.5
32	I	116	LEU	5.4
32	I	113	HIS	5.4
1	0	2237	G	5.4
7	D	134	LEU	5.4
1	0	1177	A	5.3
7	D	65	GLU	5.2
32	I	77	GLU	5.2
32	I	73	PRO	5.2
7	D	64	ARG	5.1
32	I	132	CYS	5.1
32	I	88	GLY	5.1
10	G	71	LEU	5.0
8	E	10	ASP	5.0
7	D	172	VAL	4.9
14	L	80	ASP	4.9
7	D	10	PHE	4.9
14	L	60	GLU	4.9
7	D	57	THR	4.8
4	A	36	ASP	4.8
7	D	56	ARG	4.8
7	D	85	GLN	4.8
32	I	102	VAL	4.8
7	D	170	TYR	4.8
7	D	75	LEU	4.8
1	0	497	A	4.8
7	D	61	PHE	4.7
32	I	107	GLN	4.7
7	D	40	ILE	4.7
7	D	26	GLY	4.7
30	2	41	HIS	4.7
7	D	92	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
1	0	960	G	4.5
7	D	41	LEU	4.4
26	X	88	GLU	4.4
32	I	139	ILE	4.4
1	0	735	C	4.4
32	I	103	ASP	4.4
1	0	1172	G	4.3
1	0	1951	G	4.3
32	I	135	LEU	4.3
32	I	125	ALA	4.3
10	G	24	VAL	4.3
30	2	42	TRP	4.2
1	0	1199	A	4.2
8	E	95	VAL	4.2
32	I	89	SER	4.2
32	I	117	LEU	4.2
16	N	181	ASP	4.2
2	9	3024	U	4.1
8	E	45	ASP	4.1
22	T	50	VAL	4.1
10	G	67	LEU	4.1
1	0	1279	U	4.0
32	I	85	PHE	4.0
5	B	106	HIS	4.0
1	0	1525	G	4.0
8	E	11	VAL	4.0
8	E	92	PRO	4.0
27	Y	235	GLU	4.0
2	9	3023	U	3.9
5	B	119	HIS	3.9
5	B	104	GLU	3.9
32	I	109	ALA	3.9
8	E	102	VAL	3.9
8	E	148	ILE	3.9
8	E	93	MET	3.9
30	2	47	THR	3.9
1	0	2238	A	3.8
8	E	42	VAL	3.8
30	2	35	ARG	3.8
7	D	18	ILE	3.8
10	G	28	GLU	3.8
16	N	147	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
10	G	64	ASN	3.8
1	0	284	C	3.8
8	E	99	GLY	3.8
23	U	54	THR	3.7
7	D	130	VAL	3.7
8	E	83	GLY	3.7
24	V	37	GLY	3.7
9	F	44	SER	3.7
11	H	47	ILE	3.7
9	F	119	ARG	3.7
10	G	26	MET	3.7
18	P	77	ALA	3.7
8	E	118	ILE	3.7
16	N	160	SER	3.7
16	N	182	GLY	3.7
32	I	118	SER	3.7
5	B	116	PRO	3.6
7	D	98	PHE	3.6
13	K	132	VAL	3.6
32	I	128	VAL	3.6
7	D	66	GLY	3.6
8	E	48	VAL	3.6
32	I	84	GLY	3.6
7	D	87	ALA	3.6
24	V	41	GLU	3.6
14	L	104	ASP	3.5
7	D	70	GLY	3.5
14	L	81	VAL	3.5
8	E	126	ILE	3.5
30	2	20	ARG	3.5
7	D	59	GLY	3.5
1	0	999	C	3.5
26	X	85	VAL	3.5
11	H	83	TYR	3.5
16	N	180	LEU	3.5
5	B	180	ASP	3.5
24	V	38	GLY	3.5
7	D	50	VAL	3.5
7	D	173	GLU	3.4
5	B	181	ILE	3.4
26	X	74	ALA	3.4
1	0	2004	U	3.4

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Mol	Chain	Res	Type	RSRZ
32	I	86	GLU	3.4
1	0	1000	C	3.4
10	G	20	VAL	3.4
10	G	22	ALA	3.4
1	0	285	A	3.4
23	U	47	ARG	3.4
1	0	1190	G	3.4
14	L	105	TYR	3.4
32	I	119	TYR	3.4
9	F	27	GLY	3.4
28	Z	59	TYR	3.3
32	I	75	THR	3.3
8	E	22	VAL	3.3
32	I	124	ALA	3.3
1	0	1202	A	3.3
32	I	97	VAL	3.3
16	N	166	ALA	3.3
9	F	16	ALA	3.3
16	N	172	PHE	3.3
1	0	1204	C	3.3
32	I	129	VAL	3.2
1	0	1171	A	3.2
10	G	73	ASP	3.2
32	I	104	GLN	3.2
4	A	237	GLY	3.2
7	D	27	ILE	3.2
32	I	79	ILE	3.2
1	0	280	C	3.2
8	E	97	VAL	3.2
16	N	64	SER	3.2
32	I	91	GLU	3.2
8	E	161	VAL	3.1
9	F	18	GLU	3.1
1	0	970	U	3.1
2	9	3002	U	3.1
28	Z	20	ARG	3.1
14	L	149	ARG	3.1
22	T	112	LEU	3.1
16	N	152	GLU	3.1
22	T	59	GLU	3.1
27	Y	96	GLU	3.1
4	A	32	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	0	2769	C	3.1
22	T	117	ASP	3.1
19	Q	95	GLU	3.0
7	D	55	LYS	3.0
1	0	969	G	3.0
9	F	117	GLU	3.0
21	S	81	ILE	3.0
5	B	64	GLY	3.0
16	N	175	LEU	3.0
14	L	108	VAL	3.0
8	E	105	GLU	3.0
32	I	95	ASP	3.0
8	E	82	TYR	3.0
1	0	716	G	3.0
24	V	59	ILE	3.0
30	2	45	ASN	2.9
7	D	86	THR	2.9
30	2	43	ARG	2.9
10	G	16	LYS	2.9
27	Y	97	LEU	2.9
1	0	283	U	2.9
16	N	68	GLU	2.9
1	0	1150	A	2.9
14	L	124	ASP	2.9
27	Y	95	THR	2.9
8	E	6	GLU	2.9
1	0	1163	G	2.9
16	N	183	ASP	2.9
11	H	71	ARG	2.9
16	N	159	TYR	2.9
22	T	116	ASP	2.9
13	K	3	ALA	2.9
1	0	2890	A	2.9
1	0	10	U	2.9
16	N	137	ALA	2.9
1	0	2344	G	2.9
21	S	16	ASN	2.9
7	D	166	ILE	2.9
16	N	157	PRO	2.9
1	0	1198	U	2.9
18	P	114	LEU	2.8
7	D	16	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	0	1130	U	2.8
32	I	83	ALA	2.8
1	0	1185	U	2.8
7	D	104	PHE	2.8
8	E	109	GLY	2.8
18	P	71	TYR	2.8
1	0	2588	OMG	2.8
32	I	92	PRO	2.8
7	D	11	HIS	2.8
1	0	272	A	2.8
11	H	142	ASP	2.8
1	0	1174	A	2.8
13	K	101	ASN	2.8
8	E	86	VAL	2.7
32	I	106	LYS	2.7
8	E	170	ARG	2.7
9	F	17	LEU	2.7
8	E	87	PHE	2.7
7	D	67	ASP	2.7
8	E	128	GLY	2.7
1	0	717	C	2.7
10	G	69	ARG	2.7
1	0	2768	A	2.7
4	A	35	GLY	2.7
5	B	97	LEU	2.7
5	B	140	LEU	2.7
5	B	121	PRO	2.7
1	0	1213	C	2.7
1	0	1181	A	2.7
19	Q	81	GLU	2.7
32	I	131	THR	2.7
8	E	88	TYR	2.7
16	N	127	LEU	2.7
8	E	108	LEU	2.7
31	3	92	GLU	2.6
16	N	138	ASP	2.6
1	0	1214	G	2.6
8	E	154	ILE	2.6
32	I	115	ASP	2.6
8	E	122	THR	2.6
11	H	144	GLU	2.6
5	B	196	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
14	L	100	ALA	2.6
5	B	71	VAL	2.6
1	0	2577	A	2.6
7	D	93	LEU	2.6
10	G	21	ASP	2.6
1	0	2717	C	2.6
14	L	91	VAL	2.6
1	0	370	G	2.6
31	3	56	PRO	2.6
7	D	23	VAL	2.6
7	D	171	ASP	2.6
1	0	1203	G	2.6
5	B	113	LEU	2.5
1	0	1192	A	2.5
11	H	65	SER	2.5
4	A	133	ARG	2.5
4	A	63	GLY	2.5
14	L	61	ALA	2.5
26	X	82	GLU	2.5
1	0	514	G	2.5
1	0	1186	C	2.5
7	D	25	MET	2.5
11	H	50	ILE	2.5
7	D	135	VAL	2.5
9	F	25	ASP	2.5
9	F	28	ALA	2.5
24	V	52	ALA	2.5
5	B	142	LEU	2.5
6	C	61	PHE	2.5
6	C	131	PHE	2.5
7	D	17	ARG	2.5
1	0	2239	C	2.5
16	N	163	PHE	2.5
13	K	5	GLY	2.5
19	Q	20	ASP	2.5
20	R	14	ALA	2.5
14	L	118	LEU	2.5
13	K	119	GLN	2.5
18	P	80	ARG	2.5
5	B	122	ASP	2.5
14	L	102	ASP	2.5
1	0	628	1MA	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
14	L	150	GLN	2.5
27	Y	193	LEU	2.5
24	V	9	ARG	2.5
14	L	59	GLU	2.5
32	I	87	THR	2.5
5	B	1	PRO	2.4
21	S	20	PHE	2.4
8	E	121	ASP	2.4
30	2	46	ASP	2.4
8	E	117	THR	2.4
5	B	69	VAL	2.4
5	B	65	MET	2.4
8	E	145	ALA	2.4
5	B	135	GLY	2.4
8	E	44	GLY	2.4
27	Y	108	ASP	2.4
1	0	1162	G	2.4
5	B	73	VAL	2.4
30	2	31	ARG	2.4
5	B	112	THR	2.4
4	A	38	ILE	2.4
8	E	53	GLU	2.4
1	0	1200	A	2.4
1	0	2576	A	2.4
7	D	24	HIS	2.4
11	H	150	PHE	2.4
10	G	68	GLU	2.4
27	Y	141	THR	2.4
5	B	100	VAL	2.4
5	B	328	ARG	2.4
8	E	104	ILE	2.4
16	N	179	LEU	2.4
11	H	171	ALA	2.4
11	H	161	CYS	2.4
32	I	82	GLU	2.4
1	0	2509	A	2.3
14	L	133	VAL	2.3
5	B	52	VAL	2.3
9	F	106	ALA	2.3
1	0	736	A	2.3
1	0	1626	A	2.3
6	C	132	ASP	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
12	J	62	ASP	2.3
23	U	53	ASP	2.3
7	D	106	PHE	2.3
12	J	48	GLY	2.3
21	S	76	GLU	2.3
7	D	91	ALA	2.3
32	I	90	GLY	2.3
9	F	107	ASP	2.3
32	I	74	PRO	2.3
6	C	135	GLU	2.3
8	E	40	VAL	2.3
1	0	2587	OMU	2.3
7	D	83	PHE	2.3
1	0	2508	C	2.3
8	E	157	LYS	2.3
5	B	133	GLU	2.3
11	H	141	GLU	2.3
16	N	156	GLU	2.3
31	3	22	VAL	2.3
1	0	128	A	2.3
1	0	2368	A	2.3
26	X	18	ARG	2.3
5	B	35	GLN	2.3
7	D	47	GLN	2.3
27	Y	98	GLN	2.3
7	D	139	TYR	2.3
16	N	94	GLU	2.3
7	D	45	THR	2.3
14	L	97	VAL	2.3
17	O	111	VAL	2.3
27	Y	234	VAL	2.3
28	Z	36	ASP	2.3
24	V	49	LEU	2.3
1	0	2249	G	2.3
5	B	51	VAL	2.3
26	X	10	VAL	2.3
6	C	237	GLU	2.3
12	J	57	TYR	2.3
4	A	129	LEU	2.3
9	F	103	GLU	2.2
13	K	2	GLU	2.2
1	0	1178	G	2.2

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Mol	Chain	Res	Type	RSRZ
1	0	2250	G	2.2
23	U	51	TRP	2.2
7	D	128	LEU	2.2
16	N	158	LEU	2.2
8	E	144	THR	2.2
27	Y	236	VAL	2.2
1	0	2566	A	2.2
9	F	109	GLU	2.2
32	I	94	GLU	2.2
1	0	369	G	2.2
1	0	2567	G	2.2
1	0	2716	G	2.2
4	A	62	ASP	2.2
5	B	54	VAL	2.2
32	I	76	ALA	2.2
26	X	80	GLU	2.2
5	B	296	LEU	2.2
8	E	16	ASP	2.2
8	E	39	ASP	2.2
7	D	29	HIS	2.2
16	N	97	VAL	2.2
1	0	1175	G	2.2
1	0	2570	G	2.2
7	D	62	ASP	2.2
17	O	104	ASN	2.2
1	0	372	A	2.2
1	0	1625	U	2.2
1	0	2526	C	2.2
9	F	100	ASP	2.2
1	0	1665	G	2.2
8	E	124	VAL	2.2
8	E	38	ILE	2.2
1	0	138	U	2.2
5	B	84	LEU	2.2
8	E	81	GLU	2.2
9	F	26	THR	2.2
11	H	85	MET	2.2
1	0	1210	G	2.2
1	0	2715	G	2.2
11	H	167	PRO	2.2
4	A	128	LEU	2.2
8	E	116	THR	2.1

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Mol	Chain	Res	Type	RSRZ
10	G	15	TRP	2.1
12	J	47	THR	2.1
23	U	43	GLY	2.1
1	0	2850	C	2.1
11	H	45	VAL	2.1
20	R	96	VAL	2.1
10	G	66	LEU	2.1
11	H	73	LEU	2.1
10	G	70	ALA	2.1
9	F	108	VAL	2.1
11	H	165	SER	2.1
1	0	279	C	2.1
1	0	371	U	2.1
24	V	61	GLY	2.1
27	Y	225	GLY	2.1
21	S	52	VAL	2.1
22	T	115	GLU	2.1
5	B	74	ILE	2.1
13	K	109	LEU	2.1
1	0	2718	C	2.1
2	9	3122	C	2.1
4	A	59	GLU	2.1
26	X	29	ALA	2.1
1	0	1159	G	2.1
1	0	2692	G	2.1
24	V	63	GLU	2.1
28	Z	38	ALA	2.1
1	0	2664	A	2.1
1	0	2760	C	2.1
1	0	2797	C	2.1
1	0	2713	G	2.1
32	I	98	ALA	2.1
8	E	111	LYS	2.1
13	K	131	ILE	2.1
14	L	89	PHE	2.1
1	0	2103	A	2.1
8	E	5	LEU	2.1
16	N	161	GLY	2.1
4	A	85	SER	2.1
8	E	80	TRP	2.1
8	E	134	SER	2.1
11	H	125	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
8	E	7	ILE	2.1
12	J	26	VAL	2.0
13	K	83	PRO	2.0
22	T	119	ALA	2.0
14	L	96	VAL	2.0
32	I	105	VAL	2.0
26	X	71	ARG	2.0
30	2	39	ARG	2.0
21	S	45	TYR	2.0
4	A	31	LYS	2.0
1	0	2884	G	2.0
8	E	98	GLU	2.0
9	F	15	ASP	2.0
7	D	22	VAL	2.0
4	A	211	LYS	2.0
5	B	188	HIS	2.0
31	3	41	GLU	2.0
4	A	65	ARG	2.0
16	N	165	ALA	2.0
13	K	88	VAL	2.0
1	0	2712	G	2.0
4	A	236	GLY	2.0
1	0	1179	C	2.0
1	0	2575	C	2.0
8	E	33	LEU	2.0
1	0	1118	A	2.0
1	0	2793	A	2.0
7	D	74	THR	2.0
8	E	41	SER	2.0
16	N	162	ASP	2.0
24	V	5	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	5AA	4	76	24/25	0.22	2.19	40,44,46,47	0
1	UR3	0	2619	21/22	0.20	1.42	33,38,39,42	0
1	1MA	0	628	23/24	0.20	0.20	28,34,37,38	0
1	OMG	0	2588	24/25	0.19	-1.15	30,33,38,40	0
1	PSU	0	2621	20/21	0.16	-1.32	31,34,40,41	0
1	OMU	0	2587	21/22	0.17	-1.40	31,35,40,41	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	9184	1/1	0.85	90.28	83,83,83,83	0
35	NA	B	9158	1/1	0.74	62.46	70,70,70,70	0
35	NA	0	9178	1/1	0.50	49.80	57,57,57,57	0
35	NA	0	9160	1/1	0.39	45.88	46,46,46,46	0
35	NA	0	9121	1/1	0.78	34.92	55,55,55,55	0
35	NA	0	9162	1/1	0.56	34.84	64,64,64,64	0
33	MG	0	8101	1/1	0.38	31.82	72,72,72,72	0
35	NA	0	9113	1/1	0.34	29.12	67,67,67,67	0
33	MG	0	8092	1/1	0.41	22.74	90,90,90,90	0
33	MG	0	8087	1/1	0.25	20.36	59,59,59,59	0
35	NA	0	9152	1/1	0.40	19.87	61,61,61,61	0
35	NA	0	9175	1/1	0.37	18.97	52,52,52,52	0
35	NA	0	9120	1/1	0.36	16.62	52,52,52,52	0
33	MG	0	8100	1/1	0.42	14.30	70,70,70,70	0
35	NA	0	9106	1/1	0.35	14.23	38,38,38,38	0
33	MG	0	8016	1/1	0.28	14.10	50,50,50,50	0
35	NA	0	9174	1/1	0.30	13.93	62,62,62,62	0
35	NA	L	9180	1/1	0.48	13.30	51,51,51,51	0
35	NA	0	9135	1/1	0.35	13.23	52,52,52,52	0
35	NA	0	9182	1/1	0.55	12.89	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	9123	1/1	0.36	12.70	44,44,44,44	0
33	MG	0	8049	1/1	0.38	11.99	81,81,81,81	0
35	NA	0	9169	1/1	0.36	11.80	60,60,60,60	0
35	NA	0	9176	1/1	0.33	11.07	49,49,49,49	0
35	NA	0	9177	1/1	0.39	10.50	68,68,68,68	0
35	NA	0	9170	1/1	0.32	10.19	49,49,49,49	0
36	CL	0	9315	1/1	0.24	10.00	80,80,80,80	0
35	NA	0	9156	1/1	0.28	9.63	49,49,49,49	0
35	NA	0	9118	1/1	0.26	8.31	62,62,62,62	0
35	NA	0	9165	1/1	0.27	7.17	47,47,47,47	0
35	NA	0	9107	1/1	0.23	6.95	46,46,46,46	0
35	NA	0	9179	1/1	0.31	6.69	70,70,70,70	0
35	NA	0	9129	1/1	0.23	6.61	57,57,57,57	0
35	NA	0	9185	1/1	0.28	6.08	51,51,51,51	0
35	NA	0	9155	1/1	0.48	5.93	79,79,79,79	0
35	NA	0	9142	1/1	0.24	5.78	47,47,47,47	0
35	NA	0	9164	1/1	0.23	5.74	53,53,53,53	0
33	MG	Y	8109	1/1	0.30	4.61	44,44,44,44	0
35	NA	0	9103	1/1	0.23	4.50	43,43,43,43	0
33	MG	0	8060	1/1	0.20	4.47	46,46,46,46	0
33	MG	0	8041	1/1	0.22	4.28	79,79,79,79	0
35	NA	R	9186	1/1	0.35	4.11	78,78,78,78	0
35	NA	0	9110	1/1	0.33	3.97	43,43,43,43	0
33	MG	0	8080	1/1	0.19	3.76	41,41,41,41	0
33	MG	0	8113	1/1	0.19	3.67	52,52,52,52	0
35	NA	0	9125	1/1	0.20	3.33	59,59,59,59	0
33	MG	0	8011	1/1	0.19	3.24	20,20,20,20	0
36	CL	A	9309	1/1	0.28	3.22	61,61,61,61	0
35	NA	0	9105	1/1	0.24	3.19	44,44,44,44	0
33	MG	0	8023	1/1	0.22	2.96	52,52,52,52	0
35	NA	0	9153	1/1	0.24	2.89	21,21,21,21	0
35	NA	0	9181	1/1	0.26	2.85	56,56,56,56	0
35	NA	0	9173	1/1	0.20	2.79	62,62,62,62	0
36	CL	0	9316	1/1	0.31	2.51	66,66,66,66	0
33	MG	0	8053	1/1	0.19	2.41	57,57,57,57	0
35	NA	0	9150	1/1	0.21	2.26	42,42,42,42	0
35	NA	S	9112	1/1	0.27	2.14	73,73,73,73	0
35	NA	0	9131	1/1	0.18	2.12	41,41,41,41	0
36	CL	N	9307	1/1	0.32	2.08	72,72,72,72	0
33	MG	0	8090	1/1	0.27	2.02	65,65,65,65	0
33	MG	0	8063	1/1	0.19	1.92	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	9172	1/1	0.23	1.88	62,62,62,62	0
33	MG	0	8005	1/1	0.20	1.85	36,36,36,36	0
35	NA	0	9163	1/1	0.20	1.80	65,65,65,65	0
35	NA	0	9161	1/1	0.20	1.66	56,56,56,56	0
36	CL	0	9312	1/1	0.27	1.55	59,59,59,59	0
33	MG	0	8103	1/1	0.27	1.38	65,65,65,65	0
36	CL	O	9308	1/1	0.25	1.37	79,79,79,79	0
35	NA	0	9159	1/1	0.21	1.31	50,50,50,50	0
33	MG	0	8072	1/1	0.21	1.27	60,60,60,60	0
33	MG	0	8028	1/1	0.17	1.12	41,41,41,41	0
33	MG	0	8099	1/1	0.18	1.09	53,53,53,53	0
35	NA	0	9124	1/1	0.20	1.03	66,66,66,66	0
35	NA	0	9114	1/1	0.20	0.99	64,64,64,64	0
33	MG	0	8075	1/1	0.16	0.98	57,57,57,57	0
35	NA	0	9171	1/1	0.20	0.91	52,52,52,52	0
35	NA	0	9111	1/1	0.22	0.81	61,61,61,61	0
34	K	0	9003	1/1	0.19	0.76	64,64,64,64	0
36	CL	B	9319	1/1	0.23	0.51	55,55,55,55	0
33	MG	0	8116	1/1	0.19	0.44	62,62,62,62	0
33	MG	0	8093	1/1	0.19	0.27	66,66,66,66	0
36	CL	L	9310	1/1	0.19	0.23	63,63,63,63	0
35	NA	0	9101	1/1	0.21	0.11	40,40,40,40	0
35	NA	0	9143	1/1	0.18	0.10	33,33,33,33	0
33	MG	0	8032	1/1	0.18	0.08	41,41,41,41	0
35	NA	0	9126	1/1	0.17	0.01	41,41,41,41	0
35	NA	H	9122	1/1	0.18	-0.06	72,72,72,72	0
35	NA	0	9102	1/1	0.21	-0.13	45,45,45,45	0
33	MG	0	8071	1/1	0.17	-0.20	66,66,66,66	0
35	NA	A	9145	1/1	0.19	-0.20	48,48,48,48	0
36	CL	J	9301	1/1	0.21	-0.22	78,78,78,78	0
35	NA	0	9127	1/1	0.15	-0.26	42,42,42,42	0
35	NA	0	9117	1/1	0.26	-0.52	61,61,61,61	0
33	MG	0	8045	1/1	0.19	-0.56	73,73,73,73	0
35	NA	R	9137	1/1	0.18	-0.63	44,44,44,44	0
35	NA	0	9133	1/1	0.13	-0.68	34,34,34,34	0
35	NA	0	9157	1/1	0.11	-0.73	73,73,73,73	0
35	NA	0	9166	1/1	0.13	-0.73	69,69,69,69	0
36	CL	0	9311	1/1	0.15	-0.76	53,53,53,53	0
33	MG	0	8013	1/1	0.18	-0.79	33,33,33,33	0
33	MG	0	8017	1/1	0.14	-0.80	29,29,29,29	0
35	NA	0	9140	1/1	0.20	-0.84	47,47,47,47	0
36	CL	J	9321	1/1	0.17	-0.91	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	9134	1/1	0.12	-0.92	41,41,41,41	0
36	CL	J	9302	1/1	0.19	-0.94	79,79,79,79	0
33	MG	0	8058	1/1	0.16	-0.94	56,56,56,56	0
33	MG	0	8021	1/1	0.15	-1.04	32,32,32,32	0
33	MG	0	8047	1/1	0.16	-1.06	86,86,86,86	0
33	MG	0	8086	1/1	0.11	-1.12	50,50,50,50	0
37	CD	Z	9203	1/1	0.08	-1.14	67,67,67,67	0
35	NA	Q	9148	1/1	0.16	-1.18	38,38,38,38	0
35	NA	0	9116	1/1	0.14	-1.18	42,42,42,42	0
33	MG	0	8104	1/1	0.16	-1.29	55,55,55,55	0
33	MG	0	8038	1/1	0.16	-1.34	32,32,32,32	0
33	MG	0	8030	1/1	0.15	-1.35	35,35,35,35	0
33	MG	0	8018	1/1	0.14	-1.40	42,42,42,42	0
36	CL	M	9318	1/1	0.14	-1.43	47,47,47,47	0
33	MG	0	8081	1/1	0.14	-1.43	52,52,52,52	0
35	NA	R	9138	1/1	0.15	-1.63	63,63,63,63	0
33	MG	0	8096	1/1	0.13	-1.66	53,53,53,53	0
33	MG	0	8057	1/1	0.14	-1.66	42,42,42,42	0
33	MG	0	8119	1/1	0.19	-1.67	62,62,62,62	0
33	MG	0	8050	1/1	0.13	-1.68	69,69,69,69	0
33	MG	A	8065	1/1	0.14	-1.69	45,45,45,45	0
37	CD	3	9204	1/1	0.05	-1.73	64,64,64,64	0
35	NA	C	9104	1/1	0.11	-1.76	40,40,40,40	0
33	MG	B	8055	1/1	0.17	-1.76	62,62,62,62	0
33	MG	0	8064	1/1	0.14	-1.77	30,30,30,30	0
33	MG	0	8106	1/1	0.07	-1.77	54,54,54,54	0
35	NA	0	9130	1/1	0.09	-1.80	45,45,45,45	0
34	K	0	9001	1/1	0.15	-1.87	71,71,71,71	0
35	NA	9	9151	1/1	0.10	-1.88	64,64,64,64	0
33	MG	T	8073	1/1	0.12	-1.91	59,59,59,59	0
33	MG	0	8002	1/1	0.14	-1.92	39,39,39,39	0
35	NA	0	9149	1/1	0.16	-1.93	38,38,38,38	0
33	MG	0	8019	1/1	0.13	-1.95	35,35,35,35	0
36	CL	0	9314	1/1	0.11	-1.98	49,49,49,49	0
33	MG	0	8031	1/1	0.13	-2.07	30,30,30,30	0
36	CL	R	9306	1/1	0.09	-2.10	57,57,57,57	0
35	NA	0	9144	1/1	0.13	-2.12	33,33,33,33	0
36	CL	0	9313	1/1	0.14	-2.18	60,60,60,60	0
35	NA	0	9119	1/1	0.09	-2.19	44,44,44,44	0
33	MG	0	8035	1/1	0.10	-2.20	49,49,49,49	0
36	CL	0	9305	1/1	0.11	-2.22	55,55,55,55	0
35	NA	0	9141	1/1	0.09	-2.24	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8117	1/1	0.14	-2.25	37,37,37,37	0
33	MG	0	8034	1/1	0.13	-2.36	38,38,38,38	0
33	MG	3	8078	1/1	0.10	-2.37	43,43,43,43	0
33	MG	0	8012	1/1	0.13	-2.42	32,32,32,32	0
35	NA	0	9128	1/1	0.09	-2.48	43,43,43,43	0
35	NA	0	9115	1/1	0.14	-2.49	37,37,37,37	0
36	CL	0	9317	1/1	0.09	-2.50	61,61,61,61	0
33	MG	A	8066	1/1	0.06	-2.50	66,66,66,66	0
35	NA	H	9109	1/1	0.12	-2.58	34,34,34,34	0
33	MG	0	8024	1/1	0.13	-2.76	39,39,39,39	0
33	MG	0	8070	1/1	0.10	-2.82	57,57,57,57	0
33	MG	0	8107	1/1	0.11	-2.85	53,53,53,53	0
37	CD	O	9205	1/1	0.04	-2.87	143,143,143,143	0
37	CD	1	9202	1/1	0.07	-2.90	62,62,62,62	0
33	MG	0	8074	1/1	0.07	-2.95	37,37,37,37	0
33	MG	0	8067	1/1	0.14	-2.97	49,49,49,49	0
36	CL	0	9322	1/1	0.18	-3.05	77,77,77,77	0
33	MG	0	8015	1/1	0.11	-3.06	33,33,33,33	0
33	MG	0	8037	1/1	0.11	-3.11	45,45,45,45	0
33	MG	0	8033	1/1	0.10	-3.17	38,38,38,38	0
36	CL	3	9304	1/1	0.12	-3.17	61,61,61,61	0
33	MG	0	8040	1/1	0.13	-3.24	56,56,56,56	0
35	NA	J	9146	1/1	0.06	-3.26	42,42,42,42	0
34	K	0	9002	1/1	0.11	-3.27	48,48,48,48	0
37	CD	U	9201	1/1	0.10	-3.30	74,74,74,74	0
33	MG	0	8020	1/1	0.13	-3.36	31,31,31,31	0
33	MG	0	8001	1/1	0.12	-3.38	35,35,35,35	0
33	MG	0	8108	1/1	0.09	-3.42	58,58,58,58	0
33	MG	0	8044	1/1	0.12	-3.44	55,55,55,55	0
33	MG	B	8056	1/1	0.11	-3.47	47,47,47,47	0
33	MG	4	8118	1/1	0.13	-3.60	41,41,41,41	0
33	MG	0	8085	1/1	0.16	-3.60	72,72,72,72	0
35	NA	M	9147	1/1	0.10	-3.61	25,25,25,25	0
33	MG	0	8102	1/1	0.08	-3.62	58,58,58,58	0
33	MG	0	8094	1/1	0.11	-3.64	73,73,73,73	0
35	NA	9	9183	1/1	0.12	-3.81	60,60,60,60	0
33	MG	0	8003	1/1	0.15	-3.86	31,31,31,31	0
33	MG	0	8027	1/1	0.07	-3.86	37,37,37,37	0
33	MG	0	8061	1/1	0.08	-3.97	37,37,37,37	0
33	MG	9	8095	1/1	0.10	-3.97	77,77,77,77	0
35	NA	0	9139	1/1	0.15	-3.98	31,31,31,31	0
33	MG	0	8062	1/1	0.07	-4.05	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8112	1/1	0.05	-4.05	39,39,39,39	0
33	MG	0	8097	1/1	0.08	-4.26	40,40,40,40	0
33	MG	0	8098	1/1	0.09	-4.29	47,47,47,47	0
36	CL	0	9303	1/1	0.11	-4.30	53,53,53,53	0
33	MG	2	8076	1/1	0.13	-4.33	55,55,55,55	0
33	MG	0	8008	1/1	0.08	-4.39	37,37,37,37	0
33	MG	0	8039	1/1	0.06	-4.57	52,52,52,52	0
33	MG	0	8089	1/1	0.10	-4.58	56,56,56,56	0
33	MG	0	8042	1/1	0.06	-4.74	44,44,44,44	0
33	MG	0	8110	1/1	0.12	-4.97	32,32,32,32	0
33	MG	K	8069	1/1	0.07	-4.99	52,52,52,52	0
35	NA	0	9168	1/1	0.09	-5.01	49,49,49,49	0
35	NA	0	9108	1/1	0.09	-5.05	49,49,49,49	0
33	MG	0	8115	1/1	0.08	-5.14	57,57,57,57	0
33	MG	9	8052	1/1	0.12	-5.21	54,54,54,54	0
33	MG	0	8088	1/1	0.12	-5.24	38,38,38,38	0
33	MG	0	8084	1/1	0.13	-5.30	38,38,38,38	0
33	MG	0	8043	1/1	0.10	-5.49	47,47,47,47	0
33	MG	0	8007	1/1	0.11	-5.55	27,27,27,27	0
33	MG	0	8010	1/1	0.10	-5.75	28,28,28,28	0
33	MG	0	8054	1/1	0.09	-5.84	29,29,29,29	0
35	NA	0	9154	1/1	0.10	-5.91	33,33,33,33	0
33	MG	0	8059	1/1	0.14	-5.95	51,51,51,51	0
33	MG	0	8079	1/1	0.10	-6.02	29,29,29,29	0
33	MG	0	8014	1/1	0.06	-6.05	43,43,43,43	0
33	MG	0	8009	1/1	0.13	-6.12	30,30,30,30	0
33	MG	0	8051	1/1	0.08	-6.14	72,72,72,72	0
35	NA	0	9132	1/1	0.04	-6.29	34,34,34,34	0
33	MG	0	8091	1/1	0.07	-6.73	79,79,79,79	0
33	MG	0	8077	1/1	0.09	-6.83	28,28,28,28	0
33	MG	0	8068	1/1	0.07	-7.04	60,60,60,60	0
33	MG	0	8026	1/1	0.09	-7.07	24,24,24,24	0
33	MG	0	8006	1/1	0.09	-7.26	37,37,37,37	0
35	NA	0	9167	1/1	0.06	-7.55	52,52,52,52	0
33	MG	0	8048	1/1	0.05	-7.64	56,56,56,56	0
33	MG	0	8083	1/1	0.08	-7.73	42,42,42,42	0
33	MG	0	8029	1/1	0.06	-7.76	36,36,36,36	0
36	CL	Y	9320	1/1	0.10	-7.83	52,52,52,52	0
33	MG	0	8022	1/1	0.09	-8.37	35,35,35,35	0
33	MG	0	8114	1/1	0.07	-8.55	56,56,56,56	0
33	MG	0	8025	1/1	0.13	-8.69	46,46,46,46	0
33	MG	0	8046	1/1	0.09	-9.90	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8004	1/1	0.09	-10.96	34,34,34,34	0
33	MG	0	8111	1/1	0.09	-12.95	52,52,52,52	0
35	NA	0	9136	1/1	0.08	-13.69	55,55,55,55	0
33	MG	0	8082	1/1	0.15	-14.00	76,76,76,76	0
33	MG	0	8036	1/1	0.12	-19.08	35,35,35,35	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.