



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2020 – 06:47 PM EDT

PDB ID : 1VQM
Title : The structure of the transition state analogue "DAN" bound to the large ribosomal subunit of haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.4
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4

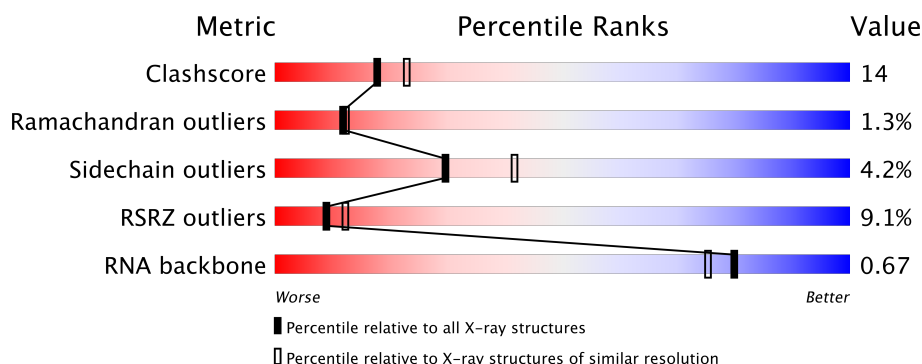
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)
RNA backbone	3102	1090 (2.70-1.90)

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

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>25%</div> <div>5%</div> <div>6%</div> </div> </div>
2	9	122	<div> <div>4%</div> <div> <div></div> <div>61%</div> <div>29%</div> <div>10%</div> <div>.</div> </div> </div>
3	4	7	<div> <div></div> <div> <div></div> <div>57%</div> <div>29%</div> <div>14%</div> </div> </div>
4	A	240	<div> <div>8%</div> <div> <div></div> <div>59%</div> <div>36%</div> <div>.</div> <div>.</div> </div> </div>
5	B	338	<div> <div>4%</div> <div> <div></div> <div>56%</div> <div>41%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
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	
15	M	195	
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	

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Mol	Chain	Length	Quality of chain
31	3	92	
32	I	162	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	MG	0	8014	-	-	-	X
33	MG	0	8022	-	-	-	X
33	MG	0	8040	-	-	-	X
33	MG	0	8047	-	-	-	X
33	MG	0	8052	-	-	-	X
33	MG	0	8065	-	-	-	X
33	MG	0	8094	-	-	-	X
35	NA	0	9140	-	-	-	X
35	NA	0	9179	-	-	-	X
35	NA	0	9185	-	-	-	X
37	SR	0	9500	-	-	-	X

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99045 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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'-R(*CP*CP*(PPU)P*(PO2)P*(DA)P*C*C')-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	7	Total	C	N	O	P	0	0	0
			135	68	24	38	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	87	Total	Mg	0	0
			87	87		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	A	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	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	2	Total	K	0	0
			2	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	62	Total 62	Na 62	0	0
35	J	1	Total 1	Na 1	0	0
35	Q	1	Total 1	Na 1	0	0
35	H	1	Total 1	Na 1	0	0
35	C	1	Total 1	Na 1	0	0
35	3	1	Total 1	Na 1	0	0
35	R	3	Total 3	Na 3	0	0
35	9	3	Total 3	Na 3	0	0
35	S	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	M	1	Total	Cl	0	0
			1	1		

- Molecule 37 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	98	Total	Sr	0	0
			98	98		
37	1	2	Total	Sr	0	0
			2	2		
37	H	1	Total	Sr	0	0
			1	1		
37	B	2	Total	Sr	0	0
			2	2		
37	3	1	Total	Sr	0	0
			1	1		
37	A	3	Total	Sr	0	0
			3	3		
37	R	1	Total	Sr	0	0
			1	1		
37	9	3	Total	Sr	0	0
			3	3		
37	L	1	Total	Sr	0	0
			1	1		
37	S	1	Total	Sr	0	0
			1	1		
37	F	1	Total	Sr	0	0
			1	1		

- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	1	Total	Cd	0	0
			1	1		
38	Z	1	Total	Cd	0	0
			1	1		
38	1	1	Total	Cd	0	0
			1	1		
38	3	1	Total	Cd	0	0
			1	1		
38	U	1	Total	Cd	0	0
			1	1		

- Molecule 39 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	0	5739	Total O 5739 5739	0	0
39	9	132	Total O 132 132	0	0
39	4	8	Total O 8 8	0	0
39	A	123	Total O 123 123	0	0
39	B	139	Total O 139 139	0	0
39	C	177	Total O 177 177	0	0
39	D	50	Total O 50 50	0	0
39	E	43	Total O 43 43	0	0
39	F	28	Total O 28 28	0	0
39	G	16	Total O 16 16	0	0
39	H	71	Total O 71 71	0	0
39	J	53	Total O 53 53	0	0
39	K	57	Total O 57 57	0	0
39	L	82	Total O 82 82	0	0
39	M	125	Total O 125 125	0	0
39	N	59	Total O 59 59	0	0
39	O	35	Total O 35 35	0	0
39	P	59	Total O 59 59	0	0
39	Q	48	Total O 48 48	0	0
39	R	86	Total O 86 86	0	0
39	S	31	Total O 31 31	0	0

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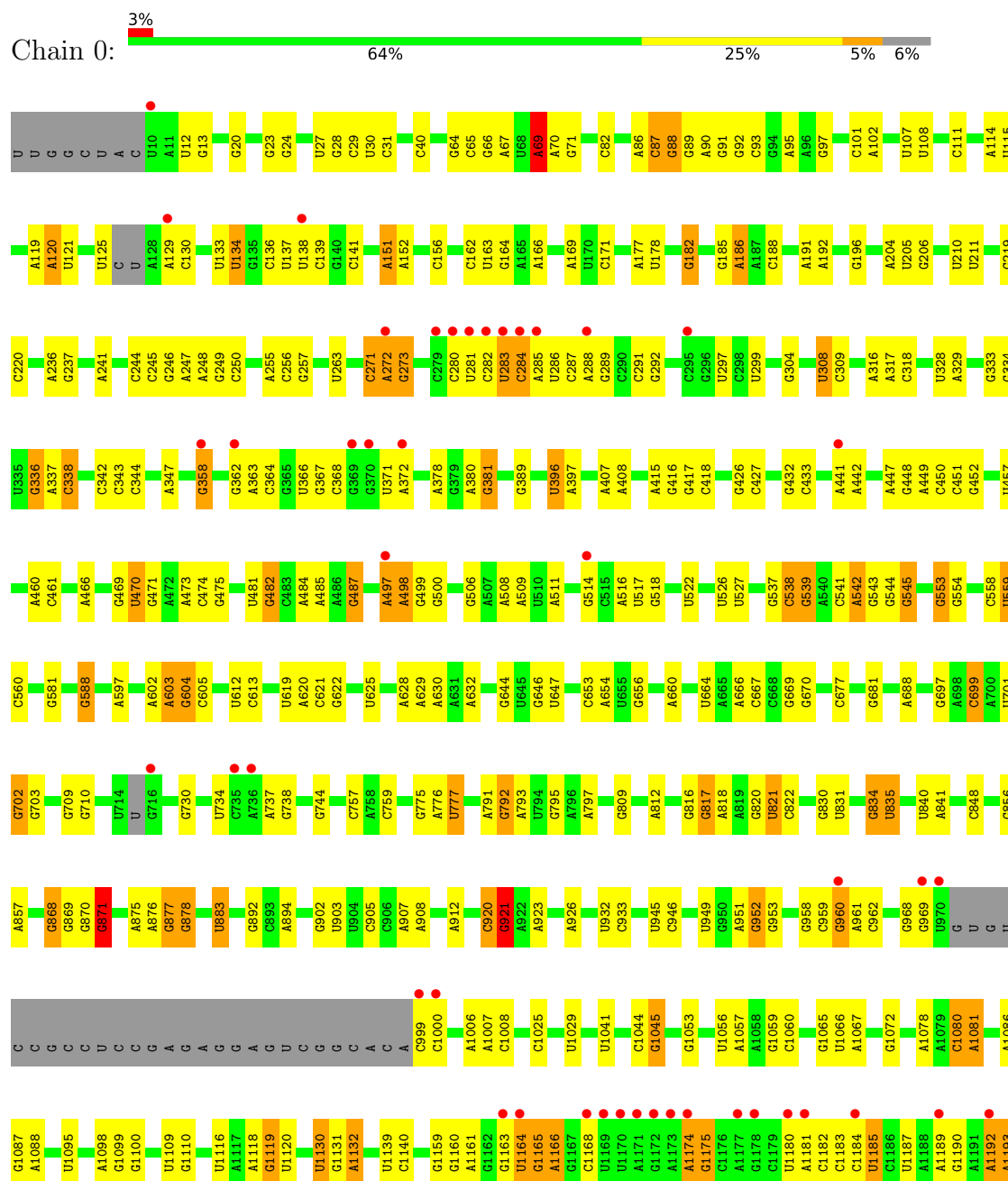
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	T	36	Total 36	O 36	0	0
39	U	26	Total 26	O 26	0	0
39	V	11	Total 11	O 11	0	0
39	W	68	Total 68	O 68	0	0
39	X	23	Total 23	O 23	0	0
39	Y	93	Total 93	O 93	0	0
39	Z	28	Total 28	O 28	0	0
39	1	51	Total 51	O 51	0	0
39	2	41	Total 41	O 41	0	0
39	3	67	Total 67	O 67	0	0
39	I	9	Total 9	O 9	0	0

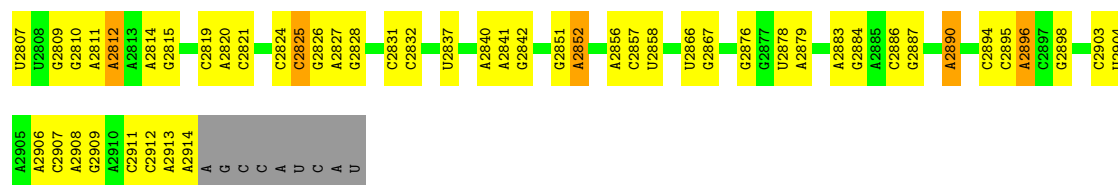
3 Residue-property plots

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

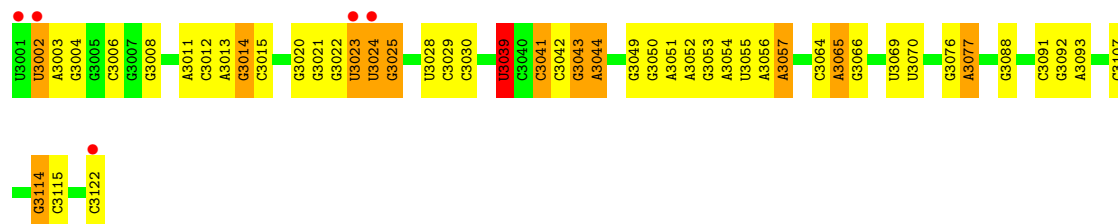
- Molecule 1: 23S ribosomal rna



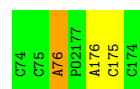
C9682	U2686	G2480	A2354	C	A	A2089	C	U1838	A1716	G1592	G1415	A1294	C1196
U2690	U2587	G2481	G2355	C	C	G2090	C	A1839	A1717	C1593	G1418	A1298	G1197
A2694	G2588	G2482	A2356	A	A	G2091	C	A1840	U1722	C1594	U1418	U1298	U1198
G2698	U2589	G2483	G2357	G	G	A2096	C	A1845	G1723	G1595	U1419	G1299	A1200
A2699	G2590	G2484	A2361	U	U	A2101	C	A1846	U1724	U1596	U1422	U1304	C1201
G2700	G2591	G2485	A2362	A	A	A2102	C	A1847	C1725	A1597	C1423	C1305	A1202
G2712	G2592	G2486	G2363	C	C	A2103	C	A1848	G1730	A1598	U1426	G1311	G1203
G2716	U2597	G2487	A2364	C	C	A2104	C	G1849	C1731	C1602	U1426	U1314	C1204
C2717	U2598	G2488	G2365	C	C	A2105	C	C1853	A1732	A1603	U1435	G1315	U1205
A2718	A2500	G2489	A2366	C	C	G2110	C	C1856	A1736	G1604	U1435	U1316	U1206
A2719	A2501	G2490	A2367	C	C	G2111	C	G1863	U1741	A1615	G1441	G1325	A1207
C2720	A2502	G2491	A2368	U	U	G2112	C	U1867	U1745	A1616	A1442	G1326	C1208
U2721	A2503	G2492	A2369	C	C	G2113	C	G1868	G1755	C1617	U1452	U1327	G1211
G2722	A2504	G2493	A2370	C	C	G2114	C	U1869	U1756	A1624	C1456	A1328	C1212
G2723	A2505	G2494	A2371	C	C	G2115	C	G1870	G1757	U1625	U1457	U1331	G1216
U2724	A2506	G2495	A2372	C	C	G2116	C	U1871	A1758	G1627	A1458	U1332	G1217
G2725	A2507	G2496	A2373	U	U	U2116	C	G1872	A1759	U1628	U1459	U1333	U1218
U2726	A2508	G2497	A2374	C	C	G2117	C	U1873	G1766	A1630	C1462	C1334	U1219
U2727	A2509	G2498	A2375	C	C	G2118	C	G1874	U1771	A1631	A1463	C1335	G1226
G2728	A2510	G2499	A2376	C	C	G2119	C	U1875	C1772	A1641	C1466	U1336	C1229
G2729	A2511	G2500	A2377	C	C	G2120	C	G1876	U1773	A1642	C1474	G1340	A1230
U2730	A2512	G2501	A2378	C	C	G2121	C	U1877	G1777	U1654	C1475	A1341	A1231
U2731	A2513	G2502	A2379	C	C	G2122	C	G1878	U1778	G1655	U1476	C1342	A1232
U2732	A2514	G2503	A2380	C	C	G2123	C	U1879	C1779	A1656	U1477	C1343	A1233
U2733	A2515	G2504	A2381	C	C	G2124	C	G1880	U1780	A1657	U1478	U1234	G1235
U2734	A2516	G2505	A2382	C	C	G2125	C	U1881	U1781	A1658	C1496	U1236	U1237
U2735	A2517	G2506	A2383	C	C	G2126	C	G1882	C1782	U1666	U1503	C1238	G1239
U2736	A2518	G2507	A2384	C	C	G2127	C	U1883	U1783	U1667	U1504	C1361	A1242
U2737	A2519	G2508	A2385	C	C	G2128	C	G1884	U1784	U1668	U1505	G1362	C1243
U2738	A2520	G2509	A2386	C	C	G2129	C	U1885	U1785	U1669	U1506	C1363	U1244
U2739	A2521	G2510	A2387	C	C	G2130	C	G1886	U1786	U1670	U1507	C1364	A1245
U2740	A2522	G2511	A2388	C	C	G2131	C	U1887	U1787	U1671	U1508	U1246	U1249
U2741	A2523	G2512	A2389	C	C	G2132	C	G1888	U1788	U1672	U1509	A1372	C1250
U2742	A2524	G2513	A2390	C	C	G2133	C	U1889	U1789	U1673	U1510	C1373	C1251
U2743	A2525	G2514	A2391	C	C	G2134	C	G1890	U1790	U1674	U1511	C1374	C1252
U2744	A2526	G2515	A2392	C	C	G2135	C	U1891	U1791	U1675	U1512	C1375	C1253
U2745	A2527	G2516	A2393	C	C	G2136	C	G1892	U1792	U1676	U1513	C1376	C1254
U2746	A2528	G2517	A2394	C	C	G2137	C	U1893	U1793	U1677	U1514	C1377	C1255
U2747	A2529	G2518	A2395	C	C	G2138	C	G1894	U1794	U1678	U1515	C1378	C1256
U2748	A2530	G2519	A2396	C	C	G2139	C	U1895	U1795	U1679	U1516	C1379	C1257
U2749	A2531	G2520	A2397	C	C	G2140	C	G1896	U1796	U1680	U1517	C1380	C1258
U2750	A2532	G2521	A2398	C	C	G2141	C	U1897	U1797	U1681	U1518	C1381	C1259
U2751	A2533	G2522	A2399	C	C	G2142	C	G1898	U1798	U1682	U1519	C1382	C1260
U2752	A2534	G2523	A2400	C	C	G2143	C	U1899	U1799	U1683	U1520	C1383	C1261
U2753	A2535	G2524	A2401	C	C	G2144	C	G1900	U1800	U1684	U1521	C1384	C1262
U2754	A2536	G2525	A2402	C	C	G2145	C	U1901	U1801	U1685	U1522	C1385	C1263
U2755	A2537	G2526	A2403	C	C	G2146	C	G1902	U1802	U1686	U1523	C1386	C1264
U2756	A2538	G2527	A2404	C	C	G2147	C	U1903	U1803	U1687	U1524	C1387	C1265
U2757	A2539	G2528	A2405	C	C	G2148	C	G1904	U1804	U1688	U1525	C1388	C1266
U2758	A2540	G2529	A2406	C	C	G2149	C	U1905	U1805	U1689	U1526	C1389	C1267
U2759	A2541	G2530	A2407	C	C	G2150	C	G1906	U1806	U1690	U1527	C1390	C1268
U2760	A2542	G2531	A2408	C	C	G2151	C	U1907	U1807	U1691	U1528	C1391	C1269
U2761	A2543	G2532	A2409	C	C	G2152	C	G1908	U1808	U1692	U1529	C1392	C1270
U2762	A2544	G2533	A2410	C	C	G2153	C	U1909	U1809	U1693	U1530	C1393	C1271
U2763	A2545	G2534	A2411	C	C	G2154	C	G1910	U1810	U1694	U1531	C1394	C1272
U2764	A2546	G2535	A2412	C	C	G2155	C	U1911	U1811	U1695	U1532	C1395	C1273
U2765	A2547	G2536	A2413	C	C	G2156	C	G1912	U1812	U1696	U1533	C1396	C1274
U2766	A2548	G2537	A2414	C	C	G2157	C	U1913	U1813	U1697	U1534	C1397	C1275
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U2768	A2550	G2539	A2416	C	C	G2159	C	U1915	U1815	U1699	U1536	C1399	C1277
U2769	A2551	G2540	A2417	C	C	G2160	C	G1916	U1816	U1700	U1537	C1400	C1278
U2770	A2552	G2541	A2418	C	C	G2161	C	U1917	U1817	U1701	U1538	C1401	C1279
U2771	A2553	G2542	A2419	C	C	G2162	C	G1918	U1818	U1702	U1539	C1402	C1280
U2772	A2554	G2543	A2420	C	C	G2163	C	U1919	U1819	U1703	U1540	C1403	C1281
U2773	A2555	G2544	A2421	C	C	G2164	C	G1920	U1820	U1704	U1541	C1404	C1282
U2774	A2556	G2545	A2422	C	C	G2165	C	U1921	U1821	U1705	U1542	C1405	C1283
U2775	A2557	G2546	A2423	C	C	G2166	C	G1922	U1822	U1706	U1543	C1406	C1284
U2776	A2558	G2547	A2424	C	C	G2167	C	U1923	U1823	U1707	U1544	C1407	C1285
U2777	A2559	G2548	A2425	C	C	G2168	C	G1924	U1824	U1708	U1545	C1408	C1286
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U2780	A2562	G2551	A2428	C	C	G2171	C	U1927	U1827	U1711	U1548	C1411	C1289
U2781	A2563	G2552	A2429	C	C	G2172	C	G1928	U1828	U1712	U1549	C1412	C1290
U2782	A2564	G2553	A2430	C	C	G2173	C	U1929	U1829	U1713	U1550	C1413	C1291
U2783	A2565	G2554	A2431	C	C	G2174	C	G1930	U1830	U1714	U1551	C1414	C1292
U2784	A2566	G2555	A2432	C	C	G2175	C	U1931	U1831	U1715	U1552	C1415	C1293
U2785	A2567	G2556	A2433	C	C	G2176	C	G1932	U1832	U1716	U1553	C1416	C1294
U2786	A2568	G2557	A2434	C	C	G2177	C	U1933	U1833	U1717	U1554	C1417	C1295
U2787	A2569	G2558	A2435	C	C	G2178	C	G1934	U1834	U1718	U1555	C1418	C1296
U2788	A2570	G2559	A2436	C	C	G2179	C	U1935	U1835	U1719	U1556	C1419	C1297
U2789	A2571	G2560	A2437	C	C	G2180	C	G1936	U1836	U1720	U1557	C1420	C1298
U2790	A2572	G2561	A2438	C	C	G2181	C	U1937	U1837	U1721	U1558	C1421	C1299
U2791	A2573	G2562	A2439	C	C	G2182	C	G1938	U1838	U1722	U1559	C1422	C1300
U2792	A2574	G2563	A2440	C	C	G2183	C	U1939	U1839	U1723	U1560	C1423	C1301
U2793	A2575	G2564	A2441	C	C	G2184	C	G1940	U1840	U1724	U1561	C1424	C1302
U2794	A2576	G2565	A2442	C	C	G2185	C	U1941	U1841	U1725	U1562	C1425	C1303
U2795	A2577	G2566	A2443	C	C	G2186	C	G1942	U1842	U1726	U1563	C1426	C1304
U2796	A2578	G2567	A2444	C	C	G2187	C	U1943	U1843	U1727	U1564	C1427	C1305
U2797	A2579	G2568	A2445	C	C	G2188	C	G1944	U1844	U1728	U1565	C1428	C1306
U2798	A2580	G2569	A2446	C	C	G2189	C	U1945	U1845	U1729	U1566	C1429	C1307
U2799	A2581	G2570	A2447	C	C	G2190	C	G1946	U1846	U1730	U1567	C1430	C1308
U2800	A2582	G2571	A2448	C	C	G2191	C	U1947	U1847	U1731	U1568	C1431	C1309
U2801	A2583	G2572	A2449	C	C	G2192	C	G1948	U1848	U1732	U1569	C1432	C1310
U2802	A2584	G2573	A2450	C	C	G2193	C	U1949	U1849	U1733	U1570	C1433	C1311
U2803	A2585	G2574	A2451	C	C	G2194	C	G1950	U1850	U1734	U1571	C1434	C1312
U2804	A2586	G2575	A2452	C	C	G2195	C	U1951	U1851	U1735	U1572	C1435	C1313
U2805	A2587	G2576	A2453	C	C	G2196	C	G1952	U1852	U1736	U1573	C1436	C1314
U2806	A2588	G2577	A2454	C	C	G2197	C	U1953	U1853	U1737	U1574	C1437	C1315
U2807	A2589	G2578	A2455	C	C	G2198	C	G1954	U1854	U1738			



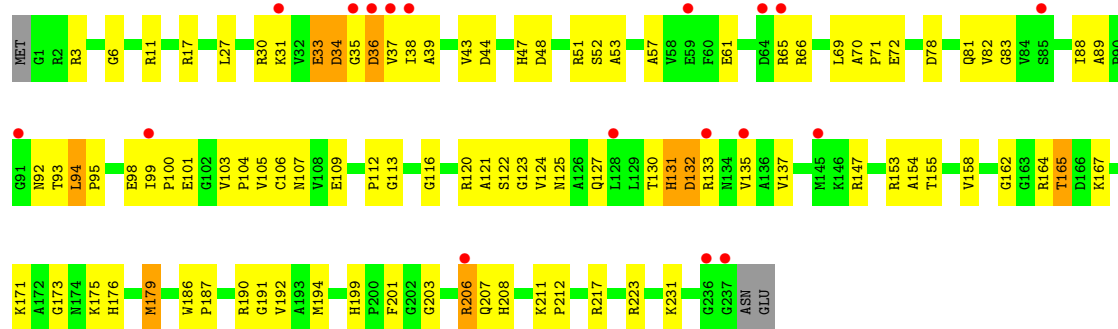
• Molecule 2: 5S ribosomal RNA



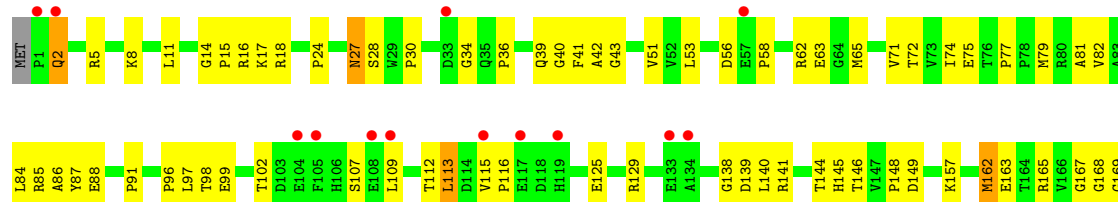
• Molecule 3: 5'-R(*CP*CP*(PPU)P*(PO2)P*(DA)P*C*C)-3'

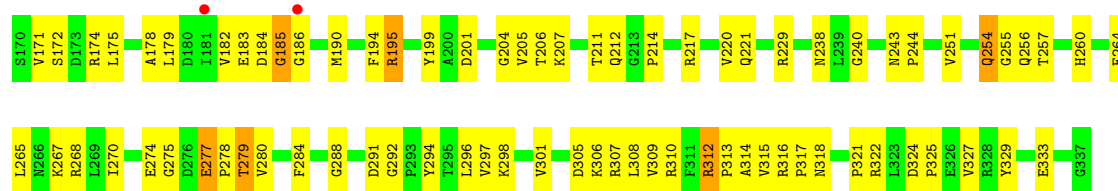


• Molecule 4: 50S ribosomal protein L2P

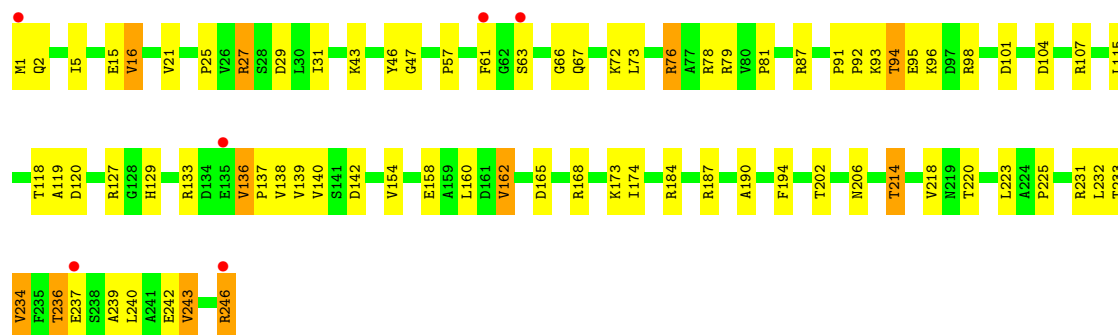


• Molecule 5: 50S ribosomal protein L3P

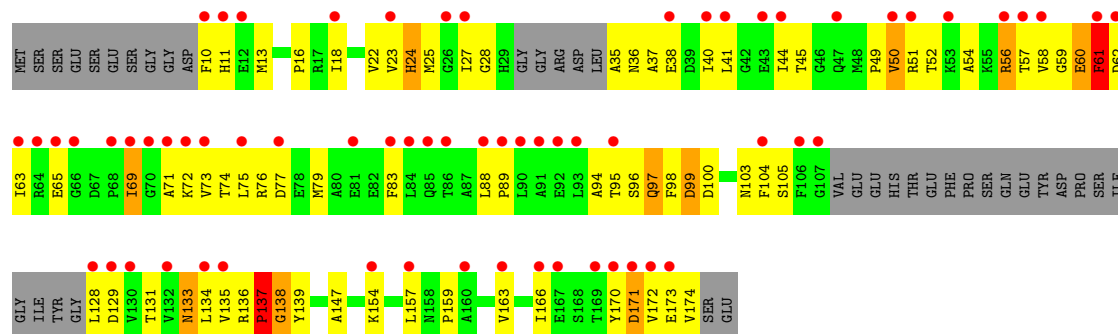




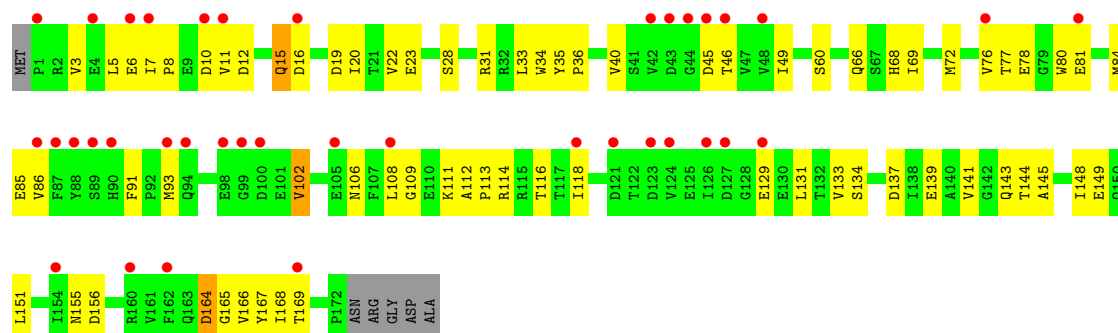
• Molecule 6: 50S ribosomal protein L4E



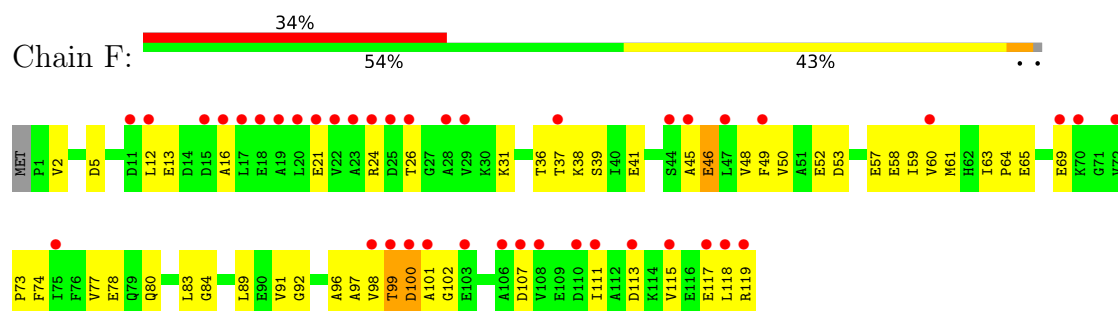
• Molecule 7: 50S ribosomal protein L5P



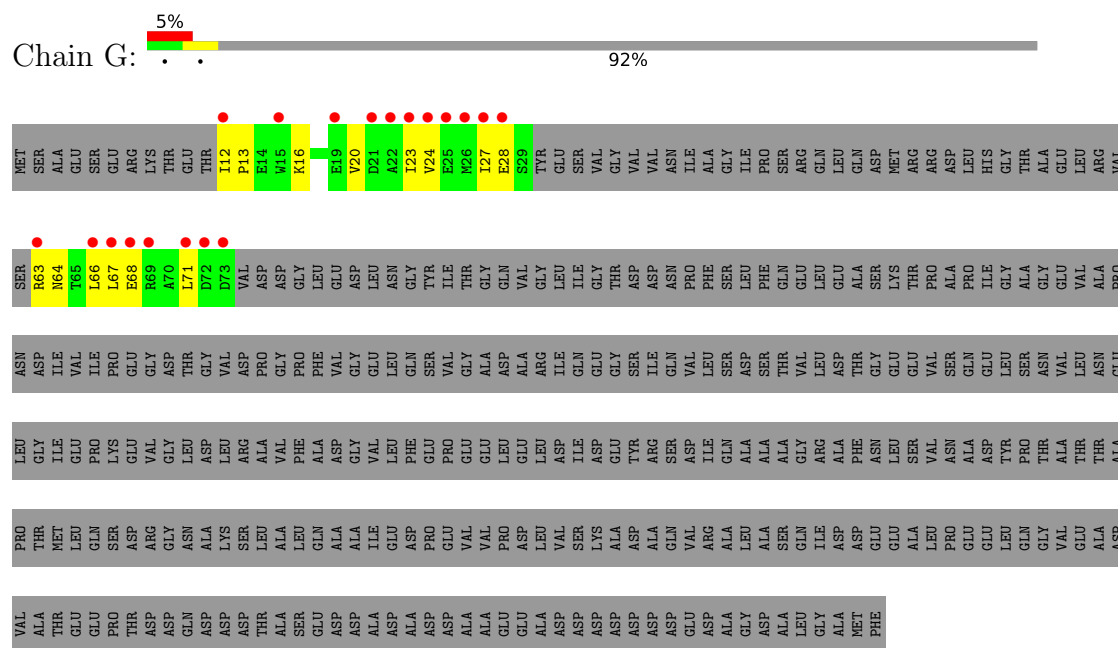
• Molecule 8: 50S ribosomal protein L6P



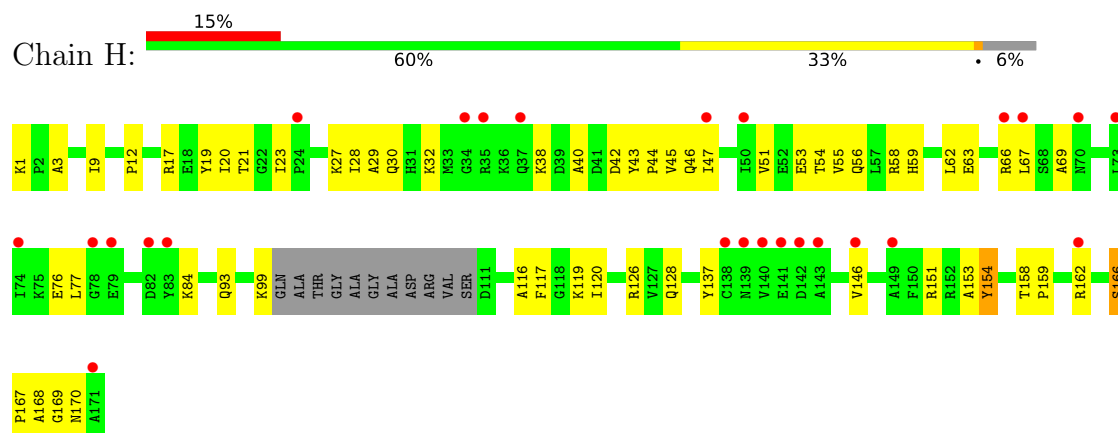
- Molecule 9: 50S ribosomal protein L7AE

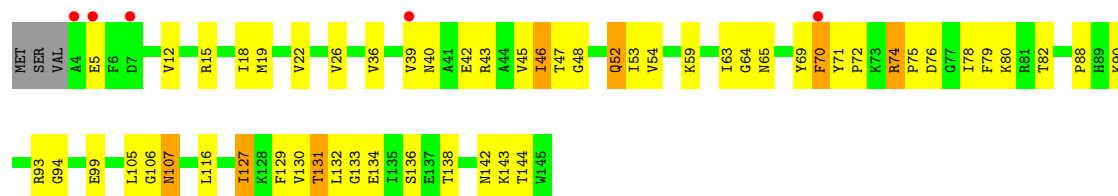


- Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

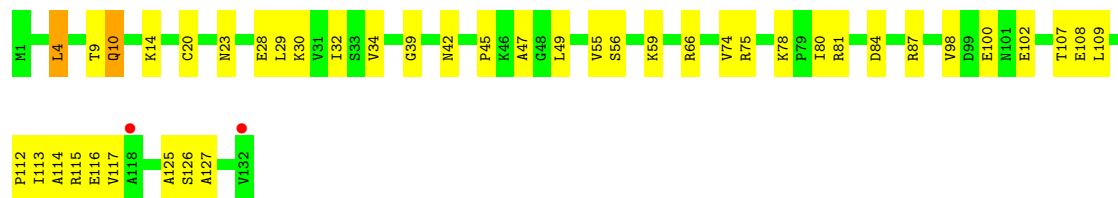


- Molecule 11: 50S RIBOSOMAL PROTEIN L10E

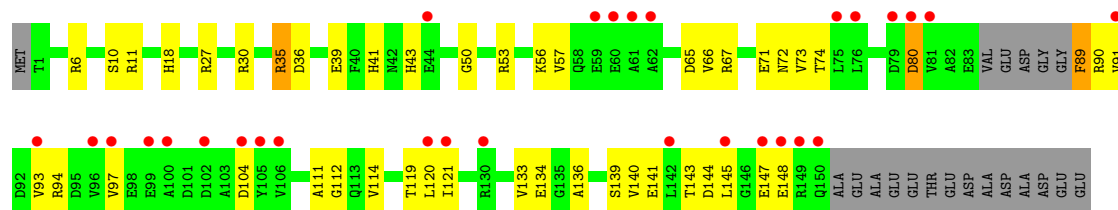




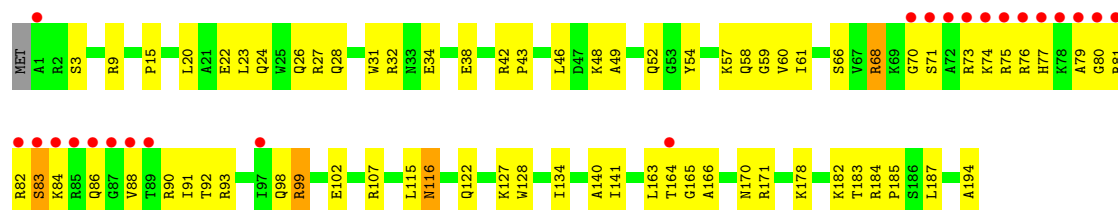
• Molecule 13: 50S ribosomal protein L14P



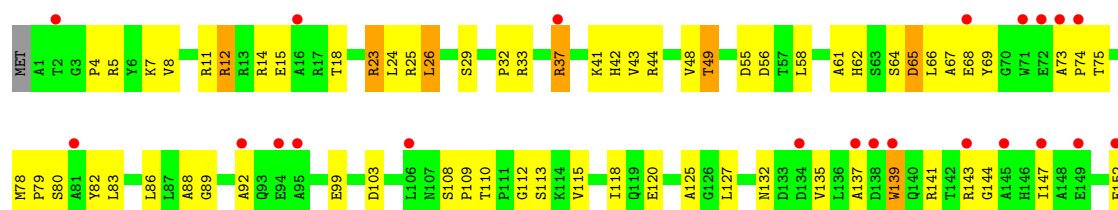
• Molecule 14: 50S ribosomal protein L15P

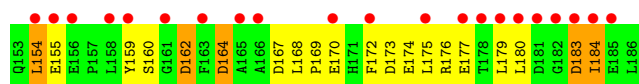


• Molecule 15: 50S Ribosomal Protein L15E



• Molecule 16: 50S ribosomal protein L18P

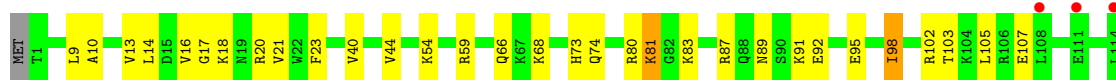




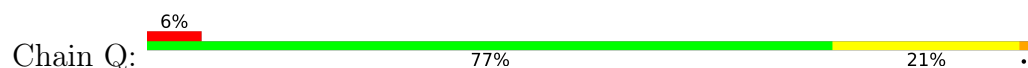
- Molecule 17: 50S ribosomal protein L18e



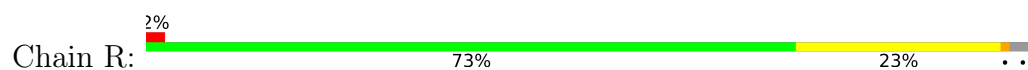
- Molecule 18: 50S ribosomal protein L19E



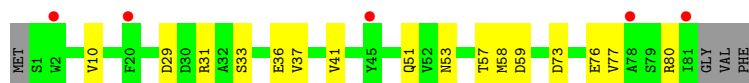
- Molecule 19: 50S ribosomal protein L21e



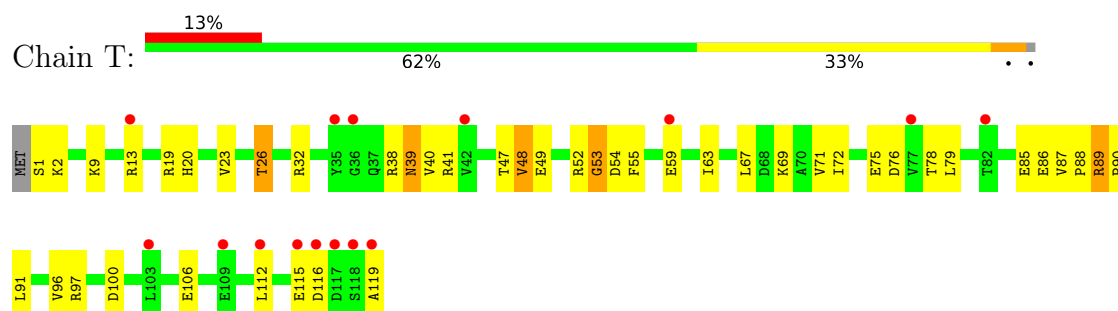
- Molecule 20: 50S ribosomal protein L22P



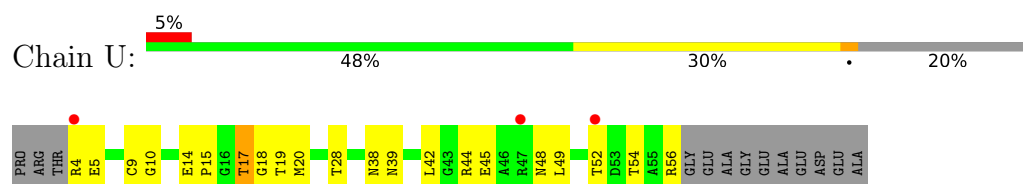
- Molecule 21: 50S ribosomal protein L23P



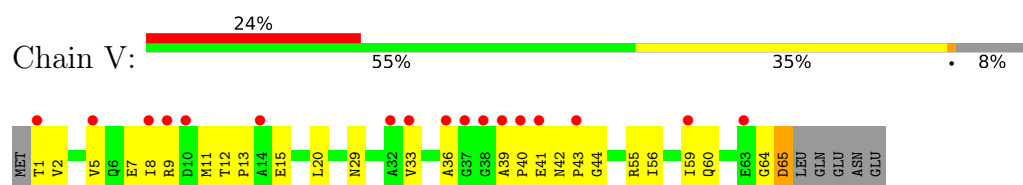
- Molecule 22: 50S ribosomal protein L24P



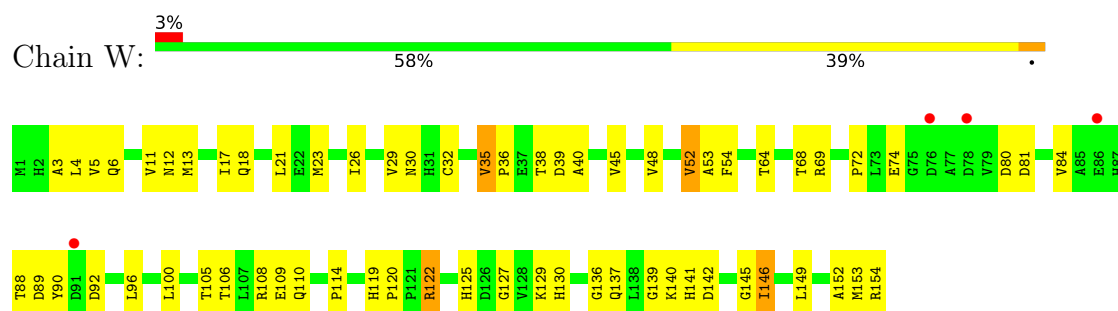
- Molecule 23: 50S ribosomal protein L24E



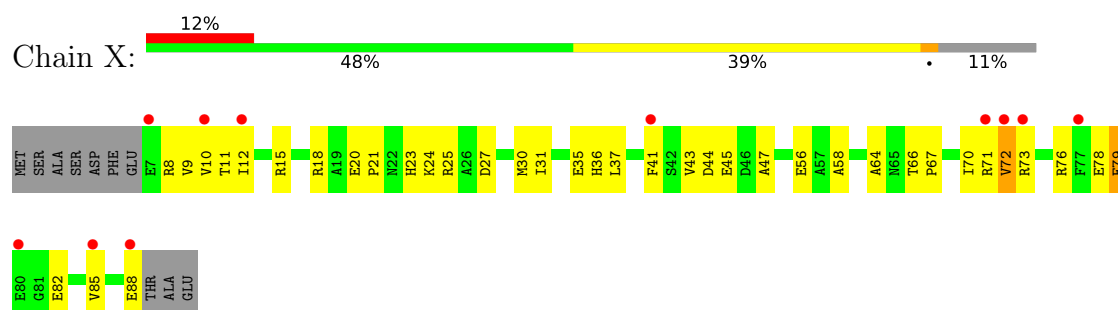
- Molecule 24: 50S ribosomal protein L29P



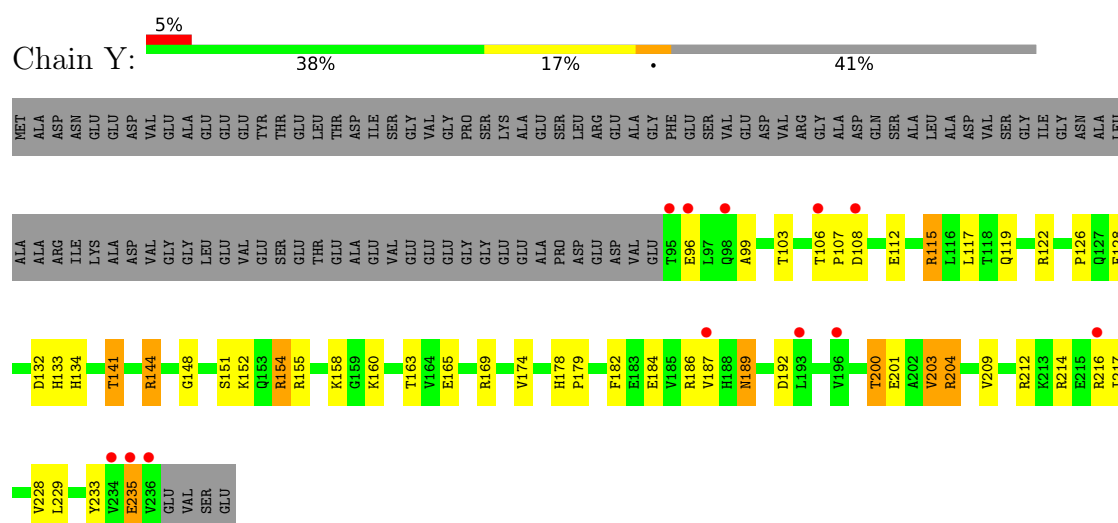
- Molecule 25: 50S ribosomal protein L30P



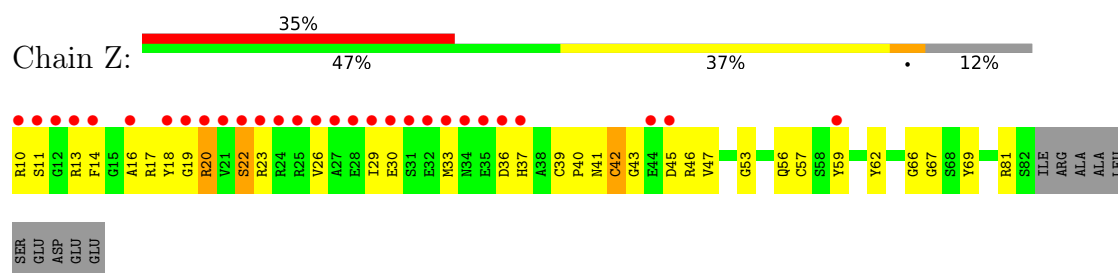
- Molecule 26: 50S ribosomal protein L31e



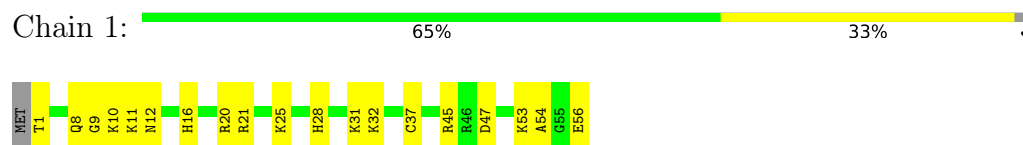
- Molecule 27: 50S ribosomal protein L32E



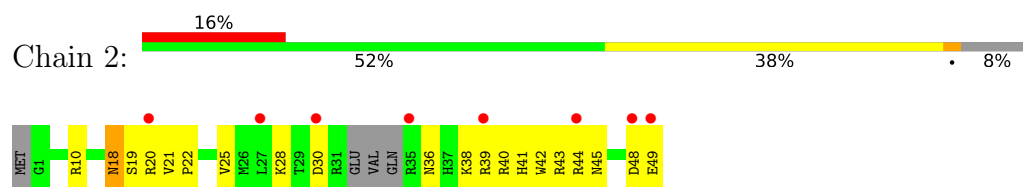
• Molecule 28: 50S ribosomal protein L37Ae



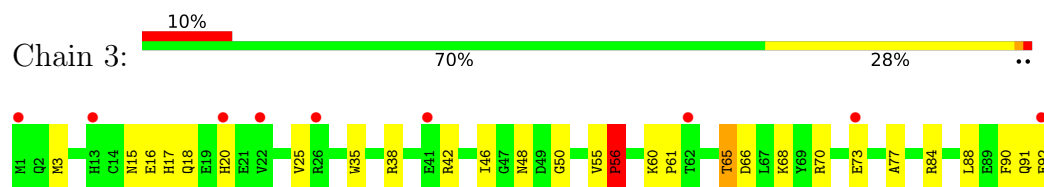
• Molecule 29: 50S ribosomal protein L37e



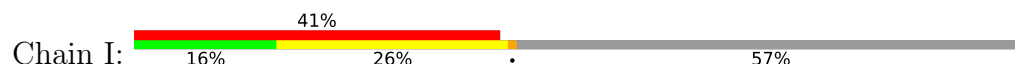
• Molecule 30: 50S ribosomal protein L39e



• Molecule 31: 50S ribosomal protein L44E



• Molecule 32: 50S RIBOSOMAL PROTEIN L11P



MET	SER		
ALA	PHE	A125	
GLY	GLU	K126	
THR	ILE	E127	
ILE	GLU	V128	
GLU	VAL	V129	
VAL	G71	G130	
LEU	T131	C132	
VAL	V72	T133	
VAL	P73	S134	
PRO	P74	L135	
GLY	T75	G136	
GLY	A76	V137	
GLU	E77	T138	
ALA	L78	I139	
ASN	I79	E140	
PRO	K80	GLY	
GLY	D81	GLU	
PRO	E82	ASN	
PRO	A83	PRO	
LEU	G84	ARG	
GLY	F85	GLU	
PRO	E86	PHE	
GLU	T87	LYS	
LEU	G88	GLU	
GLY	S89	ARG	
PRO	G90	ILE	
THR	E91	ASP	
PRO	P92	ALA	
VAL	Q93	GLY	
ASP	E94	GLU	
VAL	D95	TYR	
GLN	F96	ASP	
ALA	V97	ASP	
VAL	A98	VAL	
VAL	D99	PHE	
GLN	L100	ALA	
GLU	S101	ALA	
ILE	V102	GLU	
ASN	D103	GLN	
ASP	Q104	ALA	
GLN	V105	GLN	
THR	K106	ALA	
ALA	Q107	ALA	
ALA	I108	PHE	
PHE	A109	ASP	
ASP	E110	GLY	
GLY	Q111	THR	
THR	K112	GLU	
GLU	H113	VAL	
VAL	P114	PRO	
PRO	D115	VAL	
VAL	L116	THR	
THR	L117	VAL	
VAL	S118	LYS	
LYS	Y119	D120	
TYR	D120	L121	
ASP	L121	T122	
ASP	N123	A124	
ASP			
GLY			

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.44Å 298.56Å 574.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 49.61 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.30) 89.8 (49.61-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.247 0.206 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99045	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, PPU, CL, SR, NA, K, PO2, CD, OMU, UR3, IMA, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.38	0/65959	0.70	24/102870 (0.0%)
2	9	0.32	0/2905	0.70	1/4528 (0.0%)
3	4	0.48	0/102	0.75	0/149
4	A	0.33	0/1786	0.65	0/2408
5	B	0.32	0/2690	0.64	0/3652
6	C	0.37	0/1884	0.65	0/2551
7	D	0.29	0/1111	0.53	0/1498
8	E	0.31	0/1382	0.56	0/1880
9	F	0.30	0/901	0.53	0/1224
10	G	0.27	0/241	0.46	0/324
11	H	0.33	0/1287	0.64	0/1725
12	J	0.34	0/1136	0.60	0/1530
13	K	0.35	0/1001	0.66	0/1347
14	L	0.32	0/1130	0.63	0/1509
15	M	0.35	0/1584	0.60	0/2119
16	N	0.28	0/1474	0.60	0/1999
17	O	0.32	0/874	0.58	1/1181 (0.1%)
18	P	0.34	0/1147	0.55	0/1528
19	Q	0.35	0/749	0.68	0/1005
20	R	0.35	0/1172	0.66	1/1578 (0.1%)
21	S	0.32	0/648	0.58	0/875
22	T	0.30	0/958	0.62	0/1289
23	U	0.34	0/417	0.56	0/562
24	V	0.26	0/502	0.50	0/675
25	W	0.33	0/1219	0.59	0/1655
26	X	0.32	0/664	0.59	0/895
27	Y	0.35	0/1146	0.65	0/1536
28	Z	0.33	0/589	0.59	0/787
29	1	0.44	0/438	0.66	0/578
30	2	0.34	0/401	0.58	0/529
31	3	0.35	0/771	0.58	0/1024
32	I	0.28	0/526	0.50	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.36	0/98794	0.67	27/147726 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	44
2	9	0	1
All	All	0	45

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1819	G	C5'-C4'-C3'	7.74	128.38	116.00
1	0	871	G	C5'-C4'-O4'	-7.70	99.86	109.10
1	0	1942	A	C5'-C4'-C3'	7.40	127.83	116.00
2	9	3039	U	N1-C1'-C2'	6.97	123.06	114.00
1	0	1979	G	C2'-C3'-O3'	6.95	124.81	113.70
1	0	1592	G	N9-C1'-C2'	6.57	122.55	114.00
1	0	777	U	O4'-C1'-N1	6.41	113.33	108.20
1	0	1819	G	C4'-C3'-C2'	-6.14	96.46	102.60
1	0	1819	G	C1'-O4'-C4'	-6.12	105.01	109.90
1	0	1504	A	C1'-O4'-C4'	-6.09	105.03	109.90
1	0	389	G	C5'-C4'-C3'	-5.79	106.74	116.00
1	0	883	U	N1-C1'-C2'	5.75	121.47	114.00
1	0	2467	A	C1'-O4'-C4'	-5.66	105.37	109.90
1	0	2291	A	N9-C1'-C2'	5.62	121.31	114.00
1	0	206	G	C5'-C4'-C3'	-5.50	107.19	116.00
1	0	2726	U	N1-C1'-C2'	5.31	120.90	114.00
1	0	1261	A	N9-C1'-C2'	5.26	120.84	114.00
1	0	2313	C	C5'-C4'-O4'	5.21	115.36	109.10
1	0	1504	A	N9-C1'-C2'	5.17	120.73	114.00
17	O	66	GLY	N-CA-C	5.17	126.03	113.10
1	0	1615	A	C5'-C4'-C3'	5.12	124.18	116.00
1	0	841	A	C1'-O4'-C4'	-5.11	105.81	109.90
1	0	921	G	N9-C1'-C2'	5.09	120.62	114.00
1	0	1120	U	C5'-C4'-C3'	-5.09	107.85	116.00
1	0	69	A	C5'-C4'-O4'	-5.06	103.03	109.10
1	0	1452	G	C5'-C4'-C3'	-5.03	107.96	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	R	128	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1132	A	Sidechain
1	0	1327	G	Sidechain
1	0	1340	G	Sidechain
1	0	1342	C	Sidechain
1	0	1361	C	Sidechain
1	0	1458	A	Sidechain
1	0	1777	G	Sidechain
1	0	1809	G	Sidechain
1	0	1819	G	Sidechain
1	0	182	G	Sidechain
1	0	1829	A	Sidechain
1	0	1845	A	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1970	G	Sidechain
1	0	1979	G	Sidechain
1	0	2036	C	Sidechain
1	0	2412	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2552	C	Sidechain
1	0	2599	A	Sidechain
1	0	2607	U	Sidechain
1	0	2632	G	Sidechain
1	0	2842	G	Sidechain
1	0	396	U	Sidechain
1	0	460	A	Sidechain
1	0	469	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	518	G	Sidechain
1	0	554	G	Sidechain
1	0	619	U	Sidechain
1	0	792	G	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	868	G	Sidechain
1	0	952	G	Sidechain
2	9	3039	U	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29813	714	0
2	9	2600	0	1326	52	0
3	4	135	0	83	3	0
4	A	1753	0	1766	108	0
5	B	2625	0	2532	133	0
6	C	1859	0	1816	89	0
7	D	1094	0	1085	77	0
8	E	1357	0	1266	55	0
9	F	890	0	843	47	0
10	G	240	0	231	14	0
11	H	1266	0	1268	57	0
12	J	1120	0	1098	78	0
13	K	992	0	1031	46	0
14	L	1118	0	1076	50	0
15	M	1560	0	1568	72	0
16	N	1445	0	1401	86	0
17	O	865	0	873	37	0
18	P	1136	0	1123	38	0
19	Q	735	0	729	17	0
20	R	1149	0	1122	36	0
21	S	641	0	605	16	0
22	T	950	0	924	49	0
23	U	410	0	364	21	0
24	V	499	0	511	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	W	1196	0	1137	91	0
26	X	654	0	653	38	0
27	Y	1130	0	1133	61	0
28	Z	578	0	539	39	0
29	1	431	0	426	26	0
30	2	396	0	413	28	0
31	3	755	0	728	28	0
32	I	519	0	500	50	0
33	0	87	0	0	0	0
33	2	1	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	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	2	0	0	0	0
35	0	62	0	0	0	0
35	3	1	0	0	0	0
35	9	3	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	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	0	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	1	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	98	0	0	0	0
37	1	2	0	0	0	0
37	3	1	0	0	0	0
37	9	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	A	3	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	L	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5739	0	0	94	0
39	1	51	0	0	1	0
39	2	41	0	0	1	0
39	3	67	0	0	3	0
39	4	8	0	0	0	0
39	9	132	0	0	8	0
39	A	123	0	0	14	0
39	B	139	0	0	19	0
39	C	177	0	0	16	0
39	D	50	0	0	5	0
39	E	43	0	0	2	0
39	F	28	0	0	2	0
39	G	16	0	0	2	0
39	H	71	0	0	8	0
39	I	9	0	0	1	0
39	J	53	0	0	3	0
39	K	57	0	0	4	0
39	L	82	0	0	11	0
39	M	125	0	0	7	0
39	N	59	0	0	7	0
39	O	35	0	0	3	0
39	P	59	0	0	0	0
39	Q	48	0	0	5	0
39	R	86	0	0	2	0
39	S	31	0	0	1	0
39	T	36	0	0	1	0
39	U	26	0	0	1	0
39	V	11	0	0	1	0
39	W	68	0	0	3	0
39	X	23	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	Y	93	0	0	9	0
39	Z	28	0	0	3	0
All	All	99045	0	59983	2061	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (2061) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.23	1.17
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.31	1.10
2:9:3076:G:H3'	2:9:3077:A:H5''	1.35	1.08
6:C:236:THR:HG22	6:C:239:ALA:H	1.14	1.06
1:0:133:U:H2'	1:0:134:U:H5''	1.37	1.02
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.42	0.99
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.78	0.99
7:D:25:MET:HE2	7:D:41:LEU:HG	1.45	0.98
21:S:51:GLN:HE21	21:S:53:ASN:HD21	1.07	0.98
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.29	0.98
1:0:156:C:H5''	15:M:171:ARG:HD3	1.44	0.97
6:C:104:ASP:HA	6:C:107:ARG:HH12	1.29	0.97
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.46	0.97
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.45	0.97
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.47	0.96
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.80	0.96
30:2:18:ASN:HD21	30:2:40:ARG:H	1.05	0.96
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.48	0.96
15:M:99:ARG:HH21	15:M:170:ASN:HD22	1.13	0.95
9:F:91:VAL:HG12	9:F:92:GLY:H	1.27	0.95
1:0:2812:A:H2	1:0:2814:A:H62	1.11	0.95
29:1:25:LYS:HD2	30:2:49:GLU:H	1.29	0.94
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.46	0.94
13:K:10:GLN:H	13:K:10:GLN:NE2	1.64	0.93
1:0:542:A:H5'	1:0:542:A:H8	1.34	0.93
1:0:1242:A:H5'	12:J:82:THR:HG23	1.50	0.93
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	1.48	0.92
1:0:1160:G:H5'	1:0:1161:A:H5'	1.51	0.91
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.53	0.91
15:M:107:ARG:HH11	15:M:107:ARG:HG3	1.36	0.91
30:2:41:HIS:H	30:2:45:ASN:HD22	1.13	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:10:GLN:N	13:K:10:GLN:HE21	1.69	0.90
1:0:2717:C:H2'	1:0:2718:C:H5''	1.53	0.90
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.52	0.89
1:0:1372:A:H3'	39:0:7657:HOH:O	1.71	0.89
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.53	0.89
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.55	0.89
8:E:20:ILE:HD11	8:E:40:VAL:HG11	1.53	0.89
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.56	0.88
12:J:19:MET:HE1	12:J:132:LEU:HD21	1.54	0.88
6:C:1:MET:HG2	6:C:2:GLN:H	1.39	0.88
6:C:5:ILE:HD11	6:C:16:VAL:HG22	1.56	0.88
1:0:1466:C:H42	1:0:1476:A:H61	1.18	0.87
2:9:3056:A:H2'	2:9:3057:A:H5''	1.55	0.87
13:K:10:GLN:H	13:K:10:GLN:HE21	0.87	0.87
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.57	0.86
1:0:2506:A:HO2'	1:0:2507:G:H8	0.87	0.86
1:0:541:C:H2'	1:0:542:A:H5''	1.57	0.86
1:0:1835:U:H5	1:0:1840:A:N7	1.74	0.86
13:K:39:GLY:HA2	39:K:4183:HOH:O	1.74	0.86
5:B:238:ASN:HD22	5:B:240:GLY:H	1.20	0.86
7:D:58:VAL:HB	7:D:62:ASP:HB3	1.57	0.86
1:0:2840:A:OP1	5:B:211:THR:HG23	1.77	0.84
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.77	0.84
1:0:2717:C:C2'	1:0:2718:C:H5''	2.06	0.84
22:T:112:LEU:HD23	22:T:119:ALA:HB3	1.59	0.84
6:C:236:THR:HG22	6:C:239:ALA:N	1.91	0.84
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.12	0.84
5:B:36:PRO:HA	5:B:168:GLY:HA3	1.59	0.84
5:B:264:GLU:HG2	5:B:267:LYS:HE2	1.59	0.84
1:0:1593:C:OP1	18:P:117:SER:HB3	1.78	0.84
12:J:93:ARG:HH11	12:J:93:ARG:HB3	1.43	0.84
1:0:289:G:H22	1:0:363:A:H2	1.25	0.83
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.60	0.83
13:K:81:ARG:HB2	13:K:87:ARG:NH1	1.91	0.83
25:W:13:MET:HE1	25:W:18:GLN:HA	1.60	0.83
4:A:206:ARG:HD3	4:A:206:ARG:H	1.41	0.83
1:0:2073:G:H5''	39:0:4402:HOH:O	1.77	0.82
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.44	0.82
25:W:122:ARG:NH2	25:W:154:ARG:HG2	1.94	0.82
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.61	0.82
1:0:871:G:C8	1:0:871:G:H5'	2.15	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:81:GLN:HB2	4:A:92:ASN:ND2	1.94	0.82
4:A:191:GLY:HA2	4:A:194:MET:CE	2.09	0.82
6:C:115:LEU:HD21	6:C:243:VAL:HG13	1.62	0.82
25:W:88:THR:HB	39:W:6679:HOH:O	1.80	0.82
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.62	0.81
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.80	0.81
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.45	0.81
7:D:172:VAL:HG12	7:D:173:GLU:H	1.43	0.81
24:V:1:THR:HG23	24:V:2:VAL:H	1.46	0.81
16:N:144:GLY:O	16:N:147:ILE:HG22	1.79	0.81
4:A:69:LEU:HD23	4:A:107:ASN:HB2	1.62	0.81
6:C:104:ASP:HA	6:C:107:ARG:NH1	1.96	0.81
1:O:1116:U:O2'	1:O:1118:A:H2	1.64	0.81
1:O:2851:G:C2'	1:O:2852:A:H5'	2.11	0.81
8:E:81:GLU:HG2	8:E:134:SER:HB3	1.63	0.81
1:O:1603:A:H5'	1:O:1605:G:O4'	1.82	0.80
4:A:192:VAL:HG22	39:A:9620:HOH:O	1.79	0.80
1:O:133:U:C2'	1:O:134:U:H5''	2.11	0.80
8:E:36:PRO:HD3	12:J:127:ILE:HD12	1.63	0.80
1:O:1474:C:H6	1:O:1474:C:H5'	1.47	0.80
1:O:560:C:H42	1:O:597:A:H61	1.27	0.80
1:O:1159:G:H21	1:O:1189:A:H8	1.30	0.80
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.62	0.80
22:T:9:LYS:HE3	22:T:13:ARG:CZ	2.12	0.80
13:K:4:LEU:HD22	13:K:116:GLU:HB3	1.63	0.80
17:O:32:ARG:HD3	17:O:32:ARG:O	1.82	0.80
18:P:115:SER:H	18:P:118:GLN:HE21	1.30	0.80
1:O:541:C:C2'	1:O:542:A:H5''	2.12	0.79
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.63	0.79
16:N:113:SER:HB2	39:N:9354:HOH:O	1.82	0.79
4:A:192:VAL:HB	39:A:9583:HOH:O	1.81	0.79
39:O:5382:HOH:O	12:J:47:THR:HB	1.80	0.79
15:M:79:ALA:HB3	15:M:81:ARG:HH12	1.45	0.79
1:O:2506:A:O2'	1:O:2507:G:H8	1.64	0.79
7:D:154:LYS:HD2	7:D:154:LYS:H	1.47	0.79
15:M:28:GLN:O	15:M:32:ARG:HG3	1.83	0.79
20:R:99:ALA:HB1	20:R:109:MET:CE	2.13	0.79
1:O:2054:A:N3	20:R:128:ARG:NH2	2.31	0.79
1:O:1041:U:H5'	39:L:9490:HOH:O	1.82	0.79
1:O:1701:A:H4'	1:O:1702:U:H5''	1.65	0.79
1:O:1838:U:H1'	1:O:2644:C:H5'	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1:25:LYS:HD2	30:2:49:GLU:N	1.98	0.79
1:0:1118:A:H62	1:0:1244:U:H3	1.30	0.79
27:Y:154:ARG:HH12	27:Y:155:ARG:HG3	1.48	0.79
32:I:78:LEU:HD12	32:I:112:LYS:HZ2	1.49	0.78
4:A:191:GLY:HA2	4:A:194:MET:HE2	1.64	0.78
22:T:63:ILE:HD11	22:T:75:GLU:HB2	1.66	0.78
16:N:11:ARG:HG3	16:N:14:ARG:HH12	1.49	0.78
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.65	0.77
15:M:79:ALA:HB3	15:M:81:ARG:NH1	1.99	0.77
25:W:21:LEU:CD2	25:W:48:VAL:HG11	2.10	0.77
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.66	0.77
5:B:307:ARG:HH11	5:B:307:ARG:HG3	1.46	0.77
14:L:91:VAL:HG13	14:L:120:LEU:HD23	1.67	0.77
27:Y:235:GLU:H	27:Y:235:GLU:CD	1.85	0.77
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.66	0.77
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.67	0.77
1:0:870:G:H2'	1:0:871:G:H5''	1.67	0.77
11:H:56:GLN:HE21	11:H:126:ARG:HE	1.32	0.77
1:0:1667:A:H8	1:0:1667:A:H5'	1.50	0.77
6:C:246:ARG:HH11	6:C:246:ARG:HB3	1.49	0.76
1:0:1116:U:HO2'	1:0:1118:A:H2	0.80	0.76
1:0:1751:G:H2'	1:0:1752:G:H5''	1.67	0.76
1:0:1973:A:H5'	1:0:1973:A:H8	1.50	0.76
2:9:3039:U:H1'	2:9:3044:A:H61	1.50	0.76
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.66	0.76
1:0:1119:G:H2'	12:J:52:GLN:NE2	2.01	0.76
5:B:162:MET:HE2	5:B:310:ARG:HD3	1.68	0.76
8:E:15:GLN:HG2	8:E:19:ASP:O	1.84	0.76
1:0:1165:G:H4'	1:0:1174:A:O2'	1.86	0.76
1:0:2851:G:H2'	1:0:2852:A:H5'	1.68	0.76
4:A:192:VAL:CG1	4:A:207:GLN:HB3	2.15	0.76
1:0:1119:G:N2	1:0:1246:A:C2	2.53	0.76
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.66	0.76
6:C:107:ARG:NH1	6:C:107:ARG:HB3	2.02	0.75
1:0:544:G:H2'	1:0:545:G:H5''	1.68	0.75
11:H:27:LYS:H	11:H:59:HIS:HD2	1.30	0.75
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.68	0.75
1:0:559:U:H5'	1:0:559:U:H6	1.51	0.75
14:L:143:THR:HG22	14:L:144:ASP:H	1.49	0.75
1:0:288:A:H61	1:0:364:C:H42	1.32	0.75
32:I:78:LEU:HD12	32:I:112:LYS:NZ	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:281:U:H2'	1:0:282:C:O4'	1.86	0.74
1:0:871:G:C8	1:0:871:G:C5'	2.70	0.74
8:E:3:VAL:HG22	8:E:49:ILE:HB	1.68	0.74
18:P:115:SER:OG	18:P:118:GLN:HG3	1.87	0.74
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.68	0.74
4:A:95:PRO:HG2	4:A:98:GLU:HG2	1.69	0.74
21:S:57:THR:HG22	21:S:59:ASP:H	1.52	0.74
16:N:132:ASN:O	16:N:135:VAL:HG12	1.87	0.74
1:0:506:G:H22	1:0:509:A:H5''	1.52	0.74
5:B:217:ARG:HG3	5:B:257:THR:HG22	1.70	0.74
25:W:122:ARG:HH11	25:W:122:ARG:HG2	1.53	0.74
1:0:470:U:O2'	29:1:16:HIS:HD2	1.71	0.73
39:0:7902:HOH:O	5:B:211:THR:HG21	1.87	0.73
4:A:192:VAL:HG12	4:A:207:GLN:HB3	1.71	0.73
9:F:58:GLU:HG3	9:F:61:MET:HE1	1.70	0.73
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.70	0.73
32:I:102:VAL:HG12	32:I:106:LYS:HE3	1.69	0.73
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.18	0.73
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.19	0.73
1:0:1175:G:H1'	1:0:1193:A:H2'	1.69	0.73
1:0:2468:A:H61	31:3:48:ASN:HD21	1.37	0.73
1:0:871:G:H8	1:0:871:G:C5'	2.00	0.73
5:B:51:VAL:HG23	5:B:329:TYR:O	1.89	0.73
1:0:380:A:OP2	15:M:9:ARG:HD2	1.89	0.73
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.71	0.73
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.86	0.73
1:0:1878:G:H1'	39:0:6632:HOH:O	1.89	0.73
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.70	0.73
1:0:1160:G:C5'	1:0:1161:A:H5'	2.19	0.73
1:0:2491:G:H1'	39:0:7349:HOH:O	1.87	0.73
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.19	0.73
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.12	0.72
6:C:246:ARG:NH1	6:C:246:ARG:HB3	2.04	0.72
28:Z:30:GLU:HA	28:Z:33:MET:HE3	1.72	0.72
17:O:32:ARG:NE	17:O:35:LYS:HD2	2.03	0.72
9:F:53:ASP:OD1	9:F:80:GLN:HB2	1.90	0.72
1:0:1206:U:H6	1:0:1206:U:H5'	1.53	0.72
16:N:37:ARG:HG3	36:N:9307:CL:CL	2.26	0.72
7:D:58:VAL:HG12	7:D:60:GLU:HG2	1.70	0.72
26:X:71:ARG:HD3	39:X:2171:HOH:O	1.90	0.72
1:0:2765:C:H4'	39:0:6049:HOH:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:141:ARG:HD2	5:B:163:GLU:OE2	1.90	0.72
39:O:6049:HOH:O	5:B:298:LYS:HG2	1.88	0.72
1:O:2748:G:H2'	39:O:7984:HOH:O	1.90	0.72
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.20	0.72
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.25	0.71
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.72	0.71
1:O:960:G:H4'	39:O:7878:HOH:O	1.89	0.71
9:F:96:ALA:HA	39:F:3111:HOH:O	1.91	0.71
1:O:481:U:H5''	39:O:6176:HOH:O	1.89	0.71
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.73	0.71
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.73	0.71
6:C:236:THR:H	6:C:239:ALA:HB3	1.55	0.71
1:O:2291:A:C8	1:O:2309:C:H5'	2.26	0.71
1:O:2716:G:H5''	5:B:206:THR:HG21	1.72	0.71
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.09	0.71
21:S:51:GLN:HE21	21:S:53:ASN:ND2	1.85	0.71
2:9:3014:G:H8	2:9:3014:G:H5'	1.56	0.71
13:K:32:ILE:HD11	13:K:56:SER:HB3	1.73	0.71
14:L:143:THR:HG22	14:L:144:ASP:N	2.05	0.71
1:O:506:G:H22	1:O:509:A:C5'	2.04	0.71
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.21	0.71
21:S:51:GLN:NE2	21:S:53:ASN:HD21	1.86	0.71
27:Y:141:THR:HG23	39:Y:9388:HOH:O	1.90	0.71
1:O:93:C:H5''	24:V:1:THR:HB	1.73	0.70
26:X:25:ARG:HD3	26:X:64:ALA:O	1.90	0.70
27:Y:144:ARG:HH11	27:Y:144:ARG:CG	2.02	0.70
1:O:1118:A:H3'	1:O:1118:A:H8	1.56	0.70
5:B:179:LEU:O	5:B:183:GLU:HG2	1.92	0.70
23:U:14:GLU:O	23:U:17:THR:HB	1.92	0.70
9:F:58:GLU:HA	9:F:61:MET:HE2	1.73	0.70
24:V:12:THR:HG22	24:V:15:GLU:CG	2.20	0.70
1:O:1700:C:H5''	1:O:1701:A:OP2	1.90	0.70
6:C:27:ARG:HG3	6:C:29:ASP:OD1	1.91	0.70
10:G:12:ILE:N	10:G:13:PRO:HD3	2.06	0.70
25:W:88:THR:HG22	25:W:89:ASP:N	2.06	0.70
5:B:16:ARG:NH1	39:B:9609:HOH:O	2.25	0.70
6:C:236:THR:CG2	6:C:239:ALA:H	1.98	0.70
6:C:1:MET:HG2	6:C:2:GLN:N	2.06	0.70
17:O:32:ARG:HH21	17:O:35:LYS:NZ	1.88	0.70
11:H:59:HIS:HA	11:H:62:LEU:HD23	1.72	0.70
15:M:164:THR:HG22	15:M:166:ALA:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:80:GLY:O	15:M:81:ARG:HD2	1.91	0.70
1:O:2481:G:H5''	39:O:5097:HOH:O	1.91	0.70
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.54	0.70
1:O:1206:U:H2'	1:O:1207:A:O4'	1.92	0.70
5:B:190:MET:HE2	5:B:194:PHE:HD1	1.57	0.70
1:O:1474:C:C6	1:O:1474:C:H5'	2.27	0.70
16:N:11:ARG:HA	16:N:14:ARG:NH1	2.07	0.70
1:O:969:G:H1	1:O:999:C:H42	1.40	0.69
1:O:1182:C:H1'	1:O:1192:A:H8	1.56	0.69
4:A:105:VAL:HG11	4:A:154:ALA:HB1	1.75	0.69
1:O:1118:A:H3'	1:O:1118:A:C8	2.27	0.69
1:O:2073:G:OP2	1:O:2490:A:H5'	1.92	0.69
2:9:3039:U:H1'	2:9:3044:A:N6	2.06	0.69
6:C:2:GLN:HB3	39:C:9192:HOH:O	1.92	0.69
9:F:37:THR:O	9:F:41:GLU:HG3	1.93	0.69
25:W:80:ASP:O	25:W:84:VAL:HG23	1.90	0.69
13:K:98:VAL:HG13	13:K:102:GLU:HA	1.74	0.69
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.92	0.69
27:Y:144:ARG:HH11	27:Y:144:ARG:HG3	1.58	0.69
1:O:1184:C:H4'	32:I:126:LYS:HB3	1.75	0.69
20:R:39:THR:HB	20:R:42:GLU:HG3	1.74	0.69
1:O:1184:C:H1'	39:O:7912:HOH:O	1.93	0.69
1:O:1187:U:HO2'	1:O:1189:A:H2	1.41	0.69
1:O:545:G:H8	1:O:545:G:H5'	1.57	0.69
5:B:275:GLY:O	5:B:291:ASP:HA	1.92	0.69
11:H:56:GLN:NE2	11:H:126:ARG:HE	1.89	0.69
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.75	0.69
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.41	0.69
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.73	0.69
1:O:541:C:H2'	1:O:542:A:C5'	2.23	0.69
16:N:164:ASP:CG	16:N:167:ASP:HA	2.13	0.69
1:O:1166:A:H1'	1:O:1192:A:C2	2.28	0.69
5:B:140:LEU:HA	39:B:9575:HOH:O	1.92	0.69
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.73	0.69
1:O:542:A:C8	1:O:542:A:H5'	2.23	0.68
9:F:77:VAL:HG21	9:F:83:LEU:HD13	1.76	0.68
12:J:19:MET:CE	12:J:132:LEU:HD11	2.23	0.68
1:O:2534:C:H1'	39:O:4086:HOH:O	1.93	0.68
25:W:137:GLN:NE2	25:W:141:HIS:HE1	1.91	0.68
25:W:4:LEU:HD11	25:W:45:VAL:HG12	1.76	0.68
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:39:ALA:N	24:V:40:PRO:HD2	2.07	0.68
11:H:166:SER:HB3	11:H:167:PRO:HD3	1.73	0.68
1:O:381:G:H5''	39:M:9376:HOH:O	1.93	0.68
1:O:1730:G:H5'	1:O:1731:C:C5	2.29	0.68
22:T:115:GLU:HG3	22:T:116:ASP:N	2.08	0.68
23:U:39:ASN:ND2	23:U:44:ARG:HH11	1.90	0.68
1:O:2005:G:H3'	1:O:2005:G:OP2	1.94	0.68
7:D:170:TYR:O	7:D:171:ASP:HB3	1.94	0.68
25:W:108:ARG:HG3	25:W:114:PRO:HG3	1.76	0.68
2:9:3051:A:H5'	16:N:160:SER:HB3	1.76	0.68
25:W:48:VAL:HG12	25:W:48:VAL:O	1.93	0.68
4:A:199:HIS:HD2	4:A:201:PHE:H	1.39	0.67
1:O:2480:G:H3'	39:O:4754:HOH:O	1.94	0.67
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.77	0.67
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.76	0.67
1:O:1299:G:O6	14:L:6:ARG:HD3	1.95	0.67
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.76	0.67
1:O:1528:A:H2'	1:O:1529:G:O4'	1.95	0.67
1:O:1244:U:OP1	12:J:18:ILE:HD13	1.94	0.67
31:3:35:TRP:HB2	39:3:9488:HOH:O	1.93	0.67
17:O:96:VAL:HG13	17:O:100:GLN:HB2	1.76	0.67
15:M:24:GLN:O	15:M:28:GLN:HG3	1.94	0.67
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.76	0.67
25:W:88:THR:HG22	25:W:89:ASP:H	1.58	0.67
1:O:280:C:H2'	1:O:281:U:O4'	1.95	0.67
4:A:48:ASP:HB3	39:A:9595:HOH:O	1.94	0.67
8:E:31:ARG:HH12	8:E:68:HIS:CG	2.13	0.67
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.24	0.67
1:O:1116:U:H3	1:O:1246:A:H62	1.41	0.66
1:O:1377:C:H6	1:O:1377:C:H5'	1.59	0.66
1:O:2780:C:H1'	8:E:143:GLN:HE21	1.60	0.66
1:O:1666:C:H2'	1:O:1667:A:H5'	1.76	0.66
1:O:1681:G:H5''	1:O:1682:A:H5'	1.77	0.66
1:O:2003:U:H4'	1:O:2004:U:H5	1.61	0.66
4:A:51:ARG:HB2	39:A:9595:HOH:O	1.94	0.66
11:H:27:LYS:N	11:H:59:HIS:HD2	1.93	0.66
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.26	0.66
1:O:338:C:H4'	6:C:174:ILE:CD1	2.26	0.66
28:Z:17:ARG:HD3	39:Z:9218:HOH:O	1.95	0.66
16:N:62:HIS:HB3	16:N:65:ASP:OD1	1.96	0.66
7:D:172:VAL:HG12	7:D:173:GLU:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:112:LEU:CD2	22:T:119:ALA:HB3	2.26	0.66
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.11	0.66
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.11	0.66
1:O:1209:C:H2'	1:O:1210:G:H8	1.59	0.66
1:O:709:G:O2'	17:O:25:VAL:HG12	1.94	0.66
4:A:105:VAL:CG1	4:A:154:ALA:HB1	2.25	0.66
14:L:121:ILE:HG12	14:L:141:GLU:HB2	1.77	0.66
9:F:58:GLU:OE1	15:M:27:ARG:NH2	2.28	0.66
15:M:77:HIS:HD2	15:M:79:ALA:O	1.79	0.66
39:O:4937:HOH:O	15:M:83:SER:HB3	1.96	0.66
1:O:871:G:H8	1:O:871:G:H5'	1.60	0.65
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.26	0.65
11:H:166:SER:CB	11:H:167:PRO:CD	2.74	0.65
25:W:52:VAL:HG22	25:W:53:ALA:H	1.61	0.65
14:L:35:ARG:HB2	14:L:35:ARG:NH1	2.11	0.65
1:O:134:U:H6	1:O:134:U:C5'	2.09	0.65
30:2:18:ASN:ND2	30:2:40:ARG:H	1.86	0.65
5:B:109:LEU:HG	5:B:113:LEU:HD11	1.78	0.65
6:C:107:ARG:NE	39:C:9263:HOH:O	2.29	0.65
32:I:93:GLN:HA	32:I:96:PHE:HE2	1.60	0.65
39:O:9737:HOH:O	15:M:82:ARG:HD2	1.95	0.65
27:Y:144:ARG:CZ	39:Y:9409:HOH:O	2.44	0.65
18:P:115:SER:H	18:P:118:GLN:NE2	1.93	0.65
20:R:44:VAL:O	20:R:48:GLU:HG3	1.95	0.65
1:O:553:G:P	27:Y:204:ARG:HH22	2.19	0.65
1:O:2676:C:H4'	12:J:70:PHE:CE1	2.32	0.65
13:K:49:LEU:HD12	13:K:80:ILE:HG21	1.79	0.65
1:O:1119:G:H22	1:O:1246:A:H2	1.38	0.65
1:O:1166:A:H61	1:O:1180:U:H3	1.44	0.65
1:O:2676:C:H4'	12:J:70:PHE:CD1	2.32	0.65
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.20	0.65
24:V:20:LEU:HD22	24:V:60:GLN:HE22	1.62	0.65
1:O:1201:C:H5''	39:O:6742:HOH:O	1.97	0.65
1:O:282:C:O2'	1:O:283:U:H5'	1.96	0.65
28:Z:22:SER:O	28:Z:26:VAL:HG23	1.97	0.65
28:Z:37:HIS:O	28:Z:45:ASP:HA	1.97	0.65
1:O:544:G:C2'	1:O:545:G:H5''	2.26	0.65
9:F:2:VAL:HG22	9:F:57:GLU:OE1	1.97	0.65
21:S:57:THR:HG22	21:S:59:ASP:N	2.11	0.65
1:O:1426:C:H2'	39:O:3204:HOH:O	1.95	0.64
14:L:73:VAL:HG23	14:L:74:THR:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:99:ARG:NH2	15:M:170:ASN:HD22	1.89	0.64
1:O:263:U:O4'	9:F:59:ILE:HD13	1.98	0.64
16:N:80:SER:HB2	39:N:9333:HOH:O	1.95	0.64
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.23	0.64
4:A:125:ASN:HB3	4:A:158:VAL:HG12	1.80	0.64
18:P:91:LYS:O	18:P:95:GLU:HG3	1.97	0.64
27:Y:154:ARG:NH1	27:Y:155:ARG:HG3	2.12	0.64
1:O:2749:U:H5'	39:O:8438:HOH:O	1.96	0.64
15:M:183:THR:HG22	15:M:194:ALA:HB1	1.78	0.64
23:U:52:THR:HG22	23:U:54:THR:N	2.13	0.64
2:9:3029:C:O3'	7:D:138:GLY:HA2	1.97	0.64
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.32	0.64
1:O:1201:C:H2'	1:O:1202:A:H5'	1.79	0.64
4:A:153:ARG:HH11	4:A:153:ARG:HB2	1.62	0.64
12:J:75:PRO:HD3	12:J:136:SER:OG	1.97	0.64
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.13	0.64
17:O:32:ARG:HH21	17:O:35:LYS:HZ2	1.43	0.64
24:V:56:ILE:O	24:V:60:GLN:HG3	1.97	0.64
7:D:159:PRO:O	7:D:163:VAL:HG23	1.97	0.64
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.32	0.64
1:O:1771:U:H5'	28:Z:20:ARG:HH21	1.63	0.64
1:O:2908:A:H2'	1:O:2909:G:O4'	1.98	0.64
2:9:3056:A:C2'	2:9:3057:A:H5''	2.27	0.64
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.27	0.64
1:O:134:U:H5'	1:O:134:U:H6	1.63	0.64
2:9:3029:C:H2'	2:9:3030:C:H5'	1.80	0.64
4:A:107:ASN:OD1	4:A:120:ARG:HD2	1.97	0.64
1:O:1943:C:H4'	4:A:211:LYS:O	1.98	0.64
1:O:1119:G:H2'	12:J:52:GLN:HE22	1.61	0.64
1:O:1183:C:N4	1:O:1184:C:H41	1.96	0.63
5:B:53:LEU:HD11	5:B:327:VAL:HG22	1.78	0.63
1:O:1641:A:H2'	1:O:1642:A:H5'	1.79	0.63
31:3:65:THR:HG22	31:3:88:LEU:HD22	1.78	0.63
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.81	0.63
15:M:187:LEU:CD2	15:M:194:ALA:HB3	2.28	0.63
5:B:53:LEU:HD21	5:B:270:ILE:HD12	1.80	0.63
17:O:57:THR:HB	17:O:111:VAL:HG23	1.78	0.63
1:O:2426:G:H1'	39:O:6603:HOH:O	1.97	0.63
1:O:2541:U:H5'	39:O:3025:HOH:O	1.96	0.63
6:C:242:GLU:HG3	39:C:9189:HOH:O	1.99	0.63
7:D:105:SER:HB2	7:D:131:THR:HG23	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.80	0.63
19:Q:25:PRO:HB2	39:Q:4350:HOH:O	1.98	0.63
27:Y:165:GLU:HB3	39:Y:9393:HOH:O	1.98	0.63
1:O:834:G:H4'	1:O:835:U:OP2	1.99	0.63
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.28	0.63
1:O:282:C:H1'	1:O:368:C:N4	2.13	0.63
4:A:113:GLY:HA2	4:A:153:ARG:NH2	2.14	0.63
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.32	0.63
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.26	0.63
25:W:84:VAL:HG12	39:W:6679:HOH:O	1.98	0.63
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.34	0.63
2:9:3013:A:O2'	2:9:3014:G:H5''	1.98	0.63
7:D:57:THR:HG23	7:D:63:ILE:HA	1.80	0.63
8:E:34:TRP:O	12:J:127:ILE:HD11	1.99	0.63
9:F:91:VAL:HG12	9:F:92:GLY:N	2.05	0.63
1:O:1328:A:OP1	27:Y:169:ARG:HD2	1.98	0.63
1:O:2578:G:H5'	1:O:2578:G:H8	1.63	0.63
7:D:136:ARG:HH12	7:D:157:LEU:HA	1.63	0.63
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.80	0.63
5:B:305:ASP:O	5:B:306:LYS:HB2	1.99	0.63
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.81	0.63
32:I:99:ASP:OD1	32:I:138:THR:HB	1.98	0.63
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.79	0.63
5:B:141:ARG:HG2	5:B:165:ARG:HA	1.81	0.62
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.27	0.62
8:E:23:GLU:HG2	8:E:28:SER:HB3	1.80	0.62
9:F:21:GLU:O	9:F:24:ARG:HG3	1.99	0.62
1:O:2346:C:O2'	7:D:52:THR:HG21	1.98	0.62
1:O:2896:A:N3	1:O:2896:A:H2'	2.13	0.62
12:J:19:MET:HE1	12:J:132:LEU:HD11	1.81	0.62
1:O:902:G:N7	14:L:18:HIS:HD2	1.98	0.62
17:O:21:SER:OG	17:O:106:PRO:HB2	2.00	0.62
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.82	0.62
22:T:85:GLU:HG2	22:T:86:GLU:N	2.14	0.62
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.62	0.62
1:O:1160:G:H5'	1:O:1161:A:C5'	2.28	0.62
8:E:81:GLU:HG2	8:E:134:SER:CB	2.29	0.62
14:L:133:VAL:HA	39:L:9469:HOH:O	1.99	0.62
1:O:538:C:OP2	27:Y:134:HIS:HE1	1.82	0.62
5:B:254:GLN:HG2	5:B:255:GLY:N	2.12	0.62
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:13:GLU:OE2	9:F:78:GLU:HG2	1.99	0.62
27:Y:154:ARG:HH12	27:Y:155:ARG:CG	2.12	0.62
1:O:2064:U:H5'	1:O:2652:U:H4'	1.81	0.62
1:O:877:G:H5'	1:O:878:G:OP1	1.98	0.62
29:1:10:LYS:HG3	39:1:9489:HOH:O	1.99	0.62
5:B:238:ASN:ND2	5:B:240:GLY:H	1.96	0.62
17:O:87:THR:O	17:O:91:GLN:HG3	1.99	0.62
22:T:115:GLU:HG3	22:T:116:ASP:H	1.63	0.62
1:O:1555:G:H4'	1:O:1630:A:H2	1.65	0.62
11:H:63:GLU:HA	39:H:9544:HOH:O	1.98	0.62
32:I:110:GLU:HA	32:I:113:HIS:CE1	2.35	0.62
1:O:1666:C:O2'	1:O:1667:A:H5''	1.99	0.62
4:A:131:HIS:O	4:A:132:ASP:HB2	1.98	0.62
4:A:57:ALA:HB1	4:A:65:ARG:HE	1.64	0.62
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.29	0.62
32:I:110:GLU:HA	32:I:113:HIS:NE2	2.15	0.62
13:K:55:VAL:HG12	13:K:56:SER:N	2.15	0.62
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.14	0.62
22:T:41:ARG:NH1	22:T:41:ARG:HG2	2.15	0.62
27:Y:189:ASN:HD22	27:Y:189:ASN:C	2.03	0.62
1:O:625:U:H5''	1:O:1044:C:N4	2.14	0.62
11:H:20:ILE:HG23	11:H:120:ILE:HD11	1.82	0.62
22:T:47:THR:HB	22:T:100:ASP:HB3	1.82	0.62
1:O:2541:U:H4'	1:O:2542:C:OP1	1.99	0.61
4:A:179:MET:HG2	4:A:186:TRP:CB	2.30	0.61
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.29	0.61
11:H:30:GLN:H	11:H:66:ARG:NH1	1.98	0.61
22:T:38:ARG:NH1	39:T:6217:HOH:O	2.33	0.61
4:A:33:GLU:O	4:A:34:ASP:HB2	1.99	0.61
10:G:20:VAL:O	10:G:24:VAL:HG23	2.00	0.61
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.31	0.61
1:O:2505:G:O2'	1:O:2506:A:H5'	2.00	0.61
1:O:558:C:C2'	1:O:559:U:H5''	2.30	0.61
1:O:111:C:O2'	29:1:20:ARG:HG2	2.01	0.61
16:N:176:ARG:HG3	16:N:180:LEU:HD13	1.82	0.61
29:1:25:LYS:CD	30:2:49:GLU:H	2.09	0.61
5:B:175:LEU:O	5:B:175:LEU:HD23	2.01	0.61
7:D:25:MET:CE	7:D:41:LEU:HG	2.26	0.61
1:O:1116:U:O2'	1:O:1118:A:C2	2.45	0.61
1:O:244:C:OP2	9:F:38:LYS:HE3	2.00	0.61
12:J:39:VAL:HG13	12:J:106:GLY:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:74:ARG:O	12:J:78:ILE:HG12	2.00	0.61
15:M:76:ARG:HG3	15:M:88:VAL:HG21	1.83	0.61
4:A:33:GLU:CD	4:A:33:GLU:H	2.03	0.61
4:A:35:GLY:O	4:A:36:ASP:HB3	1.99	0.61
4:A:82:VAL:HG13	4:A:93:THR:HB	1.80	0.61
15:M:107:ARG:NH1	15:M:107:ARG:HG3	2.10	0.61
1:O:681:G:N3	1:O:681:G:H5'	2.16	0.61
5:B:307:ARG:NH1	5:B:307:ARG:HG3	2.16	0.61
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.65	0.61
1:O:1701:A:H4'	1:O:1702:U:C5'	2.30	0.61
1:O:2032:U:H2'	1:O:2033:G:C5'	2.31	0.61
1:O:2032:U:H2'	1:O:2033:G:H5''	1.83	0.61
1:O:2661:U:H3	1:O:2812:A:H62	1.48	0.61
15:M:164:THR:HG22	15:M:166:ALA:N	2.14	0.61
1:O:2890:A:H1'	23:U:56:ARG:NH2	2.15	0.61
25:W:13:MET:CE	25:W:17:ILE:HG22	2.31	0.61
1:O:2524:G:H21	1:O:2526:C:N4	1.99	0.61
1:O:2533:C:H5'	1:O:2533:C:H6	1.65	0.61
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.66	0.61
25:W:38:THR:HG22	25:W:39:ASP:N	2.15	0.61
2:9:3020:G:O2'	2:9:3021:G:H5'	2.00	0.61
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.82	0.61
8:E:68:HIS:O	8:E:72:MET:HG3	2.00	0.61
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.34	0.61
21:S:77:VAL:O	21:S:80:ARG:HG2	2.00	0.61
4:A:105:VAL:HG11	4:A:154:ALA:CB	2.31	0.60
14:L:80:ASP:HB2	14:L:90:ARG:O	2.01	0.60
1:O:447:A:P	22:T:1:SER:HB2	2.40	0.60
1:O:1406:A:H4'	1:O:1407:A:H5''	1.83	0.60
1:O:2748:G:H1'	39:O:8415:HOH:O	2.01	0.60
4:A:153:ARG:NH1	4:A:153:ARG:HB2	2.16	0.60
8:E:108:LEU:HD11	8:E:164:ASP:HB2	1.82	0.60
14:L:67:ARG:O	14:L:71:GLU:HG3	2.01	0.60
16:N:164:ASP:OD1	16:N:167:ASP:HA	2.00	0.60
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.01	0.60
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.83	0.60
1:O:558:C:H2'	1:O:559:U:C5'	2.31	0.60
5:B:221:GLN:HE22	13:K:42:ASN:HD22	1.49	0.60
7:D:94:ALA:HA	7:D:174:VAL:HA	1.84	0.60
7:D:25:MET:HE1	7:D:37:ALA:HB1	1.82	0.60
14:L:35:ARG:HB2	14:L:35:ARG:HH11	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:O:6281:HOH:O	22:T:106:GLU:HG3	2.00	0.60
5:B:41:PHE:CD1	5:B:79:MET:HE2	2.35	0.60
9:F:60:VAL:HG12	9:F:60:VAL:O	2.02	0.60
1:O:1168:C:H5''	32:I:87:THR:CG2	2.32	0.60
25:W:130:HIS:O	25:W:136:GLY:HA3	2.02	0.60
1:O:137:U:H2'	1:O:139:C:C5	2.37	0.60
1:O:2420:G:O2'	1:O:2421:G:H5'	2.02	0.60
10:G:23:ILE:HD13	10:G:67:LEU:HD23	1.82	0.60
2:9:3008:G:O6	16:N:11:ARG:NH1	2.34	0.60
25:W:141:HIS:HB2	25:W:146:ILE:HG12	1.84	0.60
1:O:1687:C:O2	29:1:9:GLY:HA2	2.02	0.60
7:D:23:VAL:HG21	7:D:45:THR:HG21	1.83	0.60
7:D:50:VAL:O	7:D:71:ALA:HA	2.02	0.60
15:M:99:ARG:HH21	15:M:170:ASN:ND2	1.93	0.60
27:Y:115:ARG:HH11	27:Y:115:ARG:HB3	1.66	0.60
1:O:1183:C:H2'	39:O:6752:HOH:O	2.01	0.60
4:A:165:THR:HG22	39:A:9608:HOH:O	2.02	0.60
6:C:107:ARG:HH11	6:C:107:ARG:HB3	1.66	0.60
11:H:58:ARG:HG3	11:H:58:ARG:HH11	1.66	0.60
13:K:107:THR:HG22	13:K:108:GLU:HG3	1.84	0.60
13:K:98:VAL:CG1	13:K:102:GLU:HA	2.31	0.60
15:M:68:ARG:HD3	15:M:68:ARG:O	2.02	0.60
16:N:115:VAL:HG22	39:N:9354:HOH:O	2.00	0.60
2:9:3014:G:C8	2:9:3014:G:H5'	2.36	0.60
6:C:127:ARG:HD3	6:C:129:HIS:HE1	1.67	0.60
1:O:271:C:H41	1:O:378:A:H2	1.46	0.59
1:O:316:A:N3	1:O:336:G:O2'	2.33	0.59
2:9:3076:G:H3'	2:9:3077:A:C5'	2.24	0.59
4:A:121:ALA:O	4:A:124:VAL:HG22	2.02	0.59
32:I:102:VAL:O	32:I:106:LYS:HG3	2.02	0.59
15:M:24:GLN:NE2	15:M:27:ARG:HH11	2.00	0.59
1:O:1838:U:O2'	1:O:2644:C:H5'	2.03	0.59
1:O:289:G:N2	1:O:363:A:H2	1.97	0.59
1:O:1168:C:H5''	32:I:87:THR:HG23	1.83	0.59
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.32	0.59
1:O:1159:G:H1	1:O:1208:C:H42	1.51	0.59
12:J:45:VAL:HG23	12:J:130:VAL:O	2.01	0.59
17:O:39:THR:O	17:O:115:ARG:NH2	2.36	0.59
22:T:19:ARG:HD3	22:T:67:LEU:O	2.03	0.59
32:I:92:PRO:C	32:I:94:GLU:H	2.05	0.59
1:O:2081:A:H4'	12:J:69:TYR:CE1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:O:3151:HOH:O	18:P:81:LYS:HG2	2.01	0.59
25:W:5:VAL:HG22	25:W:32:CYS:HB2	1.84	0.59
1:O:797:A:H4'	28:Z:10:ARG:N	2.18	0.59
10:G:24:VAL:O	10:G:28:GLU:HB2	2.02	0.59
24:V:1:THR:HG23	24:V:2:VAL:N	2.17	0.59
25:W:122:ARG:HG2	25:W:152:ALA:O	2.02	0.59
1:O:328:U:O4'	6:C:202:THR:HG22	2.03	0.59
4:A:105:VAL:HG12	4:A:106:CYS:N	2.18	0.59
1:O:2812:A:C2	1:O:2814:A:N6	2.66	0.59
6:C:236:THR:HG21	39:C:9181:HOH:O	2.03	0.59
12:J:54:VAL:HG11	12:J:138:THR:HG21	1.84	0.59
16:N:154:LEU:O	16:N:155:GLU:HB3	2.02	0.59
22:T:71:VAL:HG12	22:T:72:ILE:N	2.18	0.59
1:O:121:U:OP2	30:2:10:ARG:NH2	2.33	0.59
8:E:85:GLU:HG3	8:E:169:THR:OG1	2.03	0.59
12:J:75:PRO:HB3	12:J:132:LEU:HB3	1.85	0.59
17:O:47:ARG:HG3	17:O:47:ARG:HH11	1.68	0.59
5:B:190:MET:HE2	5:B:194:PHE:CD1	2.36	0.58
25:W:119:HIS:HD2	25:W:120:PRO:O	1.86	0.58
1:O:797:A:C4'	28:Z:10:ARG:N	2.66	0.58
1:O:1626:A:H2'	1:O:1627:G:O4'	2.03	0.58
1:O:2878:U:H2'	1:O:2879:A:O4'	2.03	0.58
1:O:775:G:OP1	29:1:16:HIS:HE1	1.85	0.58
4:A:199:HIS:CD2	4:A:201:PHE:H	2.19	0.58
1:O:1119:G:H8	12:J:52:GLN:HE22	1.52	0.58
1:O:1878:G:O2'	1:O:1879:U:OP2	2.20	0.58
4:A:206:ARG:N	4:A:206:ARG:HD3	2.14	0.58
5:B:125:GLU:O	5:B:129:ARG:HG3	2.03	0.58
1:O:2270:G:H4'	4:A:223:ARG:HH12	1.68	0.58
1:O:256:C:H2'	1:O:257:G:O4'	2.03	0.58
1:O:272:A:H5'	1:O:273:G:OP2	2.04	0.58
5:B:72:THR:HB	39:B:9598:HOH:O	2.02	0.58
25:W:149:LEU:HG	25:W:153:MET:CE	2.33	0.58
1:O:1745:G:H22	1:O:2033:G:H5'	1.68	0.58
1:O:558:C:O2'	1:O:559:U:H5''	2.04	0.58
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.17	0.58
22:T:78:THR:HB	22:T:87:VAL:O	2.04	0.58
1:O:2526:C:O2'	1:O:2527:U:H5'	2.03	0.58
39:O:9972:HOH:O	29:1:1:THR:HA	2.02	0.58
4:A:125:ASN:CB	4:A:158:VAL:HG12	2.34	0.58
8:E:20:ILE:CD1	8:E:40:VAL:HG11	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:49:ILE:HD11	8:E:69:ILE:HD12	1.86	0.58
11:H:154:TYR:HB2	39:H:9557:HOH:O	2.04	0.58
32:I:113:HIS:N	32:I:114:PRO:HD2	2.19	0.58
1:O:2721:U:H4'	13:K:87:ARG:HG3	1.85	0.58
1:O:1973:A:H5'	1:O:1973:A:C8	2.37	0.58
1:O:396:U:O2'	1:O:418:C:H4'	2.04	0.58
8:E:31:ARG:NH1	8:E:68:HIS:CG	2.72	0.58
18:P:16:VAL:HG12	18:P:17:GLY:N	2.18	0.58
27:Y:117:LEU:HA	27:Y:174:VAL:HG11	1.86	0.58
1:O:1333:U:H2'	1:O:1334:C:C6	2.40	0.57
1:O:1736:A:H1'	39:O:8095:HOH:O	2.03	0.57
1:O:871:G:H8	1:O:871:G:H5''	1.68	0.57
4:A:191:GLY:HA2	4:A:194:MET:HE3	1.85	0.57
15:M:182:LYS:O	15:M:194:ALA:HB2	2.04	0.57
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.86	0.57
1:O:2502:C:H2'	1:O:2503:A:H5'	1.86	0.57
8:E:102:VAL:HG11	8:E:148:ILE:HG12	1.86	0.57
25:W:106:THR:OG1	25:W:109:GLU:HG3	2.03	0.57
1:O:1080:C:H4'	1:O:1081:A:OP1	2.03	0.57
1:O:516:A:H5'	39:O:6176:HOH:O	2.05	0.57
18:P:40:VAL:O	18:P:44:VAL:HG23	2.04	0.57
8:E:8:PRO:HB2	8:E:11:VAL:HG23	1.86	0.57
15:M:57:LYS:HE2	15:M:140:ALA:O	2.04	0.57
15:M:71:SER:HB2	15:M:92:THR:HG22	1.85	0.57
1:O:138:U:H5''	1:O:139:C:OP2	2.04	0.57
1:O:2769:C:O2'	1:O:2770:G:H5'	2.05	0.57
1:O:447:A:OP1	22:T:2:LYS:HG2	2.05	0.57
13:K:114:ALA:HB3	13:K:117:VAL:HG23	1.85	0.57
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.70	0.57
1:O:2502:C:C2'	1:O:2503:A:H5'	2.35	0.57
1:O:2769:C:C2'	1:O:2770:G:H5'	2.35	0.57
6:C:139:VAL:HG13	39:C:9253:HOH:O	2.05	0.57
32:I:125:ALA:O	32:I:129:VAL:HG23	2.04	0.57
12:J:71:TYR:CD1	12:J:72:PRO:HD2	2.39	0.57
15:M:74:LYS:HG2	15:M:75:ARG:N	2.20	0.57
16:N:23:ARG:HD3	39:N:9344:HOH:O	2.03	0.57
25:W:125:HIS:CD2	25:W:127:GLY:H	2.23	0.57
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.87	0.57
1:O:1119:G:H8	12:J:52:GLN:NE2	2.02	0.57
5:B:297:VAL:HB	39:B:9598:HOH:O	2.03	0.57
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:485:A:N3	1:0:487:G:H5''	2.20	0.57
1:0:69:A:H5'	1:0:69:A:C8	2.39	0.57
1:0:474:C:O3'	6:C:73:LEU:HD21	2.04	0.57
32:I:134:SER:O	32:I:135:LEU:HD23	2.04	0.57
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.87	0.57
1:0:450:C:OP1	6:C:184:ARG:NH2	2.37	0.57
15:M:68:ARG:NH2	15:M:73:ARG:HD3	2.18	0.57
39:O:7990:HOH:O	15:M:91:ILE:HG23	2.04	0.57
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.34	0.57
1:0:1205:U:H2'	1:0:1206:U:C5'	2.35	0.56
1:0:475:G:OP1	6:C:73:LEU:HD22	2.05	0.56
6:C:25:PRO:HG2	39:C:9125:HOH:O	2.05	0.56
6:C:93:LYS:O	6:C:98:ARG:NH2	2.38	0.56
1:0:1786:C:OP1	18:P:74:GLN:HG2	2.05	0.56
15:M:107:ARG:CG	15:M:107:ARG:HH11	2.14	0.56
1:0:2883:A:H2'	1:0:2884:G:O4'	2.06	0.56
4:A:94:LEU:HG	4:A:99:ILE:HD11	1.86	0.56
5:B:62:ARG:HA	5:B:65:MET:CE	2.36	0.56
1:0:2524:G:H21	1:0:2526:C:H41	1.54	0.56
2:9:3024:U:H3'	2:9:3025:G:H5'	1.87	0.56
7:D:44:ILE:HG12	7:D:83:PHE:HE1	1.71	0.56
1:0:1185:U:H4'	32:I:123:ASN:HB3	1.87	0.56
16:N:169:PRO:O	16:N:172:PHE:HB3	2.05	0.56
22:T:26:THR:HA	22:T:39:ASN:HB3	1.87	0.56
28:Z:42:CYS:SG	28:Z:43:GLY:N	2.77	0.56
6:C:194:PHE:CD2	6:C:234:VAL:HG11	2.39	0.56
18:P:16:VAL:HG13	18:P:20:ARG:NH1	2.20	0.56
1:0:2586:U:H3	1:0:2592:G:H22	1.54	0.56
1:0:291:C:H2'	1:0:292:G:O4'	2.05	0.56
29:1:25:LYS:HE2	39:2:7213:HOH:O	2.04	0.56
29:1:8:GLN:HE22	29:1:11:LYS:NZ	2.03	0.56
9:F:84:GLY:O	9:F:89:LEU:HB2	2.05	0.56
13:K:28:GLU:HB3	13:K:59:LYS:HB2	1.87	0.56
15:M:15:PRO:HA	15:M:20:LEU:HD23	1.87	0.56
1:0:1189:A:H3'	39:0:8201:HOH:O	2.06	0.56
1:0:2421:G:H1'	39:0:4283:HOH:O	2.05	0.56
1:0:2670:G:O2'	1:0:2671:U:H5'	2.05	0.56
5:B:85:ARG:NH1	39:B:9628:HOH:O	2.37	0.56
11:H:99:LYS:HD3	11:H:119:LYS:HD3	1.87	0.56
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.87	0.56
1:0:710:G:H5'	17:O:25:VAL:CG1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2419:U:H5''	1:0:2420:G:H5'	1.87	0.56
24:V:5:VAL:HG23	39:V:2271:HOH:O	2.06	0.56
1:0:151:A:H2'	1:0:152:A:O4'	2.06	0.56
1:0:1979:G:O2'	1:0:1980:U:OP1	2.21	0.56
1:0:316:A:H5'	22:T:54:ASP:OD2	2.05	0.56
6:C:118:THR:HG22	6:C:137:PRO:HB3	1.88	0.56
11:H:166:SER:CB	11:H:167:PRO:HD3	2.36	0.56
12:J:90:LYS:HB2	36:J:9302:CL:CL	2.43	0.56
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.88	0.56
1:0:1118:A:H8	1:0:1119:G:H5''	1.71	0.56
1:0:1819:G:H2'	1:0:1820:G:H4'	1.87	0.56
1:0:2718:C:H6	1:0:2718:C:H5'	1.70	0.56
1:0:2866:U:H4'	1:0:2867:G:H5'	1.86	0.56
7:D:59:GLY:O	7:D:61:PHE:N	2.39	0.56
7:D:23:VAL:HG22	7:D:73:VAL:HB	1.87	0.56
23:U:17:THR:CG2	23:U:18:GLY:N	2.68	0.56
1:0:1979:G:H2'	39:0:3887:HOH:O	2.05	0.55
6:C:162:VAL:HG22	6:C:232:LEU:HD21	1.86	0.55
7:D:138:GLY:N	39:D:7597:HOH:O	2.37	0.55
7:D:136:ARG:NH1	7:D:157:LEU:HA	2.21	0.55
8:E:35:TYR:HA	12:J:127:ILE:HD12	1.88	0.55
8:E:7:ILE:HG22	8:E:45:ASP:O	2.07	0.55
18:P:9:LEU:O	18:P:13:VAL:HG12	2.05	0.55
1:0:1753:C:O2	5:B:229:ARG:NH2	2.39	0.55
5:B:71:VAL:HG11	5:B:296:LEU:HD22	1.88	0.55
16:N:110:THR:HB	16:N:113:SER:OG	2.06	0.55
1:0:2320:U:H4'	1:0:2321:A:O4'	2.06	0.55
1:0:2769:C:H2'	1:0:2770:G:O4'	2.06	0.55
1:0:2807:U:P	5:B:27:ASN:HD21	2.29	0.55
30:2:20:ARG:HD2	30:2:39:ARG:NH2	2.21	0.55
4:A:94:LEU:HD12	4:A:98:GLU:HB2	1.88	0.55
1:0:1189:A:O2'	1:0:1208:C:H2'	2.06	0.55
10:G:12:ILE:N	10:G:13:PRO:CD	2.70	0.55
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.88	0.55
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.88	0.55
25:W:26:ILE:O	25:W:26:ILE:HG13	2.06	0.55
1:0:2904:U:H4'	26:X:8:ARG:NH1	2.22	0.55
1:0:1634:G:H3'	39:0:4470:HOH:O	2.07	0.55
1:0:558:C:H2'	1:0:559:U:H5'	1.88	0.55
5:B:238:ASN:HD22	5:B:240:GLY:N	1.99	0.55
6:C:136:VAL:HG22	6:C:137:PRO:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:69:ALA:HB2	11:H:153:ALA:HB2	1.89	0.55
32:I:105:VAL:HG11	32:I:129:VAL:HG22	1.89	0.55
26:X:43:VAL:HG12	26:X:44:ASP:N	2.22	0.55
1:0:241:A:C2	1:0:378:A:H4'	2.42	0.55
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.72	0.55
31:3:55:VAL:HB	31:3:56:PRO:HD2	1.89	0.55
24:V:29:ASN:O	24:V:33:VAL:HG23	2.07	0.55
24:V:64:GLY:O	24:V:65:ASP:HB2	2.05	0.55
1:0:441:A:H1'	1:0:442:A:N7	2.21	0.55
17:O:59:VAL:HG23	17:O:111:VAL:HG22	1.88	0.55
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.89	0.55
1:0:236:A:H8	1:0:236:A:OP1	1.90	0.55
1:0:2563:U:H2'	1:0:2565:C:O5'	2.07	0.55
1:0:2645:U:OP2	1:0:2645:U:C6	2.60	0.55
12:J:39:VAL:HG11	12:J:107:ASN:CG	2.27	0.55
39:0:7355:HOH:O	15:M:178:LYS:HB2	2.05	0.55
16:N:162:ASP:HA	39:N:9328:HOH:O	2.06	0.55
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.22	0.55
5:B:268:ARG:NH2	5:B:325:PRO:HG3	2.20	0.55
12:J:19:MET:HE1	12:J:132:LEU:CD2	2.33	0.55
1:0:380:A:H2'	39:0:7695:HOH:O	2.06	0.55
1:0:90:A:H2'	1:0:91:G:O4'	2.07	0.55
1:0:1187:U:O2'	1:0:1189:A:H2	1.89	0.54
8:E:3:VAL:CG2	8:E:49:ILE:HB	2.37	0.54
10:G:12:ILE:HD12	39:G:692:HOH:O	2.06	0.54
1:0:1595:G:O2'	1:0:1596:U:H5'	2.08	0.54
1:0:848:C:H5'	39:0:7735:HOH:O	2.08	0.54
10:G:64:ASN:N	10:G:64:ASN:HD22	2.04	0.54
11:H:17:ARG:HD3	11:H:23:ILE:HD12	1.88	0.54
4:A:36:ASP:C	4:A:38:ILE:H	2.10	0.54
8:E:137:ASP:OD1	8:E:139:GLU:HB2	2.08	0.54
9:F:36:THR:HG23	9:F:97:ALA:HB2	1.90	0.54
11:H:170:ASN:N	11:H:170:ASN:HD22	2.03	0.54
11:H:27:LYS:H	11:H:59:HIS:CD2	2.18	0.54
11:H:76:GLU:O	11:H:77:LEU:HD23	2.07	0.54
39:9:1361:HOH:O	16:N:41:LYS:HE3	2.08	0.54
20:R:113:HIS:HE1	20:R:144:GLU:CD	2.10	0.54
6:C:142:ASP:OD1	6:C:236:THR:HG23	2.06	0.54
39:9:4707:HOH:O	16:N:147:ILE:HD12	2.05	0.54
2:9:3051:A:H5'	16:N:160:SER:CB	2.37	0.54
22:T:79:LEU:HG	22:T:89:ARG:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2453:G:H5''	39:L:9439:HOH:O	2.07	0.54
7:D:135:VAL:HG22	7:D:136:ARG:N	2.23	0.54
30:2:36:ASN:HB3	30:2:39:ARG:HG3	1.89	0.54
16:N:183:ASP:O	16:N:184:ILE:O	2.25	0.54
25:W:6:GLN:CB	25:W:26:ILE:HD12	2.35	0.54
9:F:46:GLU:OE1	9:F:100:ASP:HA	2.07	0.54
12:J:131:THR:HG22	12:J:134:GLU:H	1.71	0.54
17:O:25:VAL:HG23	17:O:26:TRP:N	2.22	0.54
18:P:59:ARG:HH22	18:P:66:GLN:HE22	1.55	0.54
1:O:20:G:H21	20:R:117:HIS:HD2	1.56	0.54
22:T:40:VAL:HG22	22:T:41:ARG:N	2.23	0.54
1:O:1189:A:H1'	1:O:1209:C:O4'	2.07	0.54
1:O:185:G:H4'	1:O:186:A:H4'	1.89	0.54
1:O:2032:U:C2'	1:O:2033:G:H5''	2.37	0.54
31:3:38:ARG:HB3	31:3:42:ARG:HH12	1.73	0.54
4:A:33:GLU:CD	4:A:33:GLU:N	2.61	0.54
14:L:136:ALA:HB3	39:L:9469:HOH:O	2.07	0.54
1:O:2827:A:H2'	1:O:2828:G:O4'	2.08	0.54
1:O:2851:G:O2'	1:O:2852:A:H5'	2.07	0.54
16:N:42:HIS:CE1	16:N:75:THR:HG1	2.26	0.54
17:O:98:LEU:O	17:O:102:ILE:HG13	2.08	0.54
28:Z:29:ILE:O	28:Z:33:MET:HB2	2.08	0.54
1:O:1477:C:H5'	1:O:1868:G:H5'	1.90	0.54
19:Q:26:PRO:O	19:Q:30:VAL:HG23	2.06	0.54
1:O:1730:G:H5'	1:O:1731:C:C6	2.43	0.53
1:O:949:U:H4'	19:Q:95:GLU:HA	1.89	0.53
39:O:4794:HOH:O	30:2:38:LYS:HE3	2.08	0.53
27:Y:187:VAL:HG23	27:Y:192:ASP:HB3	1.90	0.53
1:O:621:C:H5'	27:Y:132:ASP:OD2	2.07	0.53
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.37	0.53
18:P:13:VAL:HG11	18:P:40:VAL:CG1	2.37	0.53
28:Z:10:ARG:HA	39:Z:9215:HOH:O	2.07	0.53
1:O:1384:C:H5'	26:X:30:MET:HG2	1.88	0.53
11:H:38:LYS:HE2	11:H:42:ASP:HB2	1.90	0.53
1:O:1164:U:OP1	32:I:74:PRO:HA	2.08	0.53
1:O:1724:U:H5''	39:O:4314:HOH:O	2.08	0.53
39:O:9697:HOH:O	5:B:214:PRO:HD2	2.08	0.53
32:I:129:VAL:O	32:I:129:VAL:HG12	2.08	0.53
32:I:138:THR:HG22	32:I:139:ILE:N	2.23	0.53
1:O:1835:U:C5	1:O:1840:A:N7	2.66	0.53
1:O:466:A:OP1	30:2:38:LYS:HE2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:34:ASP:OD1	4:A:35:GLY:N	2.38	0.53
12:J:47:THR:HG22	12:J:48:GLY:N	2.24	0.53
13:K:109:LEU:CD1	13:K:113:ILE:HD11	2.36	0.53
1:0:1189:A:H1'	1:0:1209:C:C1'	2.37	0.53
1:0:12:U:H2'	1:0:13:G:H5'	1.91	0.53
1:0:182:G:H5'	39:M:9399:HOH:O	2.08	0.53
1:0:500:G:H21	20:R:98:ASN:HD21	1.57	0.53
1:0:2364:A:H5''	19:Q:15:LYS:HD3	1.90	0.53
25:W:4:LEU:O	25:W:32:CYS:HA	2.08	0.53
6:C:107:ARG:HH11	6:C:107:ARG:CB	2.21	0.53
21:S:10:VAL:HG11	24:V:36:ALA:CA	2.38	0.53
24:V:55:ARG:O	24:V:59:ILE:HG12	2.08	0.53
25:W:122:ARG:HH11	25:W:122:ARG:CG	2.21	0.53
26:X:9:VAL:HG22	26:X:88:GLU:OE2	2.09	0.53
1:0:1209:C:H2'	1:0:1210:G:C8	2.43	0.53
1:0:1766:U:O2	1:0:1778:A:H5'	2.09	0.53
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.39	0.53
16:N:32:PRO:HD2	16:N:99:GLU:O	2.09	0.53
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.09	0.53
1:0:1730:G:C5'	1:0:1731:C:C6	2.92	0.53
1:0:288:A:H2'	1:0:289:G:C8	2.43	0.53
9:F:46:GLU:O	9:F:73:PRO:HD2	2.08	0.53
9:F:58:GLU:HA	9:F:61:MET:CE	2.37	0.53
16:N:11:ARG:O	16:N:15:GLU:HG3	2.08	0.53
16:N:12:ARG:HD3	16:N:18:THR:OG1	2.08	0.53
16:N:74:PRO:HG2	16:N:159:TYR:CE1	2.44	0.53
22:T:49:GLU:CB	22:T:59:GLU:HG2	2.38	0.53
25:W:139:GLY:O	25:W:141:HIS:HD2	1.91	0.53
1:0:2815:G:OP2	12:J:99:GLU:HG2	2.09	0.53
7:D:104:PHE:CE2	7:D:166:ILE:HD13	2.44	0.53
7:D:24:HIS:HB2	7:D:72:LYS:HB3	1.91	0.53
7:D:99:ASP:HB2	7:D:103:ASN:O	2.08	0.53
25:W:11:VAL:O	25:W:12:ASN:HB2	2.09	0.53
1:0:1406:A:H4'	1:0:1407:A:C5'	2.39	0.52
1:0:1741:U:H3'	39:0:3367:HOH:O	2.07	0.52
1:0:2795:C:O2'	1:0:2796:U:H5'	2.09	0.52
1:0:603:A:H5''	1:0:604:G:OP1	2.08	0.52
1:0:757:C:OP1	14:L:27:ARG:HD2	2.09	0.52
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.56	0.52
2:9:3076:G:C3'	2:9:3077:A:H5''	2.24	0.52
7:D:24:HIS:HB2	7:D:72:LYS:CB	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:35:TYR:HA	12:J:127:ILE:CD1	2.39	0.52
18:P:105:LEU:CD2	18:P:137:LEU:HD21	2.39	0.52
1:O:2265:U:H2'	1:O:2266:A:C8	2.44	0.52
1:O:2591:C:H2'	1:O:2592:G:O4'	2.08	0.52
1:O:95:A:H5''	1:O:97:G:O4'	2.09	0.52
3:4:176:DA:O4'	3:4:175:C:H2'	2.09	0.52
5:B:102:THR:CG2	5:B:182:VAL:HG12	2.39	0.52
39:O:5513:HOH:O	11:H:58:ARG:HG3	2.08	0.52
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.91	0.52
1:O:447:A:OP1	22:T:1:SER:HB2	2.10	0.52
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.45	0.52
27:Y:212:ARG:HD2	39:Y:9400:HOH:O	2.08	0.52
6:C:236:THR:HG22	6:C:239:ALA:CB	2.39	0.52
1:O:475:G:C5'	6:C:73:LEU:HD23	2.39	0.52
13:K:115:ARG:HG3	13:K:116:GLU:N	2.25	0.52
17:O:59:VAL:HG23	17:O:111:VAL:CG2	2.39	0.52
1:O:1119:G:N2	1:O:1246:A:N1	2.57	0.52
1:O:1252:A:H2'	1:O:1253:C:O4'	2.10	0.52
1:O:248:A:H5'	1:O:249:G:OP2	2.10	0.52
1:O:2894:C:O2'	1:O:2895:C:H5'	2.09	0.52
1:O:920:C:H5''	1:O:921:G:O5'	2.10	0.52
5:B:171:VAL:HG23	5:B:172:SER:N	2.25	0.52
12:J:15:ARG:CZ	12:J:43:ARG:NH1	2.72	0.52
16:N:152:GLU:C	16:N:154:LEU:H	2.13	0.52
18:P:103:THR:O	18:P:107:GLU:HG3	2.09	0.52
1:O:793:A:H5''	18:P:83:LYS:HG2	1.91	0.52
21:S:57:THR:CG2	21:S:58:MET:N	2.73	0.52
1:O:1972:U:H2'	1:O:1973:A:H5'	1.92	0.52
1:O:2443:C:O3'	14:L:56:LYS:HE3	2.10	0.52
6:C:246:ARG:NE	39:C:9230:HOH:O	2.42	0.52
17:O:14:LEU:HG	17:O:102:ILE:HD11	1.91	0.52
19:Q:11:ARG:HD3	39:Q:5620:HOH:O	2.10	0.52
25:W:88:THR:HG22	25:W:90:TYR:HD1	1.74	0.52
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.39	0.52
15:M:31:TRP:HA	15:M:34:GLU:HG3	1.92	0.52
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.74	0.52
1:O:1751:G:C2'	1:O:1752:G:H5''	2.39	0.52
1:O:1926:G:H2'	1:O:1927:A:C8	2.44	0.52
1:O:870:G:C2'	1:O:871:G:H5''	2.37	0.52
4:A:192:VAL:HG11	4:A:207:GLN:HB3	1.90	0.52
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:5:GLU:HG2	23:U:10:GLY:O	2.10	0.52
25:W:64:THR:O	25:W:68:THR:HG22	2.09	0.52
1:O:2587:OMU:H6	1:O:2587:OMU:O5'	2.09	0.52
2:9:3069:U:OP1	16:N:4:PRO:HG3	2.10	0.52
39:O:5938:HOH:O	4:A:164:ARG:CZ	2.57	0.52
6:C:233:THR:HG22	6:C:234:VAL:N	2.24	0.52
7:D:41:LEU:HA	7:D:44:ILE:HG22	1.92	0.52
11:H:40:ALA:HB1	11:H:137:TYR:CE2	2.45	0.52
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.92	0.52
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.43	0.52
1:O:156:C:H5''	15:M:171:ARG:CD	2.28	0.52
1:O:2781:U:H1'	8:E:139:GLU:OE2	2.10	0.52
6:C:246:ARG:CB	6:C:246:ARG:HH11	2.20	0.52
7:D:36:ASN:HA	39:D:7500:HOH:O	2.10	0.52
1:O:1981:A:H1'	1:O:1983:C:N4	2.25	0.51
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.50	0.51
6:C:140:VAL:HB	39:C:9256:HOH:O	2.09	0.51
1:O:545:G:C8	1:O:545:G:H5'	2.41	0.51
29:1:56:GLU:OXT	29:1:56:GLU:HG2	2.10	0.51
6:C:57:PRO:HG2	6:C:73:LEU:HD13	1.92	0.51
11:H:166:SER:HB2	11:H:167:PRO:CD	2.41	0.51
12:J:99:GLU:HA	39:J:7377:HOH:O	2.11	0.51
13:K:75:ARG:HD3	13:K:112:PRO:O	2.10	0.51
1:O:164:G:H4'	14:L:30:ARG:HD3	1.93	0.51
16:N:37:ARG:NH2	39:N:9316:HOH:O	2.29	0.51
20:R:96:VAL:HG13	20:R:106:GLY:HA3	1.92	0.51
23:U:45:GLU:HB2	23:U:48:ASN:ND2	2.24	0.51
27:Y:112:GLU:OE1	27:Y:112:GLU:HA	2.11	0.51
5:B:199:TYR:CE2	5:B:268:ARG:HB2	2.45	0.51
6:C:142:ASP:CG	6:C:237:GLU:HB3	2.30	0.51
15:M:86:GLN:O	15:M:88:VAL:HG23	2.11	0.51
18:P:135:ALA:HB1	18:P:139:ARG:NH1	2.26	0.51
25:W:88:THR:CG2	25:W:89:ASP:H	2.23	0.51
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.46	0.51
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.08	0.51
1:O:969:G:H1	1:O:999:C:N4	2.08	0.51
31:3:16:GLU:HG3	31:3:18:GLN:HE21	1.75	0.51
4:A:66:ARG:HH11	4:A:66:ARG:HB2	1.75	0.51
14:L:120:LEU:HD12	14:L:133:VAL:HG21	1.92	0.51
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.09	0.51
39:K:7438:HOH:O	23:U:20:MET:HE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:119:A:H2'	1:0:120:A:H5''	1.92	0.51
7:D:173:GLU:HG3	7:D:174:VAL:N	2.25	0.51
8:E:5:LEU:HD21	8:E:66:GLN:HG3	1.93	0.51
13:K:81:ARG:HD3	13:K:87:ARG:CZ	2.40	0.51
18:P:16:VAL:HG13	18:P:20:ARG:CZ	2.40	0.51
25:W:29:VAL:O	25:W:30:ASN:HB2	2.11	0.51
28:Z:33:MET:HG3	28:Z:69:TYR:O	2.11	0.51
1:0:204:A:C2'	1:0:205:U:H5'	2.41	0.51
39:9:6497:HOH:O	16:N:23:ARG:HD2	2.09	0.51
1:0:2456:A:H2'	1:0:2457:U:C6	2.46	0.51
1:0:2649:A:H5'	1:0:2649:A:H8	1.76	0.51
8:E:84:MET:HE1	8:E:148:ILE:HD12	1.92	0.51
8:E:15:GLN:NE2	8:E:40:VAL:O	2.43	0.51
11:H:45:VAL:HA	11:H:167:PRO:O	2.10	0.51
13:K:125:ALA:C	13:K:127:ALA:H	2.13	0.51
1:0:1205:U:H2'	1:0:1206:U:H5'	1.93	0.51
30:2:20:ARG:HG3	30:2:21:VAL:N	2.26	0.51
5:B:81:ALA:O	5:B:186:GLY:HA3	2.11	0.51
5:B:212:GLN:HB2	5:B:257:THR:CG2	2.40	0.51
12:J:12:VAL:HG21	12:J:116:LEU:HD11	1.92	0.51
1:0:432:G:O2'	1:0:433:C:H5'	2.11	0.51
31:3:55:VAL:HG22	39:3:9444:HOH:O	2.10	0.51
5:B:42:ALA:HB1	5:B:308:LEU:HD11	1.92	0.51
12:J:93:ARG:NH1	12:J:93:ARG:HB3	2.19	0.51
13:K:30:LYS:O	13:K:55:VAL:HG13	2.10	0.51
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.92	0.51
25:W:88:THR:CG2	25:W:89:ASP:N	2.74	0.51
1:0:625:U:H5'	39:0:3777:HOH:O	2.11	0.51
1:0:776:A:OP1	29:1:28:HIS:HE1	1.94	0.51
4:A:153:ARG:CB	4:A:153:ARG:HH11	2.23	0.51
6:C:133:ARG:NE	6:C:138:VAL:HG22	2.26	0.51
1:0:1946:C:H2'	1:0:1971:G:C8	2.46	0.50
2:9:3003:A:H2'	39:9:2430:HOH:O	2.11	0.50
5:B:62:ARG:HA	5:B:65:MET:HE2	1.93	0.50
7:D:25:MET:HE1	7:D:37:ALA:O	2.11	0.50
1:0:2521:A:OP2	11:H:3:ALA:HB3	2.11	0.50
25:W:149:LEU:HG	25:W:153:MET:HE2	1.93	0.50
5:B:5:ARG:NH1	5:B:8:LYS:HE2	2.26	0.50
11:H:63:GLU:O	11:H:67:LEU:HB2	2.11	0.50
12:J:15:ARG:CZ	12:J:43:ARG:HH11	2.24	0.50
12:J:63:ILE:HG22	12:J:64:GLY:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3004:G:H21	16:N:44:ARG:NH1	2.09	0.50
26:X:31:ILE:O	26:X:35:GLU:HG3	2.11	0.50
1:0:653:C:H2'	1:0:654:A:C8	2.45	0.50
1:0:734:U:H1'	1:0:737:A:N6	2.26	0.50
1:0:968:G:H1'	11:H:32:LYS:HD2	1.92	0.50
30:2:20:ARG:HD2	30:2:39:ARG:HH21	1.76	0.50
4:A:39:ALA:O	4:A:61:GLU:HG3	2.11	0.50
1:0:171:C:OP2	15:M:84:LYS:HG3	2.10	0.50
26:X:20:GLU:HG3	26:X:21:PRO:HD2	1.91	0.50
39:0:5240:HOH:O	28:Z:13:ARG:HD3	2.12	0.50
1:0:2064:U:H5'	1:0:2652:U:O3'	2.11	0.50
4:A:109:GLU:HG2	4:A:116:GLY:N	2.25	0.50
4:A:123:GLY:HA3	4:A:162:GLY:HA2	1.93	0.50
5:B:41:PHE:CG	5:B:79:MET:HE2	2.47	0.50
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.94	0.50
32:I:75:THR:OG1	32:I:112:LYS:HE2	2.11	0.50
25:W:108:ARG:HE	25:W:114:PRO:CG	2.24	0.50
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.93	0.50
1:0:1268:C:O2'	27:Y:169:ARG:HB2	2.12	0.50
4:A:105:VAL:HG12	4:A:106:CYS:H	1.77	0.50
4:A:81:GLN:HB2	4:A:92:ASN:HD21	1.75	0.50
1:0:1180:U:H2'	1:0:1181:A:C8	2.46	0.50
1:0:1234:U:N3	5:B:244:PRO:HB3	2.27	0.50
1:0:284:C:H4'	1:0:285:A:H8	1.76	0.50
1:0:69:A:H5'	1:0:69:A:H8	1.77	0.50
8:E:149:GLU:OE1	8:E:167:TYR:HA	2.12	0.50
9:F:57:GLU:O	9:F:61:MET:HG3	2.12	0.50
11:H:116:ALA:O	11:H:117:PHE:C	2.50	0.50
17:O:78:ALA:C	17:O:98:LEU:HD13	2.32	0.50
1:0:2472:C:O2'	1:0:2634:G:H4'	2.11	0.50
5:B:41:PHE:CD2	5:B:190:MET:HE3	2.47	0.50
5:B:96:PRO:HG3	39:B:9628:HOH:O	2.11	0.50
8:E:11:VAL:HG12	8:E:12:ASP:N	2.27	0.50
15:M:66:SER:HB3	15:M:128:TRP:CD1	2.46	0.50
1:0:1118:A:C8	1:0:1118:A:C3'	2.90	0.50
1:0:2649:A:H5'	1:0:2649:A:C8	2.47	0.50
1:0:558:C:H2'	1:0:559:U:H5''	1.92	0.50
2:9:3028:U:H2'	2:9:3029:C:C6	2.46	0.50
4:A:192:VAL:HG12	4:A:207:GLN:CB	2.41	0.50
5:B:87:TYR:O	5:B:138:GLY:N	2.38	0.50
6:C:79:ARG:O	6:C:87:ARG:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1342:C:C2'	1:0:1343:C:H5'	2.42	0.50
1:0:1730:G:H5'	1:0:1731:C:H5	1.76	0.50
1:0:299:U:H5'	39:0:7794:HOH:O	2.11	0.50
2:9:3012:C:H5'	2:9:3070:U:O4'	2.12	0.50
5:B:145:HIS:HD2	5:B:146:THR:O	1.95	0.50
5:B:312:ARG:HD3	5:B:315:VAL:HG13	1.93	0.50
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.93	0.50
32:I:128:VAL:C	32:I:130:GLY:H	2.15	0.50
25:W:105:THR:HA	25:W:109:GLU:OE1	2.11	0.50
27:Y:154:ARG:HB3	27:Y:154:ARG:HH11	1.77	0.50
30:2:22:PRO:HG2	30:2:25:VAL:HG21	1.93	0.49
1:0:1363:G:OP1	6:C:76:ARG:NH2	2.44	0.49
14:L:145:LEU:O	14:L:145:LEU:HD23	2.12	0.49
14:L:36:ASP:HB2	39:L:9433:HOH:O	2.12	0.49
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.41	0.49
24:V:8:ILE:HA	24:V:11:MET:CE	2.42	0.49
25:W:125:HIS:HD2	25:W:127:GLY:H	1.59	0.49
28:Z:11:SER:O	28:Z:14:PHE:HB2	2.12	0.49
1:0:951:A:C2'	1:0:952:G:H5'	2.41	0.49
39:0:8006:HOH:O	31:3:60:LYS:HG3	2.12	0.49
2:9:3039:U:O2'	2:9:3042:C:C5	2.63	0.49
5:B:17:LYS:O	5:B:260:HIS:HD2	1.95	0.49
7:D:154:LYS:H	7:D:154:LYS:CD	2.22	0.49
9:F:49:PHE:HE1	9:F:98:VAL:HG23	1.77	0.49
11:H:54:THR:O	11:H:55:VAL:HG13	2.13	0.49
32:I:113:HIS:N	32:I:114:PRO:CD	2.75	0.49
14:L:89:PHE:CD1	14:L:89:PHE:N	2.80	0.49
24:V:56:ILE:HG22	24:V:60:GLN:HE21	1.77	0.49
1:0:1666:C:H2'	1:0:1667:A:C5'	2.41	0.49
1:0:1730:G:C5'	1:0:1731:C:H6	2.24	0.49
18:P:105:LEU:HD21	18:P:137:LEU:HD21	1.94	0.49
22:T:96:VAL:CG1	22:T:97:ARG:N	2.75	0.49
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.94	0.49
27:Y:96:GLU:O	27:Y:235:GLU:HA	2.12	0.49
1:0:1189:A:H1'	1:0:1209:C:H1'	1.95	0.49
1:0:1462:C:H2'	1:0:1463:A:C8	2.48	0.49
1:0:1972:U:H2'	1:0:1973:A:C5'	2.43	0.49
4:A:104:PRO:HG3	4:A:127:GLN:OE1	2.12	0.49
12:J:39:VAL:CG1	12:J:40:ASN:N	2.75	0.49
17:O:96:VAL:CG1	17:O:100:GLN:HB2	2.41	0.49
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:41:PHE:O	26:X:43:VAL:HG23	2.13	0.49
4:A:167:LYS:HB2	28:Z:29:ILE:HD13	1.94	0.49
1:0:2326:U:H4'	1:0:2412:G:C4'	2.42	0.49
1:0:949:U:O2'	19:Q:40:HIS:HE1	1.95	0.49
5:B:74:ILE:HD13	5:B:309:VAL:HG21	1.95	0.49
1:0:2548:C:OP2	5:B:5:ARG:NH2	2.45	0.49
8:E:22:VAL:O	8:E:28:SER:HA	2.12	0.49
11:H:28:ILE:HG23	39:H:9544:HOH:O	2.12	0.49
11:H:58:ARG:O	11:H:62:LEU:HD22	2.12	0.49
12:J:74:ARG:HH12	12:J:76:ASP:CB	2.25	0.49
14:L:104:ASP:HB2	39:L:9458:HOH:O	2.12	0.49
14:L:143:THR:CG2	14:L:144:ASP:N	2.75	0.49
14:L:148:GLU:HB2	39:L:9485:HOH:O	2.12	0.49
30:2:41:HIS:HD2	30:2:44:ARG:H	1.60	0.49
30:2:48:ASP:O	30:2:49:GLU:HB2	2.13	0.49
5:B:139:ASP:HB3	39:B:9547:HOH:O	2.12	0.49
9:F:39:SER:HB3	9:F:45:ALA:HB2	1.93	0.49
32:I:113:HIS:HE1	32:I:121:LEU:HD22	1.75	0.49
32:I:118:SER:HB2	32:I:123:ASN:HB2	1.94	0.49
12:J:15:ARG:NH1	12:J:43:ARG:NH1	2.61	0.49
13:K:55:VAL:CG1	13:K:56:SER:N	2.75	0.49
14:L:145:LEU:O	14:L:148:GLU:HG3	2.11	0.49
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.12	0.49
1:0:2852:A:H5''	39:0:5766:HOH:O	2.11	0.49
1:0:449:A:N7	6:C:43:LYS:HG2	2.27	0.49
7:D:103:ASN:ND2	7:D:134:LEU:H	2.10	0.49
32:I:138:THR:HG22	32:I:139:ILE:H	1.77	0.49
1:0:2815:G:N7	12:J:80:LYS:NZ	2.60	0.49
24:V:39:ALA:N	24:V:40:PRO:CD	2.73	0.49
1:0:1466:C:H42	1:0:1476:A:N6	1.98	0.49
1:0:558:C:C2'	1:0:559:U:C5'	2.91	0.49
1:0:816:G:H5'	1:0:1598:A:H4'	1.94	0.49
12:J:52:GLN:HG3	12:J:53:ILE:N	2.27	0.49
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.33	0.49
20:R:122:GLN:HB3	20:R:138:SER:HB2	1.93	0.49
27:Y:148:GLY:O	27:Y:154:ARG:HD3	2.12	0.49
1:0:1477:C:H2'	1:0:1478:U:C6	2.48	0.49
1:0:603:A:H4'	1:0:604:G:O5'	2.12	0.49
2:9:3049:G:O2'	2:9:3050:G:H5'	2.12	0.49
4:A:36:ASP:O	4:A:38:ILE:N	2.46	0.49
5:B:53:LEU:CD1	5:B:327:VAL:HG22	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:29:LYS:NZ	39:R:9453:HOH:O	2.46	0.49
1:O:2712:G:H5'	39:K:4183:HOH:O	2.13	0.49
4:A:65:ARG:C	4:A:66:ARG:HG3	2.32	0.49
6:C:168:ARG:NH2	6:C:190:ALA:O	2.46	0.49
1:O:1056:U:H2'	1:O:1057:A:O4'	2.13	0.48
1:O:1175:G:H1'	1:O:1193:A:C2'	2.41	0.48
1:O:1466:C:N4	1:O:1476:A:H61	1.98	0.48
1:O:1503:U:H2'	1:O:1504:A:O4'	2.13	0.48
1:O:247:A:H2'	39:O:4499:HOH:O	2.12	0.48
1:O:542:A:H2'	1:O:543:G:O4'	2.13	0.48
1:O:666:A:H2'	1:O:667:C:O4'	2.13	0.48
1:O:883:U:H2'	1:O:883:U:O2	2.12	0.48
4:A:105:VAL:HG13	4:A:155:THR:O	2.13	0.48
1:O:2453:G:H4'	14:L:50:GLY:C	2.33	0.48
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.95	0.48
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.43	0.48
24:V:64:GLY:O	24:V:65:ASP:CB	2.61	0.48
1:O:2779:G:H21	8:E:143:GLN:NE2	2.11	0.48
1:O:2906:A:H5'	1:O:2907:C:O4'	2.13	0.48
2:9:3054:A:O2'	2:9:3055:U:H5'	2.13	0.48
6:C:154:VAL:O	6:C:158:GLU:HG3	2.13	0.48
1:O:2090:G:H2'	1:O:2091:G:C8	2.48	0.48
1:O:2237:G:H1'	1:O:2238:A:C8	2.48	0.48
30:2:36:ASN:HB3	30:2:39:ARG:NE	2.28	0.48
5:B:75:GLU:C	5:B:77:PRO:HD3	2.32	0.48
7:D:154:LYS:HD2	7:D:154:LYS:N	2.22	0.48
8:E:81:GLU:HA	8:E:133:VAL:O	2.13	0.48
11:H:170:ASN:N	11:H:170:ASN:ND2	2.60	0.48
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.94	0.48
18:P:115:SER:N	18:P:118:GLN:HE21	2.04	0.48
27:Y:203:VAL:CG1	27:Y:228:VAL:HG22	2.43	0.48
1:O:1878:G:O2'	1:O:1879:U:C5	2.62	0.48
1:O:2414:A:H2'	1:O:2415:A:C8	2.49	0.48
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.48	0.48
2:9:3044:A:O4'	7:D:76:ARG:NE	2.46	0.48
1:O:2545:U:OP2	5:B:2:GLN:NE2	2.47	0.48
9:F:57:GLU:HB2	15:M:23:LEU:HD11	1.94	0.48
12:J:45:VAL:HG21	12:J:129:PHE:CD1	2.49	0.48
13:K:49:LEU:HD12	13:K:80:ILE:HD13	1.94	0.48
39:O:7257:HOH:O	16:N:4:PRO:HD2	2.13	0.48
1:O:1506:U:H6	1:O:1506:U:H5'	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1552:G:N2	1:0:1634:G:H1'	2.29	0.48
1:0:185:G:O3'	1:0:186:A:H4'	2.14	0.48
6:C:236:THR:HA	39:C:9256:HOH:O	2.13	0.48
9:F:91:VAL:CG1	9:F:92:GLY:H	2.11	0.48
18:P:89:ASN:OD1	18:P:92:GLU:HB2	2.13	0.48
1:0:1249:U:H2'	1:0:1250:C:C6	2.49	0.48
1:0:1667:A:C8	1:0:1667:A:H5'	2.39	0.48
4:A:88:ILE:HG22	4:A:88:ILE:O	2.13	0.48
17:O:32:ARG:HB2	39:O:4656:HOH:O	2.14	0.48
28:Z:36:ASP:HB3	28:Z:45:ASP:O	2.14	0.48
1:0:1205:U:H2'	1:0:1206:U:H5''	1.96	0.48
1:0:1377:C:H5'	1:0:1377:C:C6	2.45	0.48
1:0:602:A:O2'	1:0:605:C:H4'	2.14	0.48
1:0:120:A:H5'	29:1:20:ARG:HH21	1.79	0.48
31:3:16:GLU:HG3	31:3:18:GLN:NE2	2.29	0.48
16:N:58:LEU:N	16:N:58:LEU:HD12	2.28	0.48
24:V:39:ALA:O	24:V:41:GLU:N	2.42	0.48
25:W:21:LEU:HB3	25:W:26:ILE:CG1	2.44	0.48
1:0:1878:G:C1'	39:O:6632:HOH:O	2.56	0.48
1:0:2072:G:C6	1:0:2533:C:H1'	2.49	0.48
1:0:2365:G:H5''	39:Q:6597:HOH:O	2.12	0.48
31:3:65:THR:CG2	31:3:88:LEU:HD22	2.44	0.48
5:B:321:PRO:HA	39:B:9650:HOH:O	2.12	0.48
7:D:60:GLU:O	7:D:60:GLU:HG3	2.13	0.48
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.28	0.48
25:W:108:ARG:CG	25:W:114:PRO:HG3	2.42	0.48
28:Z:40:PRO:C	28:Z:42:CYS:H	2.17	0.48
1:0:834:G:H3'	1:0:835:U:H4'	1.96	0.48
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.13	0.48
5:B:5:ARG:HH11	5:B:8:LYS:HE2	1.77	0.48
7:D:25:MET:SD	7:D:40:ILE:HD11	2.54	0.48
15:M:187:LEU:HD23	15:M:194:ALA:HB3	1.95	0.48
21:S:33:SER:O	21:S:37:VAL:HG23	2.13	0.48
21:S:37:VAL:O	21:S:41:VAL:HG23	2.13	0.48
24:V:39:ALA:H	24:V:40:PRO:HD2	1.75	0.48
1:0:2415:A:O2'	16:N:29:SER:HB3	2.13	0.48
1:0:88:G:H2'	1:0:89:G:C8	2.49	0.48
12:J:80:LYS:NZ	39:J:7377:HOH:O	2.46	0.48
1:0:1163:G:H1	1:0:1184:C:N4	2.12	0.47
1:0:1789:G:O6	18:P:73:HIS:HE1	1.97	0.47
1:0:2851:G:H4'	5:B:157:LYS:NZ	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:396:U:OP2	31:3:38:ARG:HD2	2.13	0.47
1:0:830:G:O2'	1:0:831:U:H5'	2.14	0.47
31:3:3:MET:O	31:3:90:PHE:HA	2.14	0.47
5:B:254:GLN:HG3	39:B:9530:HOH:O	2.13	0.47
1:0:2338:G:OP1	7:D:97:GLN:HG2	2.14	0.47
32:I:116:LEU:HD22	32:I:127:GLU:OE1	2.13	0.47
32:I:139:ILE:HG22	32:I:140:GLU:N	2.29	0.47
5:B:91:PRO:O	12:J:144:THR:HG21	2.14	0.47
17:O:73:ASP:HA	17:O:92:VAL:O	2.14	0.47
23:U:52:THR:HG22	23:U:54:THR:H	1.78	0.47
24:V:1:THR:CG2	24:V:2:VAL:H	2.15	0.47
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.29	0.47
1:0:1787:C:OP1	18:P:68:LYS:HE2	2.13	0.47
1:0:2421:G:H4'	39:0:5325:HOH:O	2.13	0.47
1:0:343:C:O2'	1:0:344:C:H5'	2.13	0.47
1:0:484:A:N1	1:0:506:G:H4'	2.28	0.47
2:9:3064:C:C2'	2:9:3065:A:H5'	2.44	0.47
5:B:58:PRO:HA	5:B:63:GLU:OE2	2.14	0.47
6:C:214:THR:HG23	39:C:9243:HOH:O	2.14	0.47
16:N:69:TYR:HE2	16:N:184:ILE:HG13	1.79	0.47
19:Q:75:ILE:HD13	19:Q:84:ILE:HD11	1.95	0.47
1:0:2856:A:P	26:X:15:ARG:HH22	2.36	0.47
1:0:482:G:H4'	1:0:508:A:N1	2.29	0.47
4:A:207:GLN:O	4:A:208:HIS:HB3	2.14	0.47
6:C:246:ARG:NH1	39:C:9177:HOH:O	2.46	0.47
12:J:142:ASN:O	12:J:144:THR:N	2.48	0.47
13:K:87:ARG:NH1	39:K:4066:HOH:O	2.48	0.47
15:M:77:HIS:CD2	15:M:79:ALA:O	2.65	0.47
17:O:42:GLU:HB2	39:O:2176:HOH:O	2.14	0.47
18:P:141:ILE:C	18:P:143:ALA:H	2.17	0.47
27:Y:186:ARG:HH11	27:Y:186:ARG:HG2	1.78	0.47
1:0:1236:A:H2'	1:0:1237:U:O4'	2.14	0.47
1:0:920:C:H4'	1:0:921:G:C2	2.50	0.47
1:0:952:G:N3	1:0:2302:A:H2'	2.29	0.47
4:A:203:GLY:HA2	39:A:9535:HOH:O	2.14	0.47
39:0:5171:HOH:O	4:A:6:GLY:HA3	2.14	0.47
5:B:205:VAL:O	5:B:307:ARG:NE	2.40	0.47
11:H:58:ARG:HG3	11:H:58:ARG:NH1	2.29	0.47
17:O:15:LYS:HD3	17:O:19:ARG:NH2	2.29	0.47
20:R:132:ARG:NH2	39:R:9495:HOH:O	2.47	0.47
1:0:1086:A:C6	25:W:11:VAL:HG11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:155:ARG:NH1	39:Y:9357:HOH:O	2.46	0.47
2:9:3042:C:H5'	2:9:3043:G:OP2	2.14	0.47
4:A:223:ARG:NE	39:A:9563:HOH:O	2.47	0.47
4:A:53:ALA:HB3	39:A:9595:HOH:O	2.13	0.47
4:A:89:ALA:HB3	39:A:9614:HOH:O	2.14	0.47
5:B:41:PHE:CG	5:B:190:MET:HE3	2.50	0.47
18:P:13:VAL:HG11	18:P:40:VAL:HG11	1.96	0.47
1:0:1211:G:O2'	1:0:1212:C:H5'	2.14	0.47
1:0:622:G:P	27:Y:148:GLY:HA3	2.54	0.47
1:0:697:G:H4'	1:0:730:G:O3'	2.15	0.47
1:0:1853:C:OP1	4:A:231:LYS:HG3	2.15	0.47
1:0:2670:G:H5'	5:B:112:THR:O	2.15	0.47
12:J:22:VAL:O	12:J:26:VAL:HG23	2.15	0.47
12:J:59:LYS:O	12:J:63:ILE:HG13	2.14	0.47
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.44	0.47
17:O:53:GLN:HG2	17:O:56:GLU:OE1	2.15	0.47
22:T:71:VAL:HG13	22:T:91:LEU:O	2.14	0.47
1:0:2747:C:H4'	39:O:8438:HOH:O	2.14	0.47
5:B:277:GLU:N	5:B:278:PRO:HD2	2.29	0.47
8:E:86:VAL:HG12	8:E:129:GLU:O	2.15	0.47
14:L:57:VAL:HG12	14:L:57:VAL:O	2.14	0.47
17:O:47:ARG:HG3	17:O:47:ARG:NH1	2.29	0.47
24:V:11:MET:HB3	24:V:15:GLU:HB2	1.96	0.47
26:X:20:GLU:HG3	26:X:21:PRO:CD	2.45	0.47
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.94	0.47
1:0:1066:U:H2'	1:0:1067:A:C8	2.50	0.47
1:0:204:A:H2'	1:0:205:U:H5'	1.96	0.47
1:0:2820:A:H2'	1:0:2821:C:C6	2.50	0.47
1:0:475:G:H5'	6:C:73:LEU:HD23	1.95	0.47
31:3:42:ARG:HH11	31:3:42:ARG:HG3	1.78	0.47
1:0:2694:A:H4'	8:E:91:PHE:CE1	2.49	0.47
10:G:63:ARG:HB2	10:G:66:LEU:HG	1.96	0.47
12:J:63:ILE:CG2	12:J:64:GLY:N	2.77	0.47
1:0:1992:U:OP2	13:K:66:ARG:HD2	2.14	0.47
14:L:119:THR:HG23	14:L:139:SER:OG	2.15	0.47
14:L:143:THR:CG2	14:L:144:ASP:H	2.22	0.47
25:W:48:VAL:CG1	25:W:48:VAL:O	2.62	0.47
1:0:196:G:H2'	39:O:7143:HOH:O	2.14	0.47
1:0:2503:A:OP1	11:H:151:ARG:NH2	2.47	0.47
1:0:447:A:O2'	1:0:448:G:H5'	2.15	0.47
4:A:69:LEU:HD23	4:A:107:ASN:CB	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:22:VAL:HG22	7:D:74:THR:HG22	1.97	0.47
1:O:1242:A:C5'	12:J:82:THR:HG23	2.34	0.47
15:M:107:ARG:CG	15:M:107:ARG:NH1	2.73	0.47
15:M:60:VAL:C	15:M:61:ILE:HD12	2.35	0.47
20:R:119:VAL:HG21	20:R:142:ASP:CG	2.35	0.47
22:T:78:THR:HG22	22:T:88:PRO:HA	1.96	0.47
24:V:8:ILE:HG21	24:V:59:ILE:HG13	1.96	0.47
27:Y:144:ARG:CG	27:Y:144:ARG:NH1	2.67	0.47
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.55	0.47
1:O:1624:A:H4'	1:O:1625:U:H5'	1.96	0.47
1:O:2587:OMU:H2'	1:O:2589:U:H5''	1.96	0.47
1:O:2717:C:O2'	1:O:2718:C:H5''	2.14	0.47
1:O:677:C:H4'	6:C:246:ARG:NH2	2.30	0.47
1:O:2333:G:P	7:D:56:ARG:HH22	2.38	0.47
9:F:5:ASP:O	9:F:119:ARG:NH1	2.48	0.47
1:O:1118:A:C8	1:O:1119:G:H5''	2.49	0.47
1:O:1236:A:C8	12:J:63:ILE:HD11	2.50	0.47
1:O:1328:A:C8	27:Y:169:ARG:HD3	2.49	0.47
1:O:2296:C:H2'	1:O:2297:U:H6	1.80	0.47
1:O:2456:A:H2'	1:O:2457:U:H6	1.80	0.47
1:O:737:A:H2'	1:O:738:G:O4'	2.15	0.47
1:O:820:G:O2'	1:O:856:G:H4'	2.15	0.47
8:E:77:THR:OG1	8:E:78:GLU:N	2.47	0.47
9:F:52:GLU:HG3	9:F:77:VAL:O	2.15	0.47
32:I:87:THR:HG22	32:I:88:GLY:N	2.30	0.47
21:S:73:ASP:OD1	21:S:76:GLU:HG3	2.15	0.47
22:T:89:ARG:HG3	22:T:89:ARG:O	2.15	0.47
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.31	0.47
27:Y:235:GLU:CD	27:Y:235:GLU:N	2.58	0.47
1:O:1422:U:H2'	1:O:1423:C:C6	2.50	0.46
1:O:1755:A:H2'	1:O:1756:G:O4'	2.15	0.46
1:O:2112:A:H2'	1:O:2113:G:C8	2.50	0.46
1:O:2784:A:H1'	8:E:60:SER:OG	2.15	0.46
1:O:664:U:O4	1:O:681:G:H5''	2.15	0.46
2:9:3049:G:H5''	39:9:4707:HOH:O	2.14	0.46
6:C:127:ARG:HD3	6:C:129:HIS:CE1	2.48	0.46
14:L:93:VAL:HG12	14:L:97:VAL:HG23	1.97	0.46
23:U:39:ASN:ND2	23:U:44:ARG:NH1	2.63	0.46
24:V:5:VAL:CG1	24:V:9:ARG:NH1	2.78	0.46
26:X:23:HIS:CD2	26:X:24:LYS:HG3	2.49	0.46
26:X:30:MET:CE	26:X:58:ALA:HB3	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2372:A:H2'	1:0:2373:U:C6	2.51	0.46
1:0:2326:U:H4'	1:0:2412:G:H4'	1.98	0.46
1:0:812:A:H1'	39:0:4533:HOH:O	2.15	0.46
5:B:30:PRO:HB2	5:B:39:GLN:NE2	2.30	0.46
1:0:1180:U:O2'	32:I:92:PRO:HD2	2.15	0.46
12:J:42:GLU:O	12:J:131:THR:HG23	2.15	0.46
16:N:48:VAL:HG11	16:N:55:ASP:HB3	1.98	0.46
26:X:43:VAL:HG12	26:X:47:ALA:HB3	1.97	0.46
1:0:1192:A:H3'	1:0:1193:A:H5'	1.97	0.46
1:0:177:A:H2'	1:0:178:U:O4'	2.15	0.46
2:9:3029:C:C2'	2:9:3030:C:H5'	2.45	0.46
5:B:36:PRO:CA	5:B:168:GLY:HA3	2.40	0.46
5:B:88:GLU:HB3	5:B:97:LEU:HD12	1.98	0.46
16:N:11:ARG:CG	16:N:14:ARG:HH12	2.25	0.46
16:N:89:GLY:O	16:N:92:ALA:HB3	2.15	0.46
18:P:135:ALA:HB1	18:P:139:ARG:HH12	1.79	0.46
20:R:99:ALA:HB1	20:R:109:MET:HE3	1.95	0.46
1:0:304:G:H1'	1:0:347:A:N6	2.31	0.46
2:9:3049:G:H2'	2:9:3050:G:O4'	2.16	0.46
2:9:3114:G:O6	16:N:11:ARG:HD3	2.15	0.46
9:F:48:VAL:HG12	9:F:97:ALA:CB	2.46	0.46
11:H:66:ARG:HD3	39:H:9544:HOH:O	2.15	0.46
14:L:10:SER:O	14:L:11:ARG:HB3	2.15	0.46
39:0:5491:HOH:O	15:M:82:ARG:HD3	2.15	0.46
4:A:101:GLU:OE2	4:A:131:HIS:HB2	2.16	0.46
12:J:76:ASP:HA	39:J:5907:HOH:O	2.16	0.46
1:0:903:U:O4	14:L:18:HIS:HB2	2.15	0.46
15:M:59:GLY:HA3	15:M:141:ILE:HD12	1.96	0.46
25:W:35:VAL:HA	25:W:36:PRO:HD3	1.86	0.46
1:0:1044:C:H5''	39:0:9648:HOH:O	2.15	0.46
1:0:107:U:H2'	1:0:108:U:H5'	1.98	0.46
7:D:172:VAL:CG1	7:D:173:GLU:H	2.20	0.46
11:H:29:ALA:C	11:H:30:GLN:HG3	2.35	0.46
15:M:122:GLN:OE1	15:M:127:LYS:HE2	2.15	0.46
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.80	0.46
21:S:29:ASP:OD1	21:S:31:ARG:NH1	2.49	0.46
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.16	0.46
1:0:1829:A:H61	28:Z:18:TYR:H	1.64	0.46
1:0:2346:C:O5'	1:0:2346:C:H6	1.97	0.46
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.96	0.46
5:B:185:GLY:HA2	39:B:9627:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:254:GLN:HG2	5:B:255:GLY:H	1.81	0.46
6:C:118:THR:CG2	6:C:137:PRO:HB3	2.45	0.46
1:O:894:A:N1	6:C:87:ARG:NH2	2.63	0.46
7:D:18:ILE:HG12	7:D:134:LEU:HD23	1.97	0.46
7:D:49:PRO:HB3	39:D:5828:HOH:O	2.16	0.46
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.46	0.46
9:F:65:GLU:O	9:F:69:GLU:HG2	2.15	0.46
13:K:20:CYS:HB2	13:K:29:LEU:HG	1.98	0.46
15:M:22:GLU:HG2	15:M:26:GLN:NE2	2.31	0.46
1:O:1441:G:O2'	1:O:1442:A:H5'	2.16	0.46
1:O:1942:A:H3'	39:O:7801:HOH:O	2.16	0.46
1:O:2642:G:H2'	1:O:2643:G:O4'	2.16	0.46
39:O:8006:HOH:O	31:3:61:PRO:HG2	2.16	0.46
2:9:3024:U:H3'	2:9:3025:G:C5'	2.46	0.46
2:9:3091:C:H2'	2:9:3092:G:O4'	2.16	0.46
39:O:4967:HOH:O	4:A:11:ARG:CZ	2.64	0.46
4:A:171:LYS:NZ	39:A:9513:HOH:O	2.48	0.46
5:B:321:PRO:HG3	39:B:9593:HOH:O	2.15	0.46
10:G:64:ASN:N	10:G:64:ASN:ND2	2.63	0.46
32:I:75:THR:HA	32:I:112:LYS:NZ	2.31	0.46
16:N:154:LEU:O	16:N:155:GLU:CB	2.64	0.46
26:X:78:GLU:HG2	26:X:79:GLU:OE2	2.15	0.46
4:A:130:THR:HG22	4:A:131:HIS:O	2.15	0.46
5:B:301:VAL:HG11	5:B:309:VAL:HG11	1.97	0.46
6:C:218:VAL:HG12	39:C:9230:HOH:O	2.15	0.46
8:E:106:ASN:ND2	8:E:109:GLY:HA2	2.30	0.46
8:E:118:ILE:HG23	8:E:144:THR:HG21	1.98	0.46
8:E:114:ARG:HB3	8:E:151:LEU:HD11	1.97	0.46
11:H:9:ILE:HD12	11:H:54:THR:HG22	1.98	0.46
14:L:80:ASP:HB2	14:L:90:ARG:HB3	1.98	0.46
16:N:8:VAL:CG1	16:N:14:ARG:HE	2.29	0.46
17:O:38:ARG:NH1	39:O:7674:HOH:O	2.49	0.46
26:X:76:ARG:NH1	26:X:76:ARG:HG3	2.30	0.46
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.51	0.46
1:O:136:C:H2'	1:O:137:U:O4'	2.15	0.46
1:O:1574:C:H2'	1:O:1575:C:C6	2.52	0.46
1:O:1666:C:C2'	1:O:1667:A:C5'	2.94	0.46
1:O:1902:G:H2'	1:O:1903:U:O4'	2.16	0.46
1:O:2825:C:H4'	1:O:2826:G:O5'	2.17	0.46
39:O:7688:HOH:O	4:A:11:ARG:HA	2.16	0.46
1:O:1311:G:O6	6:C:173:LYS:HE3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:10:PHE:CE1	7:D:11:HIS:HB3	2.51	0.46
17:O:24:ALA:O	17:O:28:ASP:HB2	2.16	0.46
22:T:71:VAL:CG1	22:T:72:ILE:N	2.78	0.46
1:O:2904:U:H4'	26:X:8:ARG:HH12	1.80	0.46
27:Y:152:LYS:HB3	27:Y:160:LYS:HG3	1.98	0.46
1:O:2824:C:H5''	1:O:2825:C:H5'	1.98	0.45
5:B:36:PRO:HB3	5:B:174:ARG:CB	2.46	0.45
5:B:190:MET:CE	5:B:194:PHE:CD1	3.00	0.45
9:F:48:VAL:HG12	9:F:97:ALA:HB2	1.98	0.45
11:H:158:THR:HB	11:H:159:PRO:HD3	1.99	0.45
1:O:926:A:H5'	14:L:39:GLU:OE2	2.16	0.45
19:Q:31:GLU:CD	19:Q:93:ARG:HH12	2.19	0.45
21:S:33:SER:OG	21:S:36:GLU:HG3	2.17	0.45
25:W:72:PRO:HB2	25:W:74:GLU:O	2.15	0.45
27:Y:209:VAL:HG12	27:Y:214:ARG:HG3	1.97	0.45
1:O:2270:G:H4'	4:A:223:ARG:NH1	2.31	0.45
1:O:2821:C:H4'	5:B:116:PRO:HG3	1.97	0.45
6:C:115:LEU:O	6:C:118:THR:HB	2.16	0.45
10:G:16:LYS:O	10:G:20:VAL:HG23	2.15	0.45
11:H:54:THR:HG23	11:H:128:GLN:HA	1.97	0.45
11:H:146:VAL:HG22	39:H:9541:HOH:O	2.16	0.45
1:O:1163:G:H5'	32:I:115:ASP:O	2.17	0.45
32:I:92:PRO:C	32:I:94:GLU:N	2.70	0.45
15:M:74:LYS:HG3	39:M:9384:HOH:O	2.16	0.45
19:Q:3:SER:HB3	39:Q:5998:HOH:O	2.17	0.45
25:W:38:THR:CG2	25:W:39:ASP:N	2.78	0.45
25:W:88:THR:CG2	25:W:90:TYR:HD1	2.28	0.45
28:Z:56:GLN:HA	28:Z:62:TYR:O	2.16	0.45
1:O:1741:U:O2'	1:O:2723:G:H4'	2.17	0.45
1:O:2769:C:H2'	1:O:2770:G:C5'	2.45	0.45
39:O:7612:HOH:O	29:1:1:THR:HB	2.16	0.45
32:I:75:THR:HA	32:I:112:LYS:HZ3	1.81	0.45
17:O:60:VAL:C	17:O:62:GLY:H	2.20	0.45
19:Q:75:ILE:HD13	19:Q:84:ILE:CD1	2.46	0.45
25:W:96:LEU:O	25:W:100:LEU:HG	2.16	0.45
1:O:1165:G:H1'	1:O:1174:A:H1'	1.98	0.45
1:O:1714:C:O2'	1:O:1715:C:H5'	2.17	0.45
1:O:292:G:H2'	1:O:358:G:N2	2.32	0.45
5:B:24:PRO:HG3	5:B:204:GLY:HA2	1.97	0.45
14:L:134:GLU:HG3	39:L:9453:HOH:O	2.17	0.45
16:N:154:LEU:HG	16:N:155:GLU:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1771:U:H5'	28:Z:20:ARG:NH2	2.31	0.45
1:0:2508:C:H2'	39:0:7239:HOH:O	2.17	0.45
1:0:286:U:H2'	1:0:287:C:C6	2.52	0.45
1:0:396:U:H1'	39:0:8151:HOH:O	2.17	0.45
1:0:1881:A:OP1	4:A:199:HIS:HE1	1.99	0.45
1:0:1654:U:H2'	4:A:47:HIS:CD2	2.51	0.45
4:A:88:ILE:HD13	4:A:100:PRO:CD	2.45	0.45
4:A:94:LEU:N	4:A:94:LEU:HD23	2.32	0.45
5:B:58:PRO:HA	5:B:63:GLU:CD	2.36	0.45
6:C:133:ARG:NH1	39:C:9218:HOH:O	2.49	0.45
39:0:8228:HOH:O	6:C:94:THR:HG21	2.16	0.45
32:I:99:ASP:O	32:I:100:LEU:HD23	2.17	0.45
23:U:9:CYS:HA	23:U:52:THR:HG23	1.99	0.45
1:0:1025:C:H5'	25:W:23:MET:O	2.17	0.45
1:0:1299:G:N2	39:0:5228:HOH:O	2.49	0.45
1:0:1419:U:H2'	1:0:1685:A:C2	2.52	0.45
1:0:1878:G:O2'	1:0:1879:U:P	2.74	0.45
1:0:2072:G:H3'	1:0:2073:G:C5'	2.47	0.45
1:0:2312:G:H2'	1:0:2313:C:H5'	1.98	0.45
1:0:945:U:H2'	1:0:946:C:C6	2.51	0.45
4:A:70:ALA:HA	4:A:71:PRO:HD3	1.78	0.45
5:B:14:GLY:HA2	5:B:15:PRO:C	2.36	0.45
9:F:60:VAL:O	9:F:60:VAL:CG1	2.64	0.45
10:G:64:ASN:O	10:G:68:GLU:HG3	2.17	0.45
12:J:26:VAL:HG13	12:J:36:VAL:HG11	1.99	0.45
15:M:107:ARG:NH2	39:M:9399:HOH:O	2.48	0.45
1:0:818:A:O2'	28:Z:13:ARG:HD2	2.16	0.45
1:0:1717:A:H5''	18:P:54:LYS:HB2	1.97	0.45
1:0:2361:A:H2'	1:0:2362:A:C8	2.51	0.45
1:0:2626:C:H2'	1:0:2627:G:C8	2.52	0.45
31:3:91:GLN:O	31:3:92:GLU:HB2	2.17	0.45
7:D:49:PRO:HA	7:D:73:VAL:HG22	1.98	0.45
7:D:95:THR:OG1	7:D:174:VAL:HG22	2.16	0.45
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.32	0.45
12:J:88:PRO:O	12:J:94:GLY:HA3	2.17	0.45
9:F:38:LYS:NZ	15:M:3:SER:HA	2.32	0.45
22:T:38:ARG:HG3	22:T:38:ARG:NH1	2.32	0.45
25:W:13:MET:CE	25:W:18:GLN:HA	2.37	0.45
25:W:80:ASP:HB2	39:W:3312:HOH:O	2.15	0.45
1:0:1200:A:H3'	39:0:6280:HOH:O	2.17	0.45
1:0:2504:A:H2'	1:0:2505:G:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2568:A:C2'	1:0:2569:A:H5'	2.47	0.45
30:2:10:ARG:HH11	30:2:49:GLU:CD	2.20	0.45
6:C:5:ILE:HG13	6:C:15:GLU:HA	1.99	0.45
7:D:25:MET:CE	7:D:37:ALA:HB1	2.45	0.45
11:H:151:ARG:HA	11:H:154:TYR:CE2	2.51	0.45
25:W:122:ARG:HH22	25:W:154:ARG:HG2	1.75	0.45
25:W:88:THR:HG22	25:W:90:TYR:CD1	2.52	0.45
27:Y:112:GLU:CD	27:Y:115:ARG:NH1	2.70	0.45
1:0:1773:G:C8	28:Z:16:ALA:HA	2.52	0.45
1:0:1351:G:OP1	6:C:96:LYS:NZ	2.38	0.45
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.17	0.45
1:0:371:U:H2'	1:0:372:A:H8	1.82	0.45
1:0:702:G:O2'	1:0:703:G:H5'	2.17	0.45
1:0:958:G:H2'	1:0:959:C:C6	2.52	0.45
1:0:2250:G:OP1	4:A:31:LYS:HD3	2.16	0.45
5:B:305:ASP:O	5:B:306:LYS:CB	2.63	0.45
8:E:22:VAL:HG12	8:E:76:VAL:HG11	1.99	0.45
12:J:39:VAL:HG21	12:J:107:ASN:ND2	2.32	0.45
20:R:106:GLY:HA2	20:R:109:MET:CE	2.47	0.45
22:T:69:LYS:O	22:T:71:VAL:HG23	2.17	0.45
26:X:43:VAL:CG1	26:X:47:ALA:HB3	2.47	0.45
27:Y:107:PRO:HB3	27:Y:182:PHE:CE2	2.52	0.45
1:0:2511:A:H2'	1:0:2512:U:O4'	2.17	0.45
1:0:526:U:H2'	1:0:527:U:C6	2.52	0.45
29:1:28:HIS:HD2	29:1:31:LYS:H	1.63	0.45
5:B:265:LEU:CD2	5:B:316:ARG:HD3	2.47	0.45
32:I:96:PHE:HD2	32:I:136:GLY:HA2	1.82	0.45
14:L:72:ASN:HB2	39:L:9477:HOH:O	2.16	0.45
2:9:3006:C:H5''	16:N:37:ARG:HE	1.82	0.45
24:V:7:GLU:O	24:V:11:MET:HG3	2.17	0.45
28:Z:53:GLY:HA2	28:Z:67:GLY:O	2.17	0.45
1:0:1369:A:H4'	20:R:64:SER:OG	2.17	0.44
1:0:162:C:H2'	1:0:163:U:H5'	1.99	0.44
1:0:2011:A:H4'	1:0:2012:U:O5'	2.17	0.44
30:2:41:HIS:N	30:2:45:ASN:HD22	1.97	0.44
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.97	0.44
6:C:57:PRO:HG2	6:C:73:LEU:CD1	2.46	0.44
15:M:164:THR:CG2	15:M:166:ALA:H	2.29	0.44
1:0:317:A:OP1	22:T:52:ARG:O	2.35	0.44
1:0:1266:U:O2'	27:Y:119:GLN:NE2	2.41	0.44
1:0:1730:G:H5''	1:0:1731:C:H6	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:61:PHE:HB3	39:C:9250:HOH:O	2.17	0.44
7:D:128:LEU:HD23	7:D:128:LEU:C	2.38	0.44
12:J:70:PHE:CG	12:J:70:PHE:O	2.70	0.44
12:J:71:TYR:CG	12:J:72:PRO:HD2	2.53	0.44
15:M:98:GLN:O	15:M:102:GLU:HG3	2.17	0.44
15:M:61:ILE:N	15:M:61:ILE:HD12	2.31	0.44
21:S:57:THR:HG22	21:S:58:MET:N	2.32	0.44
22:T:48:VAL:CG2	22:T:96:VAL:CG1	2.94	0.44
1:0:1181:A:N1	1:0:1192:A:O2'	2.49	0.44
1:0:1198:U:H2'	1:0:1200:A:OP2	2.17	0.44
1:0:1592:G:O2'	1:0:1593:C:O4'	2.34	0.44
1:0:1919:A:H4'	39:0:5395:HOH:O	2.17	0.44
1:0:2720:C:O2	13:K:87:ARG:NH2	2.49	0.44
1:0:470:U:O2'	29:1:16:HIS:CD2	2.60	0.44
7:D:135:VAL:HG22	7:D:136:ARG:H	1.80	0.44
11:H:1:LYS:N	39:H:9530:HOH:O	2.49	0.44
32:I:89:SER:HB3	32:I:97:VAL:CG2	2.48	0.44
12:J:131:THR:HB	12:J:134:GLU:OE1	2.17	0.44
14:L:145:LEU:C	14:L:145:LEU:HD23	2.37	0.44
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.52	0.44
25:W:149:LEU:HG	25:W:153:MET:HE1	1.99	0.44
1:0:1007:A:H2'	11:H:19:TYR:CZ	2.52	0.44
1:0:1086:A:N6	25:W:11:VAL:HG11	2.33	0.44
1:0:1218:U:H2'	1:0:1219:U:C6	2.53	0.44
1:0:133:U:C3'	1:0:134:U:H5''	2.48	0.44
1:0:2102:G:H5''	1:0:2538:A:C2	2.52	0.44
1:0:2542:C:H5''	1:0:2608:C:N4	2.33	0.44
1:0:92:G:H4'	24:V:44:GLY:HA3	2.00	0.44
1:0:2427:C:OP2	31:3:84:ARG:HD2	2.17	0.44
2:9:3042:C:O2	7:D:76:ARG:NH1	2.50	0.44
7:D:13:MET:HA	7:D:137:PRO:HG2	1.98	0.44
27:Y:154:ARG:HH11	27:Y:154:ARG:CG	2.30	0.44
28:Z:36:ASP:CB	28:Z:45:ASP:HB3	2.34	0.44
1:0:2251:G:H2'	1:0:2252:A:C8	2.53	0.44
1:0:2518:C:H2'	1:0:2519:C:O4'	2.17	0.44
1:0:2531:U:O2'	1:0:2532:A:H5'	2.17	0.44
3:4:176:DA:H5''	3:4:175:C:H3'	2.00	0.44
6:C:194:PHE:HA	6:C:234:VAL:HG13	2.00	0.44
6:C:31:ILE:HG23	6:C:220:THR:CG2	2.47	0.44
7:D:172:VAL:CG1	7:D:173:GLU:N	2.80	0.44
39:9:5851:HOH:O	16:N:115:VAL:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:64:SER:C	16:N:66:LEU:H	2.20	0.44
27:Y:99:ALA:HB2	27:Y:233:TYR:CE2	2.52	0.44
1:0:1181:A:H2'	1:0:1182:C:H5'	2.00	0.44
1:0:125:U:H2'	39:0:4346:HOH:O	2.17	0.44
1:0:2314:G:C2'	1:0:2315:C:H5'	2.48	0.44
1:0:2353:A:H4'	1:0:2354:A:O5'	2.17	0.44
1:0:2831:C:O3'	20:R:71:LYS:HE2	2.18	0.44
1:0:2857:C:H2'	1:0:2858:U:C6	2.53	0.44
1:0:821:U:H2'	1:0:822:C:H6	1.82	0.44
4:A:36:ASP:HA	4:A:83:GLY:HA3	1.99	0.44
5:B:178:ALA:O	5:B:182:VAL:HG23	2.18	0.44
5:B:254:GLN:NE2	39:B:9585:HOH:O	2.48	0.44
5:B:8:LYS:HG3	5:B:220:VAL:HG12	1.99	0.44
7:D:60:GLU:O	7:D:61:PHE:C	2.55	0.44
9:F:31:LYS:HE3	39:F:2623:HOH:O	2.17	0.44
10:G:67:LEU:O	10:G:71:LEU:HG	2.18	0.44
11:H:169:GLY:C	11:H:170:ASN:HD22	2.21	0.44
11:H:21:THR:O	11:H:120:ILE:HD12	2.18	0.44
39:0:6242:HOH:O	13:K:87:ARG:CZ	2.64	0.44
16:N:24:LEU:HD13	19:Q:26:PRO:HB3	1.98	0.44
1:0:134:U:H5'	1:0:134:U:C6	2.47	0.44
1:0:1921:A:O2'	1:0:1922:A:H5'	2.18	0.44
1:0:2533:C:C6	1:0:2533:C:H5'	2.49	0.44
1:0:333:G:O2'	1:0:334:G:H5'	2.18	0.44
1:0:497:A:H2'	1:0:498:A:C5'	2.48	0.44
8:E:20:ILE:HD11	8:E:40:VAL:CG1	2.38	0.44
9:F:99:THR:O	9:F:100:ASP:HB2	2.17	0.44
10:G:27:ILE:HD13	10:G:71:LEU:HD23	1.99	0.44
11:H:56:GLN:HE22	11:H:93:GLN:HG2	1.83	0.44
2:9:3011:A:P	19:Q:19:ARG:HH21	2.40	0.44
1:0:249:G:O2'	1:0:250:C:H5'	2.18	0.44
1:0:2767:C:OP1	5:B:318:ASN:ND2	2.51	0.44
1:0:629:A:H2'	1:0:630:A:O4'	2.18	0.44
1:0:2101:A:H2'	6:C:63:SER:OG	2.18	0.44
1:0:1181:A:H5'	32:I:94:GLU:OE2	2.18	0.44
13:K:49:LEU:CD1	13:K:80:ILE:HD13	2.48	0.44
20:R:119:VAL:CG1	20:R:119:VAL:O	2.65	0.44
27:Y:133:HIS:HD2	39:Y:9381:HOH:O	2.00	0.44
27:Y:189:ASN:HD22	27:Y:192:ASP:H	1.66	0.44
1:0:1299:G:N7	14:L:6:ARG:NH1	2.65	0.44
1:0:1418:U:OP1	30:2:42:TRP:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2362:A:H2'	1:0:2363:G:C8	2.53	0.44
1:0:603:A:H1'	1:0:605:C:C2	2.52	0.44
1:0:951:A:O2'	1:0:952:G:H5'	2.18	0.44
2:9:3002:U:OP2	2:9:3003:A:H5'	2.18	0.44
5:B:274:GLU:HA	5:B:292:GLY:O	2.18	0.44
6:C:129:HIS:HE1	6:C:231:ARG:HA	1.83	0.44
6:C:194:PHE:CE2	6:C:234:VAL:HG11	2.53	0.44
9:F:107:ASP:O	9:F:111:ILE:HG13	2.17	0.44
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.67	0.44
1:0:656:G:OP2	17:O:37:ARG:HD2	2.17	0.43
30:2:41:HIS:CD2	30:2:44:ARG:H	2.36	0.43
4:A:201:PHE:HB3	39:A:9620:HOH:O	2.16	0.43
8:E:93:MET:HE1	8:E:165:GLY:N	2.33	0.43
25:W:122:ARG:CG	25:W:122:ARG:NH1	2.80	0.43
1:0:1205:U:C2'	1:0:1206:U:H5''	2.49	0.43
1:0:1435:U:H5'	39:0:3204:HOH:O	2.16	0.43
1:0:2568:A:H2'	1:0:2569:A:O4'	2.18	0.43
1:0:2809:G:H2'	1:0:2810:G:O4'	2.19	0.43
1:0:907:A:H2'	1:0:908:A:C8	2.52	0.43
5:B:87:TYR:HD1	39:B:9575:HOH:O	2.01	0.43
6:C:21:VAL:HG13	39:C:9202:HOH:O	2.16	0.43
12:J:131:THR:HG22	12:J:133:GLY:N	2.34	0.43
14:L:94:ARG:NH1	14:L:143:THR:HG21	2.33	0.43
22:T:52:ARG:O	22:T:53:GLY:O	2.36	0.43
1:0:1657:A:H2'	1:0:1658:A:C8	2.54	0.43
1:0:2016:U:H2'	1:0:2017:U:O4'	2.17	0.43
1:0:2416:G:O2'	16:N:25:ARG:HG2	2.18	0.43
1:0:283:U:H5''	1:0:284:C:OP2	2.19	0.43
4:A:132:ASP:OD1	4:A:133:ARG:N	2.42	0.43
5:B:175:LEU:C	5:B:175:LEU:HD23	2.38	0.43
1:0:2898:G:H4'	5:B:288:GLY:HA2	2.00	0.43
8:E:112:ALA:HA	8:E:113:PRO:HD3	1.83	0.43
22:T:32:ARG:NH1	22:T:38:ARG:HH12	2.15	0.43
23:U:38:ASN:O	23:U:42:LEU:HG	2.18	0.43
24:V:12:THR:OG1	24:V:13:PRO:HD2	2.18	0.43
1:0:1829:A:N6	28:Z:18:TYR:HA	2.33	0.43
1:0:1132:A:N6	1:0:1229:C:H2'	2.34	0.43
1:0:1641:A:C2'	1:0:1642:A:H5'	2.47	0.43
1:0:245:C:H2'	1:0:246:G:H5'	2.01	0.43
1:0:2568:A:H2'	1:0:2569:A:H5'	2.01	0.43
1:0:506:G:H22	1:0:509:A:H5'	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:41:HIS:HB3	30:2:44:ARG:HB2	2.00	0.43
4:A:211:LYS:HB2	39:A:9576:HOH:O	2.18	0.43
5:B:40:GLY:HA3	39:B:9640:HOH:O	2.17	0.43
25:W:122:ARG:CG	25:W:152:ALA:O	2.66	0.43
1:0:1067:A:H5'	39:0:4907:HOH:O	2.17	0.43
1:0:1160:G:HO2'	1:0:1190:G:H8	1.62	0.43
1:0:338:C:H4'	6:C:174:ILE:HD11	2.00	0.43
5:B:24:PRO:CG	5:B:204:GLY:HA2	2.48	0.43
5:B:307:ARG:HD2	39:B:9645:HOH:O	2.18	0.43
5:B:314:ALA:HB3	5:B:317:PRO:HG3	1.99	0.43
5:B:280:VAL:HG13	5:B:333:GLU:O	2.18	0.43
5:B:84:LEU:HD13	5:B:84:LEU:C	2.39	0.43
6:C:72:LYS:HA	6:C:76:ARG:O	2.19	0.43
7:D:173:GLU:HG3	7:D:174:VAL:H	1.82	0.43
32:I:92:PRO:O	32:I:94:GLU:HG3	2.19	0.43
12:J:74:ARG:NH1	12:J:76:ASP:CB	2.80	0.43
16:N:110:THR:HB	16:N:113:SER:HG	1.84	0.43
20:R:82:GLU:O	20:R:86:LYS:HG3	2.19	0.43
24:V:56:ILE:HG22	24:V:60:GLN:NE2	2.33	0.43
1:0:699:C:H2'	1:0:744:G:O4'	2.18	0.43
1:0:1415:G:H5'	29:1:12:ASN:O	2.19	0.43
5:B:102:THR:HG21	5:B:182:VAL:O	2.19	0.43
7:D:103:ASN:OD1	7:D:133:ASN:ND2	2.52	0.43
13:K:14:LYS:HG3	13:K:32:ILE:O	2.18	0.43
16:N:170:GLU:O	16:N:174:GLU:HG3	2.18	0.43
17:O:26:TRP:HA	17:O:26:TRP:HE3	1.82	0.43
23:U:9:CYS:O	23:U:52:THR:HG23	2.18	0.43
24:V:8:ILE:HA	24:V:11:MET:HE2	2.00	0.43
25:W:142:ASP:O	25:W:145:GLY:N	2.52	0.43
1:0:1119:G:C8	12:J:52:GLN:NE2	2.83	0.43
1:0:1667:A:H2'	1:0:1668:U:C6	2.53	0.43
1:0:2421:G:H2'	39:0:4649:HOH:O	2.18	0.43
1:0:2039:A:H4'	1:0:2760:C:O2'	2.18	0.43
1:0:297:U:H1'	39:0:4511:HOH:O	2.17	0.43
1:0:816:G:C6	1:0:817:G:N1	2.87	0.43
1:0:962:C:H1'	16:N:5:ARG:NH1	2.34	0.43
4:A:65:ARG:HH11	4:A:65:ARG:HG2	1.84	0.43
1:0:2717:C:OP1	5:B:207:LYS:HG3	2.18	0.43
5:B:85:ARG:HB2	5:B:99:GLU:HG2	2.00	0.43
12:J:130:VAL:HG12	12:J:131:THR:H	1.84	0.43
19:Q:46:SER:O	19:Q:48:PRO:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:75:GLU:O	22:T:76:ASP:HB2	2.18	0.43
1:0:1573:A:H2'	1:0:1574:C:O4'	2.18	0.43
1:0:1759:A:N3	1:0:1818:C:H2'	2.34	0.43
1:0:2506:A:O2'	1:0:2507:G:P	2.77	0.43
1:0:820:G:C6	4:A:171:LYS:HB2	2.54	0.43
5:B:243:ASN:HA	5:B:244:PRO:C	2.38	0.43
5:B:56:ASP:CG	5:B:322:ARG:HB3	2.38	0.43
6:C:138:VAL:HG11	6:C:160:LEU:HD13	2.01	0.43
7:D:96:SER:C	7:D:98:PHE:H	2.22	0.43
16:N:86:LEU:HD21	16:N:180:LEU:HD12	2.01	0.43
26:X:73:ARG:HB2	26:X:88:GLU:OE2	2.18	0.43
27:Y:216:ARG:HD2	39:Y:9369:HOH:O	2.19	0.43
1:0:1130:U:H2'	1:0:1131:G:O4'	2.19	0.43
1:0:1456:C:H2'	1:0:1457:U:C6	2.54	0.43
1:0:2506:A:O2'	1:0:2507:G:O5'	2.37	0.43
21:S:53:ASN:ND2	39:S:9480:HOH:O	2.51	0.43
22:T:23:VAL:HG23	22:T:41:ARG:HG3	2.00	0.43
23:U:14:GLU:OE1	23:U:15:PRO:HD2	2.19	0.43
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.83	0.43
25:W:54:PHE:CZ	25:W:140:LYS:HB2	2.53	0.43
25:W:3:ALA:O	25:W:54:PHE:HA	2.19	0.43
27:Y:184:GLU:HG2	27:Y:229:LEU:HD11	2.00	0.43
1:0:2356:A:H2'	1:0:2357:G:O4'	2.18	0.43
1:0:2699:A:H2'	1:0:2700:G:O4'	2.18	0.43
1:0:2726:U:O2	1:0:2749:U:O5'	2.37	0.43
1:0:2831:C:H2'	1:0:2832:C:H5'	2.01	0.43
1:0:64:G:H2'	1:0:65:C:O4'	2.19	0.43
2:9:3050:G:H5''	16:N:159:TYR:HE1	1.83	0.43
5:B:18:ARG:HE	5:B:256:GLN:NE2	2.17	0.43
5:B:279:THR:HA	5:B:284:PHE:HE1	1.84	0.43
7:D:135:VAL:HG21	7:D:139:TYR:CG	2.54	0.43
13:K:80:ILE:O	13:K:87:ARG:HA	2.19	0.43
18:P:13:VAL:HG11	18:P:40:VAL:HG12	2.00	0.43
22:T:40:VAL:HG22	22:T:41:ARG:H	1.82	0.43
28:Z:39:CYS:HB3	28:Z:42:CYS:SG	2.59	0.43
1:0:1095:U:O2	25:W:120:PRO:HG2	2.19	0.42
1:0:1298:U:H2'	1:0:1299:G:C8	2.52	0.42
1:0:2088:C:H1'	1:0:2841:A:N1	2.35	0.42
1:0:2064:U:H4'	1:0:2653:A:OP1	2.18	0.42
1:0:65:C:O2'	1:0:66:G:H5'	2.18	0.42
7:D:51:ARG:HD3	39:D:7636:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:102:VAL:CG1	32:I:106:LYS:HE3	2.44	0.42
32:I:113:HIS:CE1	32:I:121:LEU:HD22	2.53	0.42
32:I:132:CYS:C	32:I:134:SER:N	2.72	0.42
13:K:4:LEU:HD23	13:K:4:LEU:HA	1.85	0.42
15:M:115:LEU:HD13	15:M:116:ASN:HB2	2.01	0.42
16:N:137:ALA:HB1	16:N:141:ARG:HD3	2.00	0.42
17:O:97:SER:OG	17:O:100:GLN:HG3	2.19	0.42
22:T:55:PHE:CE1	22:T:89:ARG:HG2	2.54	0.42
23:U:4:ARG:HH11	23:U:4:ARG:HG2	1.84	0.42
28:Z:41:ASN:O	28:Z:42:CYS:HB3	2.19	0.42
1:0:553:G:O4'	1:0:1325:G:H5'	2.19	0.42
1:0:2239:C:H2'	1:0:2240:U:C6	2.54	0.42
1:0:2724:U:H2'	1:0:2725:G:O4'	2.19	0.42
1:0:27:U:H2'	1:0:28:G:O4'	2.19	0.42
1:0:366:U:H2'	1:0:367:G:O4'	2.19	0.42
29:1:21:ARG:HD3	29:1:45:ARG:NE	2.34	0.42
31:3:70:ARG:HB3	39:3:9502:HOH:O	2.18	0.42
4:A:36:ASP:CG	4:A:36:ASP:O	2.57	0.42
5:B:146:THR:C	5:B:148:PRO:HD3	2.40	0.42
8:E:6:GLU:HA	8:E:46:THR:HG22	2.01	0.42
15:M:184:ARG:HG3	15:M:185:PRO:HA	2.01	0.42
15:M:82:ARG:O	15:M:83:SER:C	2.57	0.42
16:N:152:GLU:HA	16:N:152:GLU:OE1	2.19	0.42
20:R:114:VAL:HG13	20:R:114:VAL:O	2.19	0.42
20:R:84:ALA:O	20:R:88:PHE:HD1	2.02	0.42
25:W:52:VAL:HG13	25:W:53:ALA:N	2.33	0.42
26:X:20:GLU:CG	26:X:21:PRO:HD2	2.48	0.42
27:Y:106:THR:CG2	27:Y:107:PRO:HD2	2.49	0.42
1:0:1099:G:H2'	1:0:1100:G:O4'	2.19	0.42
1:0:912:A:C4	1:0:1294:A:C2	3.06	0.42
1:0:1603:A:H5''	1:0:1604:G:H3'	2.00	0.42
1:0:188:C:H5''	15:M:163:LEU:HD21	2.02	0.42
1:0:1940:C:H4'	39:0:7801:HOH:O	2.18	0.42
1:0:2541:U:O2	3:4:76:PPU:HA	2.20	0.42
1:0:2676:C:H4'	12:J:70:PHE:HE1	1.84	0.42
1:0:2807:U:OP2	5:B:27:ASN:ND2	2.50	0.42
1:0:2911:C:O2'	1:0:2912:C:H5'	2.19	0.42
1:0:308:U:C4	1:0:342:C:H1'	2.54	0.42
1:0:415:A:O2'	1:0:416:G:H5'	2.19	0.42
5:B:62:ARG:CB	5:B:65:MET:HE3	2.49	0.42
6:C:46:TYR:CE1	6:C:92:PRO:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:7:ILE:HD11	8:E:11:VAL:C	2.39	0.42
8:E:166:VAL:HG12	39:E:3134:HOH:O	2.18	0.42
15:M:34:GLU:HB3	15:M:38:GLU:HG3	2.01	0.42
27:Y:187:VAL:HB	27:Y:203:VAL:CG2	2.50	0.42
28:Z:26:VAL:HG12	28:Z:30:GLU:OE1	2.18	0.42
1:O:1159:G:H1	1:O:1208:C:N4	2.15	0.42
1:O:1342:C:O2'	1:O:1343:C:H5'	2.19	0.42
2:9:3039:U:HO2'	2:9:3042:C:H5	1.57	0.42
2:9:3107:C:H5	39:9:3167:HOH:O	2.01	0.42
7:D:76:ARG:O	7:D:77:ASP:HB2	2.20	0.42
12:J:132:LEU:HA	12:J:132:LEU:HD23	1.84	0.42
16:N:173:ASP:O	16:N:177:GLU:HB2	2.19	0.42
39:O:5821:HOH:O	25:W:122:ARG:NH2	2.51	0.42
26:X:66:THR:HG23	26:X:67:PRO:HD2	2.01	0.42
1:O:1181:A:C2'	1:O:1182:C:H5'	2.49	0.42
1:O:1226:G:H5'	39:O:5084:HOH:O	2.19	0.42
1:O:2263:G:O2'	15:M:70:GLY:HA2	2.20	0.42
1:O:793:A:C5'	18:P:83:LYS:HG2	2.49	0.42
1:O:87:C:H2'	30:2:28:LYS:O	2.19	0.42
2:9:3039:U:O2'	2:9:3042:C:H5	2.02	0.42
4:A:130:THR:HB	4:A:137:VAL:HB	2.02	0.42
5:B:294:TYR:HE2	39:B:9642:HOH:O	2.01	0.42
7:D:136:ARG:HB3	7:D:137:PRO:HD2	2.01	0.42
9:F:111:ILE:O	9:F:115:VAL:HG23	2.20	0.42
9:F:48:VAL:CG2	9:F:74:PHE:HB3	2.48	0.42
11:H:154:TYR:C	11:H:154:TYR:CD1	2.93	0.42
12:J:39:VAL:HG11	12:J:107:ASN:CB	2.50	0.42
16:N:108:SER:HA	16:N:109:PRO:HD3	1.80	0.42
1:O:497:A:H2'	1:O:498:A:H5'	2.01	0.42
1:O:588:G:O6	25:W:154:ARG:NH1	2.53	0.42
1:O:945:U:H2'	1:O:946:C:H6	1.84	0.42
5:B:41:PHE:HA	5:B:79:MET:CE	2.49	0.42
6:C:119:ALA:HA	6:C:137:PRO:HD3	2.01	0.42
7:D:99:ASP:N	7:D:103:ASN:O	2.47	0.42
26:X:45:GLU:HG3	39:X:6178:HOH:O	2.19	0.42
27:Y:154:ARG:HH11	27:Y:154:ARG:CB	2.33	0.42
1:O:1314:U:H2'	39:O:6398:HOH:O	2.20	0.42
1:O:1616:A:H5''	1:O:1617:C:OP1	2.20	0.42
1:O:2449:G:H2'	1:O:2450:C:O4'	2.19	0.42
1:O:2436:U:H5'	31:3:68:LYS:HE2	2.01	0.42
4:A:93:THR:C	4:A:94:LEU:HD23	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:62:ARG:HA	5:B:65:MET:HE3	2.02	0.42
5:B:41:PHE:HA	5:B:79:MET:HE2	2.02	0.42
5:B:86:ALA:HA	39:B:9575:HOH:O	2.19	0.42
7:D:88:LEU:N	7:D:89:PRO:CD	2.82	0.42
11:H:43:TYR:HA	11:H:44:PRO:HD3	1.79	0.42
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.49	0.42
16:N:167:ASP:C	16:N:168:LEU:HG	2.39	0.42
18:P:18:LYS:O	18:P:21:VAL:HG13	2.20	0.42
20:R:39:THR:CG2	20:R:107:GLU:O	2.68	0.42
22:T:85:GLU:CG	22:T:86:GLU:N	2.80	0.42
23:U:20:MET:CG	23:U:28:THR:HG23	2.50	0.42
1:0:1065:G:H5'	39:0:4138:HOH:O	2.19	0.42
1:0:1218:U:H2'	1:0:1219:U:H6	1.84	0.42
1:0:1119:G:N2	1:0:1246:A:H2	2.08	0.42
1:0:1778:A:H2'	1:0:1779:A:H5'	2.01	0.42
1:0:220:C:H1'	39:0:6282:HOH:O	2.18	0.42
1:0:2649:A:O4'	1:0:2650:U:H5	2.02	0.42
1:0:2769:C:H2'	1:0:2770:G:H5'	2.01	0.42
1:0:2787:C:H5	39:0:5181:HOH:O	2.02	0.42
1:0:362:G:H2'	1:0:363:A:C8	2.54	0.42
1:0:426:G:H2'	1:0:427:C:O4'	2.20	0.42
1:0:612:U:H2'	1:0:613:C:C6	2.55	0.42
1:0:820:G:C5	4:A:171:LYS:HB2	2.55	0.42
1:0:835:U:P	5:B:229:ARG:HH12	2.43	0.42
1:0:932:U:H2'	1:0:933:C:C6	2.55	0.42
1:0:960:G:N3	1:0:960:G:H2'	2.34	0.42
4:A:100:PRO:HG2	4:A:103:VAL:CG2	2.45	0.42
8:E:145:ALA:HB1	8:E:168:ILE:CD1	2.49	0.42
10:G:12:ILE:HG13	39:G:6833:HOH:O	2.19	0.42
11:H:51:VAL:CG1	11:H:53:GLU:O	2.67	0.42
12:J:74:ARG:HH11	12:J:74:ARG:CB	2.28	0.42
15:M:48:LYS:O	15:M:52:GLN:HG3	2.20	0.42
16:N:43:VAL:CG1	16:N:118:ILE:HD11	2.49	0.42
23:U:17:THR:HG23	23:U:18:GLY:N	2.34	0.42
39:0:3167:HOH:O	25:W:119:HIS:HE1	2.03	0.42
1:0:2269:C:H2'	1:0:2270:G:O4'	2.19	0.42
31:3:17:HIS:O	31:3:18:GLN:HG3	2.20	0.42
4:A:122:SER:O	4:A:124:VAL:HG13	2.19	0.42
4:A:52:SER:HB2	4:A:164:ARG:HH11	1.85	0.42
5:B:51:VAL:HG23	5:B:327:VAL:HG13	2.01	0.42
6:C:129:HIS:HD2	6:C:165:ASP:OD2	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:162:VAL:CG2	6:C:232:LEU:HD21	2.50	0.42
32:I:92:PRO:HB3	39:I:6825:HOH:O	2.19	0.42
14:L:91:VAL:CG1	14:L:120:LEU:HD23	2.43	0.42
14:L:144:ASP:O	14:L:147:GLU:HB2	2.19	0.42
15:M:164:THR:CG2	15:M:165:GLY:N	2.81	0.42
16:N:82:TYR:HE1	16:N:120:GLU:HG2	1.84	0.42
1:O:1398:G:H5'	18:P:23:PHE:O	2.19	0.42
1:O:1849:G:H1'	1:O:2011:A:N1	2.34	0.42
1:O:2015:A:H2'	1:O:2016:U:O4'	2.20	0.42
1:O:2296:C:H2'	1:O:2297:U:C6	2.55	0.42
1:O:2338:G:H2'	7:D:129:ASP:OD1	2.20	0.42
1:O:2837:U:H2'	39:O:7320:HOH:O	2.20	0.42
1:O:40:C:H6	1:O:40:C:O5'	2.03	0.42
2:9:3003:A:H2	2:9:3021:G:N3	2.18	0.42
8:E:10:ASP:HA	39:E:3707:HOH:O	2.20	0.42
8:E:20:ILE:HD12	8:E:33:LEU:HD12	2.02	0.42
9:F:16:ALA:HA	9:F:111:ILE:HD13	2.02	0.42
9:F:113:ASP:O	9:F:117:GLU:HG3	2.19	0.42
18:P:14:LEU:O	18:P:16:VAL:HG23	2.19	0.42
24:V:42:ASN:O	24:V:44:GLY:N	2.53	0.42
1:O:1400:C:H4'	26:X:56:GLU:HG2	2.01	0.42
27:Y:115:ARG:NE	39:Y:9355:HOH:O	2.52	0.42
1:O:2505:G:C2'	1:O:2506:A:H5'	2.50	0.41
1:O:2819:C:H2'	1:O:2820:A:C8	2.55	0.41
1:O:449:A:C8	6:C:43:LYS:HG2	2.55	0.41
2:9:3041:C:C6	7:D:50:VAL:HG21	2.54	0.41
4:A:43:VAL:O	4:A:44:ASP:HB2	2.20	0.41
22:T:48:VAL:O	22:T:59:GLU:HA	2.20	0.41
25:W:108:ARG:HE	25:W:114:PRO:HG2	1.85	0.41
26:X:8:ARG:HE	26:X:8:ARG:HB3	1.63	0.41
39:O:6789:HOH:O	27:Y:158:LYS:HD3	2.19	0.41
1:O:1203:G:O2'	1:O:1204:C:H5'	2.20	0.41
1:O:907:A:H2'	1:O:908:A:H8	1.85	0.41
5:B:115:VAL:HA	5:B:116:PRO:HD3	1.94	0.41
5:B:41:PHE:CD1	5:B:79:MET:CE	3.03	0.41
39:O:3827:HOH:O	32:I:92:PRO:HD3	2.19	0.41
16:N:24:LEU:HD22	39:Q:2847:HOH:O	2.19	0.41
1:O:1603:A:H5''	1:O:1605:G:H5'	2.01	0.41
1:O:451:C:O2'	1:O:452:G:H5'	2.20	0.41
1:O:522:U:O2'	1:O:1366:C:H5'	2.20	0.41
1:O:538:C:H5''	1:O:539:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:926:A:O2'	14:L:41:HIS:HD2	2.03	0.41
6:C:120:ASP:C	6:C:120:ASP:OD1	2.58	0.41
32:I:112:LYS:C	32:I:114:PRO:HD2	2.40	0.41
14:L:6:ARG:NH2	39:L:9445:HOH:O	2.53	0.41
14:L:80:ASP:CB	14:L:90:ARG:HB3	2.50	0.41
15:M:82:ARG:HA	39:M:9339:HOH:O	2.19	0.41
23:U:4:ARG:NH1	23:U:4:ARG:HG2	2.35	0.41
1:0:2323:G:H5'	39:0:7497:HOH:O	2.19	0.41
1:0:2886:C:O2'	1:0:2887:G:H5'	2.20	0.41
1:0:407:A:H2'	1:0:408:A:C8	2.55	0.41
1:0:82:C:OP1	22:T:67:LEU:HB2	2.20	0.41
2:9:3050:G:H5''	16:N:159:TYR:CE1	2.55	0.41
4:A:192:VAL:HG13	39:A:9546:HOH:O	2.20	0.41
4:A:30:ARG:HB3	4:A:30:ARG:HE	1.72	0.41
6:C:133:ARG:HG3	6:C:133:ARG:HH11	1.84	0.41
11:H:76:GLU:C	11:H:77:LEU:HD23	2.41	0.41
32:I:103:ASP:HA	32:I:106:LYS:HD2	2.02	0.41
16:N:33:ARG:NH1	16:N:103:ASP:OD2	2.51	0.41
26:X:18:ARG:NH1	39:X:4132:HOH:O	2.41	0.41
28:Z:41:ASN:O	28:Z:41:ASN:ND2	2.53	0.41
1:0:1098:A:O3'	25:W:129:LYS:HE2	2.20	0.41
1:0:1131:G:C6	1:0:1230:A:C4	3.08	0.41
1:0:1139:U:H2'	1:0:1140:C:C6	2.56	0.41
1:0:1797:A:H2'	1:0:1799:G:O5'	2.21	0.41
1:0:2415:A:N3	16:N:26:LEU:HD13	2.35	0.41
1:0:2676:C:H4'	12:J:70:PHE:HD1	1.82	0.41
1:0:2748:G:H4'	1:0:2749:U:H5'	2.02	0.41
4:A:186:TRP:CG	4:A:187:PRO:HA	2.56	0.41
4:A:192:VAL:HG12	4:A:192:VAL:O	2.19	0.41
5:B:16:ARG:NH2	39:B:9552:HOH:O	2.44	0.41
5:B:183:GLU:O	5:B:184:ASP:C	2.58	0.41
7:D:88:LEU:HB2	7:D:89:PRO:HD3	2.02	0.41
11:H:47:ILE:HG21	39:H:9541:HOH:O	2.19	0.41
12:J:15:ARG:NH1	12:J:43:ARG:HH11	2.17	0.41
14:L:66:VAL:HG23	14:L:67:ARG:N	2.35	0.41
39:C:9165:HOH:O	17:O:3:THR:HG21	2.19	0.41
1:0:1335:C:H2'	1:0:1336:U:C6	2.56	0.41
1:0:1552:G:H2'	1:0:1553:C:C6	2.56	0.41
1:0:1829:A:H2'	1:0:1830:C:H5'	2.03	0.41
1:0:2717:C:H2'	1:0:2718:C:C5'	2.37	0.41
1:0:29:C:C2'	1:0:30:U:H5'	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:517:U:H1'	39:0:8071:HOH:O	2.19	0.41
29:1:28:HIS:O	29:1:32:LYS:N	2.47	0.41
2:9:3088:G:OP1	25:W:130:HIS:NE2	2.47	0.41
13:K:23:ASN:HD21	13:K:107:THR:HB	1.84	0.41
24:V:8:ILE:CG2	24:V:59:ILE:HG13	2.50	0.41
25:W:122:ARG:NH1	25:W:152:ALA:O	2.54	0.41
1:0:1044:C:H3'	1:0:1045:G:H5''	2.02	0.41
1:0:1182:C:H1'	1:0:1192:A:C8	2.45	0.41
1:0:1183:C:H5	1:0:1192:A:OP1	2.03	0.41
1:0:2379:G:N3	1:0:2418:G:H2'	2.35	0.41
1:0:255:A:H2'	1:0:256:C:C6	2.55	0.41
1:0:329:A:OP2	6:C:206:ASN:HB2	2.20	0.41
1:0:892:G:H5''	29:1:54:ALA:HB2	2.02	0.41
8:E:133:VAL:HG12	8:E:141:VAL:HG13	2.03	0.41
32:I:102:VAL:HG23	32:I:140:GLU:O	2.20	0.41
15:M:49:ALA:C	15:M:54:TYR:HB3	2.40	0.41
1:0:1495:C:H2'	1:0:1496:G:C8	2.56	0.41
1:0:1795:G:H2'	1:0:1796:A:O4'	2.20	0.41
1:0:1867:G:O2'	1:0:1868:G:H5'	2.21	0.41
1:0:1943:C:O4'	4:A:212:PRO:HA	2.20	0.41
1:0:2346:C:H4'	7:D:52:THR:CG2	2.51	0.41
1:0:2690:U:H4'	8:E:111:LYS:HE3	2.03	0.41
1:0:441:A:H8	1:0:441:A:O5'	2.03	0.41
30:2:19:SER:O	30:2:36:ASN:ND2	2.53	0.41
5:B:43:GLY:O	5:B:308:LEU:HD12	2.20	0.41
5:B:312:ARG:HG2	5:B:313:PRO:N	2.35	0.41
7:D:75:LEU:HD22	7:D:79:MET:HB3	2.02	0.41
39:0:7990:HOH:O	15:M:91:ILE:HG12	2.19	0.41
27:Y:122:ARG:NH2	39:Y:9335:HOH:O	2.53	0.41
28:Z:30:GLU:HB2	39:Z:9215:HOH:O	2.20	0.41
1:0:2053:G:H4'	20:R:136:TRP:CE2	2.56	0.41
1:0:2134:G:C6	1:0:2258:A:C8	3.09	0.41
2:9:3092:G:H2'	2:9:3093:A:C8	2.56	0.41
8:E:80:TRP:O	8:E:134:SER:HA	2.19	0.41
8:E:7:ILE:HA	8:E:8:PRO:HD3	1.95	0.41
32:I:101:SER:OG	32:I:104:GLN:HG3	2.21	0.41
13:K:9:THR:HG21	13:K:78:LYS:HE2	2.03	0.41
14:L:67:ARG:HB2	14:L:112:GLY:HA3	2.02	0.41
15:M:90:ARG:HB2	31:3:46:ILE:HD11	2.03	0.41
18:P:16:VAL:HG12	18:P:17:GLY:H	1.84	0.41
20:R:9:ASP:O	20:R:13:THR:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:189:ASN:ND2	27:Y:189:ASN:C	2.73	0.41
1:O:101:C:H2'	1:O:102:A:C8	2.56	0.41
1:O:1268:C:O2'	1:O:1269:G:H5'	2.20	0.41
1:O:2032:U:H2'	1:O:2033:G:H5'	2.02	0.41
1:O:210:U:H2'	1:O:211:U:C6	2.55	0.41
1:O:2453:G:H5'	39:O:5235:HOH:O	2.21	0.41
1:O:2456:A:H5'	39:O:6223:HOH:O	2.21	0.41
1:O:499:G:O2'	1:O:500:G:H5'	2.20	0.41
2:9:3052:A:H2'	2:9:3053:G:O4'	2.21	0.41
6:C:236:THR:HG22	6:C:239:ALA:HB2	2.03	0.41
14:L:73:VAL:HG23	14:L:74:THR:N	2.31	0.41
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.50	0.41
23:U:19:THR:HG22	23:U:20:MET:N	2.35	0.41
25:W:26:ILE:O	25:W:26:ILE:CG1	2.68	0.41
26:X:43:VAL:CG1	26:X:44:ASP:N	2.83	0.41
1:O:1555:G:H4'	1:O:1630:A:C2	2.50	0.41
1:O:1929:G:H1'	39:O:5691:HOH:O	2.20	0.41
1:O:2044:G:OP1	26:X:23:HIS:HE1	2.04	0.41
1:O:2115:U:H2'	1:O:2116:U:C6	2.56	0.41
1:O:2597:U:H2'	1:O:2598:U:H5'	2.02	0.41
1:O:2698:G:H2'	1:O:2699:A:C8	2.56	0.41
2:9:3054:A:H2	39:9:3535:HOH:O	2.04	0.41
4:A:130:THR:HG22	4:A:131:HIS:N	2.36	0.41
7:D:37:ALA:O	7:D:40:ILE:HG12	2.21	0.41
11:H:20:ILE:HG23	11:H:120:ILE:CD1	2.50	0.41
1:O:1235:G:O4'	12:J:63:ILE:HG23	2.20	0.41
14:L:145:LEU:C	14:L:147:GLU:N	2.74	0.41
15:M:74:LYS:HA	39:M:9375:HOH:O	2.20	0.41
16:N:69:TYR:CE2	16:N:184:ILE:HG13	2.55	0.41
1:O:1098:A:H2'	1:O:1099:G:O4'	2.21	0.40
1:O:2523:U:O2'	1:O:2524:G:H5'	2.21	0.40
1:O:646:G:H2'	1:O:647:U:C6	2.56	0.40
2:9:3023:U:O2'	2:9:3024:U:H4'	2.21	0.40
4:A:103:VAL:O	4:A:105:VAL:HG23	2.21	0.40
4:A:179:MET:HG2	4:A:186:TRP:HB2	2.02	0.40
4:A:72:GLU:HG3	28:Z:66:GLY:HA2	2.02	0.40
5:B:195:ARG:NH1	5:B:324:ASP:OD1	2.55	0.40
39:O:4099:HOH:O	6:C:81:PRO:HD3	2.21	0.40
11:H:162:ARG:HD3	39:H:9548:HOH:O	2.20	0.40
11:H:29:ALA:H	11:H:66:ARG:HH12	1.69	0.40
12:J:45:VAL:HG22	12:J:46:ILE:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:112:GLY:HA2	16:N:137:ALA:N	2.36	0.40
27:Y:108:ASP:N	27:Y:108:ASP:OD1	2.53	0.40
1:0:1333:U:H2'	1:0:1334:C:H6	1.85	0.40
1:0:2032:U:C2'	1:0:2033:G:C5'	2.97	0.40
1:0:2101:A:OP2	6:C:66:GLY:HA2	2.21	0.40
1:0:2442:G:H3'	39:0:7117:HOH:O	2.20	0.40
1:0:23:G:C6	1:0:24:G:N1	2.89	0.40
1:0:2672:C:H1'	39:B:9628:HOH:O	2.20	0.40
1:0:2782:G:O6	1:0:2790:C:H5''	2.21	0.40
31:3:20:HIS:HA	31:3:70:ARG:O	2.21	0.40
2:9:3014:G:H2'	2:9:3015:C:H5'	2.03	0.40
5:B:144:THR:HG22	5:B:145:HIS:N	2.36	0.40
9:F:99:THR:HG23	9:F:99:THR:O	2.22	0.40
15:M:58:GLN:HG3	39:M:9408:HOH:O	2.21	0.40
16:N:167:ASP:O	16:N:168:LEU:HG	2.21	0.40
16:N:67:ALA:C	16:N:69:TYR:H	2.24	0.40
20:R:39:THR:HG22	20:R:107:GLU:O	2.21	0.40
20:R:25:PHE:CZ	20:R:29:LYS:HE2	2.55	0.40
1:0:1304:U:H2'	1:0:1305:C:C6	2.56	0.40
1:0:1314:U:H5''	1:0:1316:G:O4'	2.21	0.40
1:0:1462:C:H2'	1:0:1463:A:H8	1.85	0.40
1:0:2072:G:H3'	1:0:2073:G:H5''	2.03	0.40
1:0:669:G:O2'	1:0:670:G:H5'	2.21	0.40
1:0:791:A:H2'	1:0:792:G:O4'	2.22	0.40
1:0:999:C:H2'	1:0:1000:C:O4'	2.21	0.40
1:0:87:C:C2	30:2:30:ASP:OD2	2.74	0.40
4:A:17:ARG:HD2	39:A:9532:HOH:O	2.20	0.40
7:D:35:ALA:O	7:D:38:GLU:HG3	2.21	0.40
14:L:114:VAL:HB	39:L:9469:HOH:O	2.21	0.40
15:M:82:ARG:O	15:M:84:LYS:N	2.55	0.40
23:U:49:LEU:HG	39:U:3805:HOH:O	2.22	0.40
26:X:10:VAL:HG12	26:X:11:THR:N	2.36	0.40
28:Z:39:CYS:O	28:Z:42:CYS:O	2.39	0.40
1:0:1525:G:H5'	1:0:1526:A:OP2	2.21	0.40
1:0:1636:G:O2'	1:0:1637:A:H5'	2.20	0.40
1:0:2238:A:O2'	1:0:2239:C:H5'	2.21	0.40
1:0:2912:C:H2'	1:0:2913:A:O4'	2.21	0.40
1:0:710:G:H5'	17:O:25:VAL:HG13	2.04	0.40
1:0:876:A:H2'	1:0:876:A:N3	2.37	0.40
29:1:53:LYS:HD3	29:1:53:LYS:HA	1.89	0.40
31:3:25:VAL:HB	31:3:66:ASP:OD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3114:G:H2'	2:9:3115:C:C6	2.57	0.40
4:A:135:VAL:HG21	4:A:147:ARG:NH1	2.37	0.40
4:A:173:GLY:O	4:A:176:HIS:HB3	2.22	0.40
5:B:217:ARG:CG	5:B:257:THR:HG22	2.43	0.40
5:B:36:PRO:HA	5:B:167:GLY:O	2.22	0.40
7:D:57:THR:HA	39:D:5728:HOH:O	2.22	0.40
9:F:118:LEU:O	9:F:119:ARG:HB3	2.21	0.40
15:M:42:ARG:HA	15:M:43:PRO:HD3	1.90	0.40
16:N:110:THR:HG22	39:N:9349:HOH:O	2.20	0.40
16:N:143:ARG:HE	16:N:143:ARG:HB3	1.70	0.40
17:O:32:ARG:HD3	17:O:32:ARG:C	2.41	0.40
1:O:949:U:C4'	19:Q:95:GLU:HA	2.52	0.40
22:T:20:HIS:HB3	22:T:41:ARG:HD2	2.03	0.40
26:X:70:ILE:O	26:X:70:ILE:HG23	2.22	0.40
1:O:1602:C:OP2	28:Z:46:ARG:NH2	2.54	0.40
1:O:1834:C:H2'	1:O:1840:A:N6	2.37	0.40
1:O:2408:A:H4'	31:3:15:ASN:O	2.22	0.40
31:3:48:ASN:ND2	31:3:50:GLY:H	2.20	0.40
9:F:26:THR:HG21	9:F:102:GLY:C	2.42	0.40
1:O:1053:G:OP1	11:H:12:PRO:HG3	2.21	0.40
25:W:38:THR:HG22	25:W:40:ALA:H	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	235/240 (98%)	213 (91%)	17 (7%)	5 (2%)	7	5
5	B	335/338 (99%)	312 (93%)	18 (5%)	5 (2%)	10	10
6	C	244/246 (99%)	226 (93%)	18 (7%)	0	100	100
7	D	134/177 (76%)	104 (78%)	18 (13%)	12 (9%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	E	170/178 (96%)	164 (96%)	6 (4%)	0	100	100
9	F	117/120 (98%)	104 (89%)	11 (9%)	2 (2%)	9	8
10	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
11	H	156/171 (91%)	141 (90%)	13 (8%)	2 (1%)	12	12
12	J	140/145 (97%)	132 (94%)	5 (4%)	3 (2%)	7	5
13	K	130/132 (98%)	121 (93%)	8 (6%)	1 (1%)	19	23
14	L	141/165 (86%)	120 (85%)	20 (14%)	1 (1%)	22	26
15	M	192/195 (98%)	180 (94%)	11 (6%)	1 (0%)	29	35
16	N	184/187 (98%)	162 (88%)	15 (8%)	7 (4%)	3	1
17	O	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
18	P	141/149 (95%)	137 (97%)	4 (3%)	0	100	100
19	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
20	R	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
21	S	79/85 (93%)	74 (94%)	5 (6%)	0	100	100
22	T	117/120 (98%)	108 (92%)	8 (7%)	1 (1%)	17	20
23	U	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
24	V	63/71 (89%)	55 (87%)	7 (11%)	1 (2%)	9	9
25	W	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
26	X	80/92 (87%)	71 (89%)	9 (11%)	0	100	100
27	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
28	Z	71/83 (86%)	58 (82%)	10 (14%)	3 (4%)	3	1
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	2	42/50 (84%)	40 (95%)	2 (5%)	0	100	100
31	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	14	15
32	I	68/162 (42%)	52 (76%)	14 (21%)	2 (3%)	4	3
All	All	3705/4431 (84%)	3409 (92%)	249 (7%)	47 (1%)	12	12

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	37	VAL
7	D	137	PRO
9	F	101	ALA

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Mol	Chain	Res	Type
11	H	166	SER
12	J	143	LYS
14	L	80	ASP
16	N	154	LEU
16	N	183	ASP
16	N	184	ILE
28	Z	42	CYS
28	Z	81	ARG
4	A	34	ASP
5	B	169	GLY
7	D	60	GLU
7	D	171	ASP
11	H	168	ALA
22	T	53	GLY
28	Z	20	ARG
32	I	129	VAL
4	A	132	ASP
5	B	34	GLY
7	D	16	PRO
7	D	56	ARG
7	D	138	GLY
7	D	147	ALA
12	J	65	ASN
15	M	83	SER
16	N	162	ASP
4	A	27	LEU
5	B	185	GLY
7	D	61	PHE
12	J	5	GLU
13	K	126	SER
16	N	68	GLU
24	V	43	PRO
31	3	56	PRO
7	D	65	GLU
7	D	97	GLN
16	N	65	ASP
16	N	164	ASP
5	B	107	SER
9	F	100	ASP
4	A	112	PRO
7	D	27	ILE
7	D	69	ILE

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Mol	Chain	Res	Type
32	I	114	PRO
5	B	2	GLN

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%)	21	29
5	B	282/283 (100%)	268 (95%)	14 (5%)	24	34
6	C	193/193 (100%)	174 (90%)	19 (10%)	8	9
7	D	117/148 (79%)	110 (94%)	7 (6%)	19	26
8	E	152/156 (97%)	145 (95%)	7 (5%)	27	38
9	F	93/94 (99%)	90 (97%)	3 (3%)	39	54
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	130 (98%)	2 (2%)	65	79
12	J	118/121 (98%)	110 (93%)	8 (7%)	16	21
13	K	106/106 (100%)	102 (96%)	4 (4%)	33	47
14	L	113/127 (89%)	109 (96%)	4 (4%)	36	50
15	M	158/159 (99%)	153 (97%)	5 (3%)	39	54
16	N	149/150 (99%)	142 (95%)	7 (5%)	26	37
17	O	93/94 (99%)	91 (98%)	2 (2%)	52	69
18	P	113/117 (97%)	110 (97%)	3 (3%)	44	61
19	Q	79/80 (99%)	75 (95%)	4 (5%)	24	33
20	R	117/122 (96%)	117 (100%)	0	100	100
21	S	71/74 (96%)	71 (100%)	0	100	100
22	T	105/106 (99%)	101 (96%)	4 (4%)	33	47
23	U	44/52 (85%)	43 (98%)	1 (2%)	50	67
24	V	51/57 (90%)	50 (98%)	1 (2%)	55	72
25	W	130/130 (100%)	126 (97%)	4 (3%)	40	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	X	66/74 (89%)	62 (94%)	4 (6%)	18	25
27	Y	120/196 (61%)	109 (91%)	11 (9%)	9	11
28	Z	60/68 (88%)	59 (98%)	1 (2%)	60	76
29	1	46/47 (98%)	45 (98%)	1 (2%)	52	69
30	2	42/46 (91%)	41 (98%)	1 (2%)	49	66
31	3	79/79 (100%)	77 (98%)	2 (2%)	47	65
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3612 (86%)	2964 (96%)	129 (4%)	30	42

All (129) 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	78	ASP
4	A	94	LEU
4	A	131	HIS
4	A	165	THR
4	A	179	MET
4	A	206	ARG
4	A	217	ARG
5	B	11	LEU
5	B	27	ASN
5	B	28	SER
5	B	82	VAL
5	B	98	THR
5	B	113	LEU
5	B	149	ASP
5	B	162	MET
5	B	195	ARG
5	B	251	VAL
5	B	254	GLN
5	B	277	GLU
5	B	279	THR
5	B	312	ARG
6	C	16	VAL
6	C	27	ARG
6	C	67	GLN
6	C	76	ARG

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Mol	Chain	Res	Type
6	C	78	ARG
6	C	91	PRO
6	C	94	THR
6	C	95	GLU
6	C	101	ASP
6	C	136	VAL
6	C	162	VAL
6	C	187	ARG
6	C	214	THR
6	C	223	LEU
6	C	234	VAL
6	C	236	THR
6	C	240	LEU
6	C	243	VAL
6	C	246	ARG
7	D	24	HIS
7	D	50	VAL
7	D	61	PHE
7	D	99	ASP
7	D	100	ASP
7	D	133	ASN
7	D	137	PRO
8	E	15	GLN
8	E	16	ASP
8	E	102	VAL
8	E	131	LEU
8	E	155	ASN
8	E	156	ASP
8	E	164	ASP
9	F	12	LEU
9	F	46	GLU
9	F	99	THR
11	H	84	LYS
11	H	154	TYR
12	J	46	ILE
12	J	52	GLN
12	J	70	PHE
12	J	74	ARG
12	J	79	PHE
12	J	107	ASN
12	J	127	ILE
12	J	131	THR

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Mol	Chain	Res	Type
13	K	4	LEU
13	K	10	GLN
13	K	84	ASP
13	K	100	GLU
14	L	35	ARG
14	L	43	HIS
14	L	89	PHE
14	L	140	VAL
15	M	46	LEU
15	M	68	ARG
15	M	93	ARG
15	M	99	ARG
15	M	116	ASN
16	N	12	ARG
16	N	23	ARG
16	N	26	LEU
16	N	37	ARG
16	N	49	THR
16	N	127	LEU
16	N	139	TRP
17	O	3	THR
17	O	111	VAL
18	P	81	LYS
18	P	98	ILE
18	P	117	SER
19	Q	16	ASN
19	Q	18	PRO
19	Q	57	ASP
19	Q	95	GLU
22	T	26	THR
22	T	39	ASN
22	T	48	VAL
22	T	89	ARG
23	U	17	THR
24	V	65	ASP
25	W	35	VAL
25	W	52	VAL
25	W	122	ARG
25	W	146	ILE
26	X	27	ASP
26	X	72	VAL
26	X	79	GLU

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Mol	Chain	Res	Type
26	X	82	GLU
27	Y	103	THR
27	Y	115	ARG
27	Y	141	THR
27	Y	144	ARG
27	Y	154	ARG
27	Y	163	THR
27	Y	189	ASN
27	Y	200	THR
27	Y	203	VAL
27	Y	204	ARG
27	Y	235	GLU
28	Z	22	SER
29	1	47	ASP
30	2	18	ASN
31	3	56	PRO
31	3	65	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	29	HIS
4	A	199	HIS
5	B	27	ASN
5	B	145	HIS
5	B	221	GLN
5	B	238	ASN
5	B	256	GLN
5	B	260	HIS
5	B	320	GLN
5	B	332	ASN
6	C	39	GLN
6	C	129	HIS
7	D	47	GLN
7	D	103	ASN
7	D	133	ASN
8	E	106	ASN
8	E	143	GLN
10	G	64	ASN
11	H	31	HIS
11	H	56	GLN
11	H	59	HIS

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Mol	Chain	Res	Type
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
14	L	43	HIS
14	L	116	HIS
15	M	24	GLN
15	M	26	GLN
15	M	58	GLN
15	M	77	HIS
15	M	143	ASN
15	M	170	ASN
16	N	93	GLN
16	N	107	ASN
16	N	153	GLN
17	O	53	GLN
17	O	100	GLN
18	P	50	GLN
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	53	ASN
22	T	37	GLN
22	T	39	ASN
23	U	39	ASN
23	U	48	ASN
24	V	29	ASN
24	V	60	GLN
25	W	27	HIS
25	W	110	GLN

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Mol	Chain	Res	Type
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	22	ASN
27	Y	119	GLN
27	Y	134	HIS
27	Y	149	GLN
27	Y	189	ASN
28	Z	41	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	30	GLN
31	3	48	ASN
32	I	113	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	235 (8%)	36 (1%)
2	9	121/122 (99%)	14 (11%)	1 (0%)
3	4	1/7 (14%)	0	0
All	All	2867/3051 (93%)	249 (8%)	37 (1%)

All (249) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	86	A
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U

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Mol	Chain	Res	Type
1	0	120	A
1	0	130	C
1	0	134	U
1	0	141	C
1	0	151	A
1	0	166	A
1	0	186	A
1	0	191	A
1	0	192	A
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	308	U
1	0	309	C
1	0	318	C
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	457	U
1	0	461	C
1	0	473	A
1	0	487	G
1	0	497	A
1	0	498	A
1	0	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

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Mol	Chain	Res	Type
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	702	G
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	875	A
1	0	877	G
1	0	878	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	1087	G
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1164	U

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Mol	Chain	Res	Type
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	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1331	A
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1378	G
1	0	1407	A
1	0	1409	G
1	0	1474	C
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1528	A
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U

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Mol	Chain	Res	Type
1	0	1723	G
1	0	1725	C
1	0	1731	C
1	0	1732	A
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1873	G
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1967	U
1	0	1971	G
1	0	1973	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2004	U
1	0	2006	C
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	2103	A
1	0	2110	G
1	0	2238	A
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G

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Mol	Chain	Res	Type
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	2379	G
1	0	2422	U
1	0	2462	G
1	0	2467	A
1	0	2469	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2542	C
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2634	G
1	0	2637	A
1	0	2644	C
1	0	2645	U
1	0	2648	U
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2726	U
1	0	2727	A
1	0	2747	C
1	0	2748	G
1	0	2749	U

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Mol	Chain	Res	Type
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2812	A
1	0	2825	C
1	0	2852	A
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
2	9	3044	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (37) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A
1	0	129	A
1	0	169	A
1	0	338	C
1	0	603	A
1	0	644	G
1	0	699	C
1	0	834	G
1	0	857	A

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Mol	Chain	Res	Type
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1232	A
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1506	U
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1730	G
1	0	1819	G
1	0	1856	C
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2536	C
1	0	2541	U
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2761	A
1	0	2791	U
1	0	2852	A
2	9	3065	A

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

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	PSU	0	2621	1	17,21,22	1.68	3 (17%)	20,30,33	5.43	4 (20%)
3	PPU	4	76	1,3	32,40,41	1.19	1 (3%)	33,57,60	0.84	2 (6%)
1	UR3	0	2619	1	14,22,23	0.87	1 (7%)	15,32,35	0.59	0
1	OMG	0	2588	1,3	18,26,27	1.06	2 (11%)	20,38,41	2.61	5 (25%)
1	1MA	0	628	1	15,25,26	0.72	0	15,37,40	1.36	1 (6%)
1	OMU	0	2587	1	14,22,23	0.99	1 (7%)	14,31,34	1.17	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
3	PPU	4	76	1,3	-	0/21/43/44	0/4/4/4
1	UR3	0	2619	1	-	0/5/25/26	0/2/2/2
1	OMG	0	2588	1,3	-	2/5/27/28	0/3/3/3
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3
1	OMU	0	2587	1	-	0/7/27/28	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	76	PPU	OC-CM	-5.45	1.26	1.42
1	0	2621	PSU	C5-C1'	-4.96	1.48	1.52
1	0	2588	OMG	C6-N1	3.28	1.38	1.33
1	0	2621	PSU	C4-N3	3.02	1.38	1.33
1	0	2621	PSU	C2-N1	2.79	1.43	1.38
1	0	2587	OMU	C4-N3	2.61	1.37	1.33
1	0	2619	UR3	C6-C5	-2.16	1.33	1.38
1	0	2588	OMG	C8-N7	-2.03	1.31	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-17.24	114.72	128.43
1	0	2621	PSU	C4-N3-C2	14.32	127.23	115.14
1	0	2588	OMG	C5-C6-N1	-8.61	111.65	123.43
1	0	2621	PSU	C5-C4-N3	-8.22	114.76	125.36
1	0	2588	OMG	C6-N1-C2	5.84	125.22	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	628	1MA	C2-N3-C4	-4.63	110.79	116.58
1	0	2587	OMU	C5-C4-N3	-3.85	114.84	123.31
1	0	2588	OMG	C2-N3-C4	-3.03	111.90	115.36
1	0	2621	PSU	C6-N1-C2	2.52	119.51	115.36
1	0	2588	OMG	N3-C2-N1	-2.44	123.97	127.22
3	4	76	PPU	C3'-N3'-C	-2.18	119.92	123.21
3	4	76	PPU	CM-OC-CZ	2.07	122.00	117.51
1	0	2588	OMG	C6-C5-C4	-2.04	118.85	120.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	2588	OMG	C3'-C2'-O2'-CM2
1	0	2588	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	4	76	PPU	1	0
1	0	2587	OMU	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 312 ligands modelled in this entry, 312 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2922 (94%)	-0.12	75 (2%) 54 62	26, 50, 94, 154	0
2	9	122/122 (100%)	0.14	5 (4%) 37 44	45, 70, 97, 154	0
3	4	5/7 (71%)	-0.62	0 100 100	46, 48, 54, 54	0
4	A	237/240 (98%)	0.54	18 (7%) 13 18	31, 55, 88, 108	0
5	B	337/338 (99%)	0.41	15 (4%) 33 40	32, 57, 83, 94	0
6	C	246/246 (100%)	0.19	6 (2%) 59 66	29, 51, 76, 90	0
7	D	140/177 (79%)	2.40	65 (46%) 0 0	64, 100, 128, 135	0
8	E	172/178 (96%)	1.14	38 (22%) 0 1	47, 71, 89, 96	0
9	F	119/120 (99%)	1.46	41 (34%) 0 0	51, 77, 106, 112	0
10	G	29/348 (8%)	2.78	19 (65%) 0 0	75, 97, 105, 106	0
11	H	160/171 (93%)	0.89	25 (15%) 2 2	49, 66, 97, 105	0
12	J	142/145 (97%)	0.28	5 (3%) 44 51	40, 55, 76, 95	0
13	K	132/132 (100%)	0.08	2 (1%) 73 79	36, 52, 74, 83	0
14	L	145/165 (87%)	1.00	29 (20%) 1 1	29, 70, 114, 125	0
15	M	194/195 (99%)	0.99	23 (11%) 4 6	36, 49, 90, 98	0
16	N	186/187 (99%)	1.27	43 (23%) 0 1	48, 70, 117, 121	0
17	O	115/116 (99%)	0.39	4 (3%) 44 51	42, 60, 75, 81	0
18	P	143/149 (95%)	0.30	4 (2%) 53 60	41, 56, 69, 81	0
19	Q	95/96 (98%)	0.38	6 (6%) 20 25	42, 54, 70, 78	0
20	R	150/155 (96%)	0.12	3 (2%) 65 71	33, 49, 69, 77	0
21	S	81/85 (95%)	0.43	5 (6%) 20 26	42, 60, 81, 98	0
22	T	119/120 (99%)	0.89	15 (12%) 3 5	46, 59, 89, 113	0
23	U	53/66 (80%)	0.38	3 (5%) 23 30	46, 57, 77, 84	0
24	V	65/71 (91%)	1.83	17 (26%) 0 0	55, 80, 116, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	0.34	4 (2%) 56 63	42, 56, 79, 88	0
26	X	82/92 (89%)	0.91	11 (13%) 3 4	46, 60, 88, 105	0
27	Y	142/241 (58%)	0.40	12 (8%) 10 14	32, 49, 70, 90	0
28	Z	73/83 (87%)	2.19	29 (39%) 0 0	51, 83, 99, 106	0
29	1	56/57 (98%)	-0.28	0 100 100	30, 36, 45, 54	0
30	2	46/50 (92%)	1.06	8 (17%) 1 1	39, 63, 88, 100	0
31	3	92/92 (100%)	0.62	9 (9%) 7 10	39, 61, 76, 90	0
32	I	70/162 (43%)	6.05	66 (94%) 0 0	114, 127, 144, 146	0
All	All	6651/7482 (88%)	0.43	605 (9%) 9 12	26, 56, 102, 154	0

All (605) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	71	GLY	20.6
24	V	1	THR	16.1
7	D	63	ILE	14.8
15	M	70	GLY	13.7
32	I	133	THR	13.6
16	N	166	ALA	12.8
7	D	57	THR	12.6
32	I	79	ILE	11.6
24	V	39	ALA	11.5
15	M	80	GLY	11.4
22	T	119	ALA	11.2
28	Z	22	SER	11.2
32	I	109	ALA	11.1
28	Z	11	SER	11.0
32	I	75	THR	10.5
32	I	105	VAL	10.5
15	M	79	ALA	10.4
32	I	137	VAL	10.3
32	I	76	ALA	10.2
24	V	40	PRO	10.1
32	I	96	PHE	9.8
32	I	121	LEU	9.4
32	I	102	VAL	9.3
32	I	118	SER	9.1
26	X	88	GLU	8.9
15	M	74	LYS	8.7

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Mol	Chain	Res	Type	RSRZ
32	I	85	PHE	8.6
2	9	3001	U	8.5
32	I	116	LEU	8.5
30	2	49	GLU	8.4
32	I	125	ALA	8.1
32	I	81	ASP	8.0
32	I	107	GLN	7.8
15	M	87	GLY	7.8
32	I	126	LYS	7.8
32	I	111	GLN	7.8
32	I	77	GLU	7.8
28	Z	21	VAL	7.7
28	Z	20	ARG	7.7
32	I	108	ILE	7.7
32	I	129	VAL	7.7
32	I	114	PRO	7.6
32	I	113	HIS	7.5
15	M	86	GLN	7.4
32	I	93	GLN	7.4
32	I	104	GLN	7.4
15	M	71	SER	7.3
32	I	132	CYS	7.2
32	I	78	LEU	7.2
15	M	77	HIS	7.2
28	Z	19	GLY	7.1
7	D	61	PHE	7.1
24	V	38	GLY	7.0
32	I	91	GLU	6.9
10	G	26	MET	6.9
10	G	23	ILE	6.9
1	0	1951	G	6.7
4	A	37	VAL	6.7
32	I	87	THR	6.7
1	0	282	C	6.6
32	I	88	GLY	6.6
15	M	78	LYS	6.6
7	D	88	LEU	6.6
32	I	138	THR	6.6
8	E	45	ASP	6.5
28	Z	29	ILE	6.5
32	I	83	ALA	6.4
4	A	237	GLY	6.3

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Mol	Chain	Res	Type	RSRZ
28	Z	18	TYR	6.3
15	M	76	ARG	6.2
7	D	166	ILE	6.2
7	D	90	LEU	6.1
28	Z	24	ARG	6.0
32	I	97	VAL	6.0
28	Z	25	ARG	6.0
16	N	175	LEU	6.0
30	2	35	ARG	6.0
32	I	117	LEU	6.0
7	D	170	TYR	5.9
10	G	27	ILE	5.9
1	0	1199	A	5.9
7	D	134	LEU	5.9
28	Z	23	ARG	5.9
15	M	83	SER	5.8
7	D	64	ARG	5.8
32	I	136	GLY	5.7
32	I	74	PRO	5.6
16	N	165	ALA	5.6
16	N	147	ILE	5.6
28	Z	12	GLY	5.5
7	D	27	ILE	5.5
21	S	81	ILE	5.5
28	Z	31	SER	5.5
9	F	16	ALA	5.5
1	0	2004	U	5.4
1	0	497	A	5.4
28	Z	45	ASP	5.4
28	Z	34	ASN	5.4
32	I	89	SER	5.4
2	9	3024	U	5.3
15	M	75	ARG	5.3
7	D	104	PHE	5.3
16	N	163	PHE	5.3
7	D	44	ILE	5.3
24	V	36	ALA	5.2
1	0	1177	A	5.1
32	I	86	GLU	5.1
7	D	135	VAL	5.1
15	M	73	ARG	5.1
7	D	69	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
14	L	93	VAL	5.0
1	0	1173	A	5.0
28	Z	33	MET	5.0
9	F	119	ARG	5.0
32	I	103	ASP	4.9
9	F	106	ALA	4.9
28	Z	32	GLU	4.9
1	0	1172	G	4.9
22	T	118	SER	4.9
14	L	75	LEU	4.8
4	A	133	ARG	4.8
16	N	155	GLU	4.8
1	0	1198	U	4.8
2	9	3023	U	4.8
1	0	272	A	4.8
15	M	81	ARG	4.7
8	E	86	VAL	4.7
7	D	10	PHE	4.7
7	D	62	ASP	4.7
1	0	970	U	4.7
16	N	68	GLU	4.7
32	I	123	ASN	4.6
16	N	95	ALA	4.6
7	D	81	GLU	4.6
9	F	22	VAL	4.6
14	L	91	VAL	4.6
7	D	40	ILE	4.6
22	T	116	ASP	4.6
11	H	171	ALA	4.6
7	D	92	GLU	4.6
11	H	73	LEU	4.6
1	0	280	C	4.5
1	0	960	G	4.5
7	D	73	VAL	4.5
14	L	106	VAL	4.5
14	L	76	LEU	4.5
24	V	41	GLU	4.5
7	D	26	GLY	4.5
8	E	4	GLU	4.5
9	F	118	LEU	4.4
32	I	99	ASP	4.4
1	0	285	A	4.4

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Mol	Chain	Res	Type	RSRZ
26	X	80	GLU	4.4
7	D	93	LEU	4.4
9	F	110	ASP	4.4
1	0	735	C	4.4
24	V	37	GLY	4.3
25	W	86	GLU	4.3
28	Z	30	GLU	4.3
13	K	132	VAL	4.3
11	H	74	ILE	4.3
1	0	999	C	4.3
6	C	61	PHE	4.3
9	F	49	PHE	4.3
12	J	70	PHE	4.3
7	D	85	GLN	4.3
32	I	122	THR	4.3
17	O	22	GLY	4.3
15	M	84	LYS	4.2
1	0	1202	A	4.2
14	L	105	TYR	4.2
30	2	39	ARG	4.2
7	D	18	ILE	4.2
1	0	1525	G	4.1
28	Z	14	PHE	4.1
9	F	28	ALA	4.1
4	A	36	ASP	4.1
15	M	82	ARG	4.1
16	N	159	TYR	4.1
9	F	117	GLU	4.1
1	0	2645	U	4.1
8	E	108	LEU	4.1
1	0	2238	A	4.0
32	I	112	LYS	4.0
32	I	72	VAL	4.0
10	G	24	VAL	4.0
14	L	102	ASP	4.0
31	3	92	GLU	4.0
10	G	73	ASP	4.0
7	D	11	HIS	4.0
1	0	1965	C	4.0
7	D	56	ARG	3.9
8	E	10	ASP	3.9
1	0	514	G	3.9

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Mol	Chain	Res	Type	RSRZ
1	0	2237	G	3.9
8	E	6	GLU	3.9
15	M	88	VAL	3.9
16	N	184	ILE	3.9
27	Y	235	GLU	3.9
14	L	80	ASP	3.9
1	0	1948	G	3.9
2	9	3002	U	3.9
9	F	17	LEU	3.9
7	D	172	VAL	3.9
8	E	87	PHE	3.9
32	I	134	SER	3.9
11	H	37	GLN	3.8
9	F	25	ASP	3.7
31	3	62	THR	3.7
28	Z	36	ASP	3.7
10	G	69	ARG	3.7
27	Y	216	ARG	3.7
26	X	85	VAL	3.7
7	D	41	LEU	3.7
10	G	71	LEU	3.7
24	V	8	ILE	3.7
28	Z	26	VAL	3.7
7	D	89	PRO	3.7
22	T	117	ASP	3.7
24	V	43	PRO	3.7
1	0	288	A	3.7
9	F	100	ASP	3.7
16	N	161	GLY	3.7
11	H	146	VAL	3.7
32	I	110	GLU	3.6
7	D	130	VAL	3.6
1	0	1169	U	3.6
1	0	284	C	3.6
32	I	98	ALA	3.6
32	I	115	ASP	3.6
9	F	108	VAL	3.6
16	N	152	GLU	3.6
32	I	80	LYS	3.6
32	I	106	LYS	3.6
24	V	63	GLU	3.6
1	0	2769	C	3.6

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Mol	Chain	Res	Type	RSRZ
15	M	85	ARG	3.6
10	G	67	LEU	3.6
10	G	25	GLU	3.6
19	Q	95	GLU	3.6
1	O	1200	A	3.6
11	H	78	GLY	3.6
16	N	158	LEU	3.6
28	Z	37	HIS	3.5
9	F	99	THR	3.5
22	T	82	THR	3.5
1	O	2508	C	3.5
16	N	181	ASP	3.5
16	N	154	LEU	3.5
26	X	10	VAL	3.5
7	D	167	GLU	3.5
14	L	60	GLU	3.5
7	D	84	LEU	3.5
1	O	1163	G	3.5
4	A	145	MET	3.5
14	L	104	ASP	3.5
14	L	120	LEU	3.5
28	Z	28	GLU	3.5
30	2	27	LEU	3.5
10	G	22	ALA	3.5
14	L	62	ALA	3.5
15	M	72	ALA	3.5
11	H	35	ARG	3.5
1	O	10	U	3.5
26	X	7	GLU	3.5
7	D	23	VAL	3.4
14	L	81	VAL	3.4
32	I	95	ASP	3.4
14	L	148	GLU	3.4
32	I	120	ASP	3.4
8	E	88	TYR	3.4
9	F	19	ALA	3.4
13	K	118	ALA	3.4
14	L	145	LEU	3.4
26	X	77	PHE	3.4
9	F	98	VAL	3.4
16	N	178	THR	3.4
8	E	42	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
32	I	119	TYR	3.4
23	U	47	ARG	3.4
8	E	76	VAL	3.3
26	X	71	ARG	3.3
1	0	969	G	3.3
7	D	68	PRO	3.3
1	0	1171	A	3.3
1	0	2748	G	3.3
27	Y	96	GLU	3.3
27	Y	108	ASP	3.3
8	E	11	VAL	3.3
16	N	185	GLU	3.3
27	Y	236	VAL	3.3
1	0	1168	C	3.3
8	E	160	ARG	3.3
7	D	157	LEU	3.3
14	L	97	VAL	3.3
1	0	1000	C	3.3
7	D	106	PHE	3.3
14	L	121	ILE	3.3
5	B	108	GLU	3.3
1	0	2511	A	3.2
8	E	94	GLN	3.2
9	F	21	GLU	3.2
28	Z	10	ARG	3.2
6	C	1	MET	3.2
9	F	12	LEU	3.2
9	F	107	ASP	3.2
14	L	79	ASP	3.2
16	N	183	ASP	3.2
30	2	48	ASP	3.2
28	Z	16	ALA	3.2
4	A	35	GLY	3.2
8	E	100	ASP	3.2
16	N	180	LEU	3.2
32	I	94	GLU	3.1
4	A	85	SER	3.1
12	J	4	ALA	3.1
16	N	134	ASP	3.1
5	B	57	GLU	3.1
7	D	66	GLY	3.1
10	G	66	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
9	F	15	ASP	3.1
1	0	1966	U	3.1
14	L	99	GLU	3.1
9	F	11	ASP	3.1
4	A	31	LYS	3.1
8	E	1	PRO	3.1
1	0	138	U	3.1
1	0	281	U	3.1
9	F	101	ALA	3.1
26	X	72	VAL	3.0
8	E	43	ASP	3.0
27	Y	95	THR	3.0
30	2	44	ARG	3.0
16	N	71	TRP	3.0
8	E	118	ILE	3.0
21	S	45	TYR	3.0
32	I	124	ALA	3.0
9	F	72	VAL	3.0
11	H	143	ALA	3.0
7	D	65	GLU	3.0
8	E	127	ASP	3.0
11	H	138	CYS	2.9
16	N	137	ALA	2.9
7	D	58	VAL	2.9
1	0	1950	G	2.9
8	E	98	GLU	2.9
9	F	69	GLU	2.9
16	N	139	TRP	2.9
14	L	142	LEU	2.9
14	L	44	GLU	2.9
14	L	100	ALA	2.9
16	N	143	ARG	2.9
16	N	156	GLU	2.9
1	0	1178	G	2.9
19	Q	76	VAL	2.9
11	H	82	ASP	2.9
7	D	53	LYS	2.9
22	T	115	GLU	2.9
16	N	172	PHE	2.9
7	D	160	ALA	2.9
31	3	41	GLU	2.9
32	I	92	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
8	E	7	ILE	2.8
8	E	89	SER	2.8
11	H	141	GLU	2.8
7	D	75	LEU	2.8
24	V	10	ASP	2.8
4	A	91	GLY	2.8
9	F	44	SER	2.8
22	T	112	LEU	2.8
25	W	76	ASP	2.8
28	Z	59	TYR	2.8
1	0	1170	U	2.8
7	D	154	LYS	2.8
2	9	3122	C	2.8
21	S	20	PHE	2.8
1	0	2344	G	2.8
14	L	130	ARG	2.8
32	I	127	GLU	2.8
5	B	104	GLU	2.8
9	F	18	GLU	2.8
4	A	38	ILE	2.8
8	E	154	ILE	2.8
7	D	51	ARG	2.8
15	M	1	ALA	2.7
22	T	42	VAL	2.7
16	N	94	GLU	2.7
8	E	93	MET	2.7
16	N	138	ASP	2.7
5	B	2	GLN	2.7
11	H	149	ALA	2.7
16	N	179	LEU	2.7
7	D	77	ASP	2.7
10	G	21	ASP	2.7
16	N	72	GLU	2.7
18	P	111	GLU	2.7
24	V	5	VAL	2.7
31	3	1	MET	2.7
11	H	79	GLU	2.7
16	N	16	ALA	2.7
10	G	72	ASP	2.7
12	J	7	ASP	2.7
18	P	108	LEU	2.7
27	Y	196	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
11	H	83	TYR	2.7
22	T	35	TYR	2.7
25	W	91	ASP	2.6
16	N	2	THR	2.6
16	N	106	LEU	2.6
1	0	1279	U	2.6
14	L	61	ALA	2.6
24	V	59	ILE	2.6
31	3	20	HIS	2.6
1	0	1929	G	2.6
27	Y	234	VAL	2.6
32	I	100	LEU	2.6
32	I	135	LEU	2.6
1	0	283	U	2.6
7	D	91	ALA	2.6
8	E	90	HIS	2.6
26	X	73	ARG	2.6
7	D	129	ASP	2.6
18	P	114	LEU	2.6
1	0	362	G	2.6
32	I	73	PRO	2.6
4	A	236	GLY	2.6
11	H	139	ASN	2.6
14	L	149	ARG	2.6
28	Z	13	ARG	2.6
32	I	82	GLU	2.6
7	D	107	GLY	2.6
9	F	45	ALA	2.6
21	S	78	ALA	2.6
24	V	32	ALA	2.6
7	D	171	ASP	2.6
8	E	121	ASP	2.6
1	0	372	A	2.6
7	D	173	GLU	2.6
4	A	99	ILE	2.6
9	F	75	ILE	2.6
15	M	89	THR	2.5
5	B	105	PHE	2.5
32	I	128	VAL	2.5
8	E	44	GLY	2.5
8	E	99	GLY	2.5
12	J	5	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
30	2	20	ARG	2.5
5	B	109	LEU	2.5
7	D	38	GLU	2.5
1	0	1181	A	2.5
18	P	141	ILE	2.5
19	Q	18	PRO	2.5
27	Y	98	GLN	2.5
11	H	34	GLY	2.5
7	D	132	VAL	2.5
8	E	162	PHE	2.5
1	0	736	A	2.5
8	E	123	ASP	2.5
7	D	12	GLU	2.5
8	E	124	VAL	2.5
10	G	28	GLU	2.5
1	0	1208	C	2.5
1	0	1625	U	2.5
1	0	1967	U	2.5
6	C	246	ARG	2.5
9	F	111	ILE	2.5
4	A	59	GLU	2.5
5	B	117	GLU	2.5
27	Y	187	VAL	2.5
28	Z	27	ALA	2.5
4	A	65	ARG	2.4
16	N	92	ALA	2.4
1	0	279	C	2.4
10	G	15	TRP	2.4
1	0	370	G	2.4
4	A	64	ASP	2.4
8	E	126	ILE	2.4
22	T	59	GLU	2.4
1	0	358	G	2.4
27	Y	193	LEU	2.4
20	R	96	VAL	2.4
7	D	70	GLY	2.4
16	N	37	ARG	2.4
16	N	149	GLU	2.4
11	H	67	LEU	2.4
9	F	24	ARG	2.4
9	F	29	VAL	2.4
31	3	22	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
11	H	47	ILE	2.4
6	C	135	GLU	2.4
7	D	43	GLU	2.4
16	N	177	GLU	2.4
28	Z	44	GLU	2.4
5	B	1	PRO	2.4
5	B	134	ALA	2.4
20	R	150	PRO	2.4
1	0	369	G	2.4
11	H	140	VAL	2.4
8	E	105	GLU	2.4
5	B	119	HIS	2.4
1	0	1189	A	2.3
19	Q	92	ARG	2.3
8	E	129	GLU	2.3
10	G	12	ILE	2.3
11	H	24	PRO	2.3
7	D	128	LEU	2.3
7	D	50	VAL	2.3
1	0	295	C	2.3
16	N	73	ALA	2.3
9	F	37	THR	2.3
15	M	164	THR	2.3
1	0	1192	A	2.3
1	0	716	G	2.3
5	B	33	ASP	2.3
7	D	95	THR	2.3
4	A	206	ARG	2.3
16	N	170	GLU	2.3
16	N	145	ALA	2.3
16	N	182	GLY	2.3
22	T	36	GLY	2.3
10	G	63	ARG	2.3
22	T	13	ARG	2.3
8	E	46	THR	2.2
1	0	441	A	2.2
6	C	237	GLU	2.2
9	F	23	ALA	2.2
19	Q	84	ILE	2.2
1	0	1164	U	2.2
23	U	52	THR	2.2
1	0	1947	G	2.2

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Mol	Chain	Res	Type	RSRZ
11	H	66	ARG	2.2
1	0	1180	U	2.2
9	F	70	LYS	2.2
1	0	1196	C	2.2
8	E	169	THR	2.2
17	O	23	GLY	2.2
32	I	84	GLY	2.2
17	O	98	LEU	2.2
28	Z	35	GLU	2.2
22	T	77	VAL	2.2
24	V	33	VAL	2.2
32	I	90	GLY	2.2
7	D	86	THR	2.2
9	F	47	LEU	2.2
8	E	48	VAL	2.2
9	F	115	VAL	2.2
32	I	140	GLU	2.2
26	X	41	PHE	2.2
7	D	71	ALA	2.2
1	0	1981	A	2.2
11	H	162	ARG	2.2
22	T	103	LEU	2.2
22	T	109	GLU	2.2
1	0	1203	G	2.1
4	A	135	VAL	2.1
31	3	26	ARG	2.1
1	0	1206	U	2.1
1	0	1174	A	2.1
1	0	2345	A	2.1
10	G	68	GLU	2.1
9	F	20	LEU	2.1
19	Q	17	LYS	2.1
21	S	2	TRP	2.1
5	B	115	VAL	2.1
5	B	133	GLU	2.1
8	E	81	GLU	2.1
1	0	129	A	2.1
11	H	50	ILE	2.1
26	X	12	ILE	2.1
9	F	60	VAL	2.1
9	F	113	ASP	2.1
4	A	128	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
5	B	186	GLY	2.1
10	G	19	GLU	2.1
31	3	73	GLU	2.1
1	0	1184	C	2.1
17	O	31	GLU	2.1
20	R	104	PHE	2.1
8	E	16	ASP	2.1
30	2	30	ASP	2.1
14	L	59	GLU	2.1
9	F	26	THR	2.1
11	H	70	ASN	2.1
7	D	163	VAL	2.1
14	L	96	VAL	2.1
5	B	181	ILE	2.1
7	D	47	GLN	2.1
9	F	103	GLU	2.1
14	L	147	GLU	2.1
27	Y	106	THR	2.1
24	V	14	ALA	2.1
14	L	150	GLN	2.0
15	M	97	ILE	2.0
7	D	72	LYS	2.0
7	D	169	THR	2.0
16	N	74	PRO	2.0
7	D	83	PHE	2.0
23	U	4	ARG	2.0
16	N	81	ALA	2.0
11	H	142	ASP	2.0
12	J	39	VAL	2.0
31	3	13	HIS	2.0
6	C	63	SER	2.0
24	V	9	ARG	2.0
25	W	78	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	OMG	0	2588	24/25	0.97	0.12	34,37,42,43	0
3	PPU	4	76	37/38	0.98	0.12	38,43,49,54	0
1	UR3	0	2619	21/22	0.98	0.14	39,40,43,47	0
1	PSU	0	2621	20/21	0.98	0.13	35,39,43,44	0
1	1MA	0	628	23/24	0.98	0.15	35,37,40,44	0
1	OMU	0	2587	21/22	0.98	0.12	35,40,43,43	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	SR	0	9537	1/1	0.14	0.21	159,159,159,159	0
33	MG	0	8047	1/1	0.18	1.13	111,111,111,111	0
35	NA	0	9129	1/1	0.29	0.32	82,82,82,82	0
37	SR	0	9547	1/1	0.38	0.28	184,184,184,184	0
33	MG	0	8102	1/1	0.43	0.16	76,76,76,76	0
33	MG	0	8108	1/1	0.47	0.13	107,107,107,107	0
38	CD	Z	9203	1/1	0.48	0.19	93,93,93,93	0
33	MG	0	8094	1/1	0.51	0.68	93,93,93,93	0
35	NA	0	9184	1/1	0.56	0.21	83,83,83,83	0
35	NA	0	9111	1/1	0.67	0.27	70,70,70,70	0
35	NA	0	9185	1/1	0.67	0.47	62,62,62,62	0
35	NA	0	9179	1/1	0.69	1.23	96,96,96,96	0
35	NA	9	9151	1/1	0.71	0.23	83,83,83,83	0
33	MG	0	8050	1/1	0.72	0.18	86,86,86,86	0
35	NA	S	9112	1/1	0.72	0.31	85,85,85,85	0
33	MG	0	8059	1/1	0.72	0.40	71,71,71,71	0
33	MG	0	8065	1/1	0.74	0.47	90,90,90,90	0
35	NA	0	9178	1/1	0.75	0.26	57,57,57,57	0
33	MG	0	8042	1/1	0.76	0.09	58,58,58,58	0
33	MG	0	8052	1/1	0.76	0.41	87,87,87,87	0
33	MG	0	8022	1/1	0.76	1.07	123,123,123,123	0
36	CL	0	9316	1/1	0.77	0.24	86,86,86,86	0
33	MG	0	8091	1/1	0.77	0.08	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8014	1/1	0.77	0.86	94,94,94,94	0
37	SR	0	9484	1/1	0.77	0.08	139,139,139,139	0
37	SR	9	9588	1/1	0.78	0.14	141,141,141,141	0
33	MG	0	8032	1/1	0.78	0.10	47,47,47,47	0
33	MG	0	8040	1/1	0.78	0.44	100,100,100,100	0
33	MG	0	8072	1/1	0.79	0.33	78,78,78,78	0
37	SR	0	9500	1/1	0.79	1.25	200,200,200,200	0
35	NA	0	9140	1/1	0.79	0.55	67,67,67,67	0
35	NA	0	9171	1/1	0.81	0.25	66,66,66,66	0
35	NA	H	9122	1/1	0.81	0.19	78,78,78,78	0
33	MG	0	8089	1/1	0.81	0.23	64,64,64,64	0
35	NA	0	9168	1/1	0.82	0.15	68,68,68,68	0
33	MG	0	8107	1/1	0.82	0.16	67,67,67,67	0
35	NA	0	9182	1/1	0.82	0.14	81,81,81,81	0
33	MG	0	8084	1/1	0.83	0.33	84,84,84,84	0
35	NA	0	9102	1/1	0.83	0.24	64,64,64,64	0
35	NA	0	9174	1/1	0.83	0.51	71,71,71,71	0
35	NA	0	9163	1/1	0.83	0.19	65,65,65,65	0
35	NA	0	9170	1/1	0.84	0.38	87,87,87,87	0
33	MG	0	8041	1/1	0.84	0.12	56,56,56,56	0
35	NA	0	9158	1/1	0.84	0.23	62,62,62,62	0
33	MG	0	8099	1/1	0.84	0.19	74,74,74,74	0
33	MG	0	8116	1/1	0.84	0.08	59,59,59,59	0
33	MG	0	8092	1/1	0.84	0.49	79,79,79,79	0
35	NA	0	9164	1/1	0.84	0.34	62,62,62,62	0
35	NA	0	9125	1/1	0.85	0.56	87,87,87,87	0
33	MG	0	8054	1/1	0.85	0.14	60,60,60,60	0
33	MG	0	8101	1/1	0.85	0.15	68,68,68,68	0
33	MG	0	8114	1/1	0.86	0.39	79,79,79,79	0
33	MG	0	8093	1/1	0.86	0.18	52,52,52,52	0
35	NA	0	9157	1/1	0.86	0.17	52,52,52,52	0
35	NA	9	9152	1/1	0.87	0.48	76,76,76,76	0
33	MG	0	8113	1/1	0.87	0.13	49,49,49,49	0
35	NA	0	9161	1/1	0.88	0.20	61,61,61,61	0
37	SR	0	9504	1/1	0.88	0.12	107,107,107,107	0
37	SR	0	9626	1/1	0.88	0.38	147,147,147,147	0
34	K	0	9001	1/1	0.88	0.71	92,92,92,92	0
35	NA	9	9183	1/1	0.88	0.13	80,80,80,80	0
35	NA	0	9118	1/1	0.88	0.30	71,71,71,71	0
35	NA	0	9172	1/1	0.88	0.36	78,78,78,78	0
35	NA	0	9107	1/1	0.89	0.25	59,59,59,59	0
33	MG	0	8063	1/1	0.89	0.12	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	3	9169	1/1	0.89	0.40	98,98,98,98	0
33	MG	0	8117	1/1	0.89	0.15	48,48,48,48	0
38	CD	O	9205	1/1	0.89	0.04	138,138,138,138	0
37	SR	B	9521	1/1	0.89	0.40	184,184,184,184	0
35	NA	R	9137	1/1	0.89	0.11	43,43,43,43	0
33	MG	0	8090	1/1	0.89	0.18	67,67,67,67	0
35	NA	0	9173	1/1	0.89	0.37	69,69,69,69	0
34	K	0	9002	1/1	0.89	0.12	90,90,90,90	0
33	MG	0	8046	1/1	0.90	0.10	47,47,47,47	0
35	NA	0	9126	1/1	0.90	0.11	64,64,64,64	0
35	NA	0	9110	1/1	0.90	0.15	49,49,49,49	0
33	MG	0	8045	1/1	0.90	0.32	82,82,82,82	0
35	NA	0	9156	1/1	0.90	0.34	59,59,59,59	0
33	MG	0	8024	1/1	0.90	0.42	76,76,76,76	0
35	NA	0	9130	1/1	0.90	0.14	53,53,53,53	0
35	NA	0	9167	1/1	0.91	0.16	57,57,57,57	0
35	NA	0	9149	1/1	0.91	0.21	52,52,52,52	0
37	SR	0	9459	1/1	0.91	0.07	107,107,107,107	0
35	NA	0	9175	1/1	0.91	0.19	55,55,55,55	0
33	MG	B	8055	1/1	0.91	0.27	94,94,94,94	0
33	MG	0	8079	1/1	0.91	0.14	33,33,33,33	0
33	MG	9	8095	1/1	0.91	0.26	61,61,61,61	0
36	CL	B	9319	1/1	0.91	0.23	62,62,62,62	0
35	NA	0	9131	1/1	0.91	0.21	52,52,52,52	0
35	NA	0	9113	1/1	0.91	0.11	74,74,74,74	0
33	MG	0	8051	1/1	0.91	0.29	33,33,33,33	0
37	SR	0	9467	1/1	0.92	0.10	91,91,91,91	0
35	NA	0	9154	1/1	0.92	0.26	57,57,57,57	0
37	SR	0	9517	1/1	0.92	0.04	117,117,117,117	0
37	SR	0	9529	1/1	0.92	0.09	120,120,120,120	0
33	MG	0	8082	1/1	0.92	0.41	89,89,89,89	0
33	MG	0	8115	1/1	0.92	0.17	61,61,61,61	0
33	MG	0	8021	1/1	0.92	0.18	58,58,58,58	0
33	MG	0	8080	1/1	0.92	0.20	58,58,58,58	0
33	MG	0	8085	1/1	0.93	0.32	68,68,68,68	0
35	NA	C	9104	1/1	0.93	0.11	33,33,33,33	0
35	NA	0	9155	1/1	0.93	0.29	62,62,62,62	0
35	NA	0	9177	1/1	0.93	0.35	78,78,78,78	0
35	NA	0	9132	1/1	0.93	0.15	57,57,57,57	0
33	MG	0	8103	1/1	0.93	0.20	74,74,74,74	0
33	MG	0	8075	1/1	0.93	0.05	41,41,41,41	0
33	MG	T	8073	1/1	0.93	0.12	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8039	1/1	0.93	0.09	66,66,66,66	0
35	NA	J	9146	1/1	0.93	0.12	58,58,58,58	0
33	MG	0	8043	1/1	0.93	0.06	57,57,57,57	0
37	SR	0	9539	1/1	0.93	0.50	162,162,162,162	0
37	SR	0	9532	1/1	0.93	0.05	127,127,127,127	0
37	SR	0	9475	1/1	0.94	0.12	84,84,84,84	0
36	CL	0	9322	1/1	0.94	0.20	58,58,58,58	0
33	MG	Y	8109	1/1	0.94	0.12	47,47,47,47	0
37	SR	0	9581	1/1	0.94	0.10	136,136,136,136	0
35	NA	0	9159	1/1	0.94	0.21	54,54,54,54	0
33	MG	0	8096	1/1	0.94	0.12	51,51,51,51	0
35	NA	0	9141	1/1	0.94	0.08	64,64,64,64	0
33	MG	2	8076	1/1	0.94	0.20	64,64,64,64	0
33	MG	0	8097	1/1	0.94	0.23	63,63,63,63	0
35	NA	0	9124	1/1	0.94	0.12	54,54,54,54	0
35	NA	0	9181	1/1	0.94	0.20	55,55,55,55	0
37	SR	0	9590	1/1	0.94	0.10	98,98,98,98	0
35	NA	0	9127	1/1	0.94	0.19	71,71,71,71	0
33	MG	0	8060	1/1	0.94	0.17	97,97,97,97	0
33	MG	0	8106	1/1	0.94	0.08	50,50,50,50	0
33	MG	0	8083	1/1	0.94	0.08	59,59,59,59	0
36	CL	N	9307	1/1	0.95	0.14	65,65,65,65	0
33	MG	0	8002	1/1	0.95	0.10	37,37,37,37	0
33	MG	0	8027	1/1	0.95	0.25	40,40,40,40	0
36	CL	J	9302	1/1	0.95	0.08	63,63,63,63	0
37	SR	0	9560	1/1	0.95	0.08	98,98,98,98	0
35	NA	0	9128	1/1	0.95	0.09	48,48,48,48	0
35	NA	Q	9148	1/1	0.95	0.12	48,48,48,48	0
33	MG	0	8058	1/1	0.95	0.56	92,92,92,92	0
33	MG	0	8015	1/1	0.95	0.10	33,33,33,33	0
35	NA	0	9116	1/1	0.95	0.45	55,55,55,55	0
37	SR	0	9468	1/1	0.95	0.03	120,120,120,120	0
36	CL	J	9321	1/1	0.95	0.13	68,68,68,68	0
36	CL	0	9315	1/1	0.95	0.10	59,59,59,59	0
35	NA	0	9134	1/1	0.95	0.06	52,52,52,52	0
35	NA	0	9162	1/1	0.95	0.18	50,50,50,50	0
33	MG	0	8088	1/1	0.95	0.08	39,39,39,39	0
37	SR	0	9505	1/1	0.95	0.08	91,91,91,91	0
35	NA	0	9160	1/1	0.95	0.16	45,45,45,45	0
33	MG	0	8104	1/1	0.95	0.10	59,59,59,59	0
37	SR	0	9465	1/1	0.96	0.09	101,101,101,101	0
36	CL	0	9317	1/1	0.96	0.07	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8098	1/1	0.96	0.07	47,47,47,47	0
35	NA	0	9166	1/1	0.96	0.08	68,68,68,68	0
33	MG	0	8013	1/1	0.96	0.37	24,24,24,24	0
33	MG	0	8028	1/1	0.96	0.12	37,37,37,37	0
33	MG	0	8074	1/1	0.96	0.19	32,32,32,32	0
33	MG	0	8019	1/1	0.96	0.05	51,51,51,51	0
37	SR	0	9489	1/1	0.96	0.08	92,92,92,92	0
33	MG	0	8067	1/1	0.96	0.10	44,44,44,44	0
37	SR	0	9515	1/1	0.96	0.16	94,94,94,94	0
33	MG	A	8066	1/1	0.96	0.13	53,53,53,53	0
33	MG	0	8057	1/1	0.96	0.34	68,68,68,68	0
33	MG	0	8012	1/1	0.96	0.22	46,46,46,46	0
35	NA	0	9165	1/1	0.96	0.23	46,46,46,46	0
36	CL	A	9309	1/1	0.96	0.11	60,60,60,60	0
36	CL	J	9301	1/1	0.96	0.10	59,59,59,59	0
35	NA	0	9120	1/1	0.96	0.26	61,61,61,61	0
37	SR	F	9595	1/1	0.96	0.15	104,104,104,104	0
35	NA	R	9186	1/1	0.96	0.19	71,71,71,71	0
35	NA	0	9150	1/1	0.96	0.16	52,52,52,52	0
37	SR	9	9503	1/1	0.96	0.04	116,116,116,116	0
35	NA	R	9138	1/1	0.96	0.11	76,76,76,76	0
37	SR	0	9522	1/1	0.96	0.07	118,118,118,118	0
33	MG	0	8061	1/1	0.96	0.12	81,81,81,81	0
33	MG	0	8068	1/1	0.96	0.13	55,55,55,55	0
35	NA	0	9139	1/1	0.96	0.08	50,50,50,50	0
35	NA	M	9147	1/1	0.96	0.18	45,45,45,45	0
36	CL	0	9311	1/1	0.96	0.10	64,64,64,64	0
37	SR	0	9585	1/1	0.96	0.10	94,94,94,94	0
37	SR	0	9452	1/1	0.96	0.11	107,107,107,107	0
35	NA	0	9106	1/1	0.97	0.37	44,44,44,44	0
37	SR	0	9566	1/1	0.97	0.07	80,80,80,80	0
35	NA	0	9136	1/1	0.97	0.14	38,38,38,38	0
37	SR	0	9455	1/1	0.97	0.07	77,77,77,77	0
37	SR	0	9508	1/1	0.97	0.07	91,91,91,91	0
37	SR	0	9417	1/1	0.97	0.13	61,61,61,61	0
36	CL	Y	9320	1/1	0.97	0.10	49,49,49,49	0
33	MG	0	8017	1/1	0.97	0.12	30,30,30,30	0
37	SR	0	9482	1/1	0.97	0.26	122,122,122,122	0
37	SR	0	9534	1/1	0.97	0.17	108,108,108,108	0
37	SR	0	9473	1/1	0.97	0.02	79,79,79,79	0
36	CL	L	9310	1/1	0.97	0.09	58,58,58,58	0
36	CL	0	9314	1/1	0.97	0.09	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	SR	0	9442	1/1	0.97	0.11	65,65,65,65	0
37	SR	0	9429	1/1	0.97	0.11	71,71,71,71	0
37	SR	0	9464	1/1	0.97	0.05	83,83,83,83	0
35	NA	0	9115	1/1	0.97	0.17	47,47,47,47	0
37	SR	A	9437	1/1	0.97	0.12	73,73,73,73	0
35	NA	0	9135	1/1	0.97	0.18	54,54,54,54	0
35	NA	0	9114	1/1	0.97	0.13	46,46,46,46	0
37	SR	0	9530	1/1	0.97	0.14	73,73,73,73	0
37	SR	H	9486	1/1	0.97	0.22	114,114,114,114	0
33	MG	0	8030	1/1	0.97	0.05	37,37,37,37	0
37	SR	0	9477	1/1	0.97	0.07	83,83,83,83	0
37	SR	0	9629	1/1	0.97	0.08	77,77,77,77	0
33	MG	0	8031	1/1	0.97	0.09	55,55,55,55	0
37	SR	0	9469	1/1	0.97	0.03	91,91,91,91	0
37	SR	0	9509	1/1	0.97	0.12	91,91,91,91	0
35	NA	0	9108	1/1	0.98	0.15	35,35,35,35	0
33	MG	0	8008	1/1	0.98	0.19	22,22,22,22	0
37	SR	0	9433	1/1	0.98	0.13	75,75,75,75	0
37	SR	0	9435	1/1	0.98	0.08	75,75,75,75	0
37	SR	0	9488	1/1	0.98	0.12	84,84,84,84	0
33	MG	0	8037	1/1	0.98	0.07	42,42,42,42	0
37	SR	0	9427	1/1	0.98	0.13	58,58,58,58	0
33	MG	0	8029	1/1	0.98	0.31	37,37,37,37	0
37	SR	0	9466	1/1	0.98	0.04	101,101,101,101	0
36	CL	O	9308	1/1	0.98	0.08	66,66,66,66	0
33	MG	0	8025	1/1	0.98	0.40	33,33,33,33	0
33	MG	0	8003	1/1	0.98	0.16	38,38,38,38	0
33	MG	K	8069	1/1	0.98	0.19	26,26,26,26	0
37	SR	0	9446	1/1	0.98	0.11	93,93,93,93	0
36	CL	0	9305	1/1	0.98	0.07	58,58,58,58	0
37	SR	0	9490	1/1	0.98	0.09	108,108,108,108	0
37	SR	S	9470	1/1	0.98	0.12	99,99,99,99	0
37	SR	0	9450	1/1	0.98	0.07	76,76,76,76	0
37	SR	0	9405	1/1	0.98	0.15	59,59,59,59	0
33	MG	0	8020	1/1	0.98	0.19	38,38,38,38	0
35	NA	0	9105	1/1	0.98	0.10	45,45,45,45	0
33	MG	0	8118	1/1	0.98	0.15	30,30,30,30	0
37	SR	0	9495	1/1	0.98	0.10	102,102,102,102	0
37	SR	0	9420	1/1	0.98	0.14	73,73,73,73	0
37	SR	0	9483	1/1	0.98	0.07	80,80,80,80	0
37	SR	B	9458	1/1	0.98	0.08	83,83,83,83	0
35	NA	0	9117	1/1	0.98	0.12	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8056	1/1	0.98	0.18	47,47,47,47	0
35	NA	0	9143	1/1	0.98	0.08	46,46,46,46	0
33	MG	0	8026	1/1	0.98	0.18	35,35,35,35	0
35	NA	0	9123	1/1	0.98	0.09	42,42,42,42	0
37	SR	0	9447	1/1	0.98	0.11	69,69,69,69	0
37	SR	0	9570	1/1	0.98	0.04	105,105,105,105	0
37	SR	0	9414	1/1	0.98	0.11	58,58,58,58	0
37	SR	0	9431	1/1	0.98	0.15	66,66,66,66	0
37	SR	0	9568	1/1	0.98	0.07	77,77,77,77	0
33	MG	0	8044	1/1	0.98	0.06	44,44,44,44	0
33	MG	0	8036	1/1	0.98	0.10	60,60,60,60	0
33	MG	0	8070	1/1	0.98	0.16	28,28,28,28	0
37	SR	0	9426	1/1	0.98	0.08	72,72,72,72	0
37	SR	0	9449	1/1	0.98	0.07	66,66,66,66	0
36	CL	3	9304	1/1	0.99	0.10	65,65,65,65	0
37	SR	0	9441	1/1	0.99	0.07	68,68,68,68	0
36	CL	0	9303	1/1	0.99	0.10	50,50,50,50	0
37	SR	0	9474	1/1	0.99	0.11	61,61,61,61	0
37	SR	0	9423	1/1	0.99	0.09	58,58,58,58	0
37	SR	0	9422	1/1	0.99	0.12	59,59,59,59	0
37	SR	0	9545	1/1	0.99	0.05	79,79,79,79	0
37	SR	A	9497	1/1	0.99	0.10	91,91,91,91	0
37	SR	0	9415	1/1	0.99	0.11	58,58,58,58	0
37	SR	0	9506	1/1	0.99	0.04	71,71,71,71	0
33	MG	0	8004	1/1	0.99	0.11	36,36,36,36	0
38	CD	3	9204	1/1	0.99	0.05	63,63,63,63	0
37	SR	0	9448	1/1	0.99	0.06	63,63,63,63	0
35	NA	0	9101	1/1	0.99	0.17	50,50,50,50	0
37	SR	1	9460	1/1	0.99	0.11	53,53,53,53	0
36	CL	M	9318	1/1	0.99	0.18	43,43,43,43	0
37	SR	0	9407	1/1	0.99	0.15	46,46,46,46	0
37	SR	0	9601	1/1	0.99	0.04	95,95,95,95	0
37	SR	0	9413	1/1	0.99	0.12	50,50,50,50	0
33	MG	0	8038	1/1	0.99	0.26	27,27,27,27	0
36	CL	0	9312	1/1	0.99	0.09	60,60,60,60	0
37	SR	0	9440	1/1	0.99	0.04	73,73,73,73	0
33	MG	0	8112	1/1	0.99	0.07	43,43,43,43	0
37	SR	0	9432	1/1	0.99	0.13	67,67,67,67	0
36	CL	R	9306	1/1	0.99	0.07	48,48,48,48	0
33	MG	0	8001	1/1	0.99	0.24	19,19,19,19	0
38	CD	U	9201	1/1	0.99	0.09	60,60,60,60	0
37	SR	0	9438	1/1	0.99	0.10	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	SR	0	9462	1/1	0.99	0.12	73,73,73,73	0
37	SR	0	9445	1/1	0.99	0.10	59,59,59,59	0
37	SR	0	9411	1/1	0.99	0.18	46,46,46,46	0
33	MG	0	8005	1/1	0.99	0.10	34,34,34,34	0
37	SR	0	9416	1/1	0.99	0.10	47,47,47,47	0
37	SR	3	9439	1/1	0.99	0.03	74,74,74,74	0
37	SR	0	9456	1/1	0.99	0.09	64,64,64,64	0
33	MG	0	8110	1/1	0.99	0.10	46,46,46,46	0
37	SR	0	9425	1/1	0.99	0.12	59,59,59,59	0
37	SR	0	9434	1/1	0.99	0.13	68,68,68,68	0
33	MG	0	8009	1/1	0.99	0.13	26,26,26,26	0
37	SR	0	9501	1/1	0.99	0.11	76,76,76,76	0
37	SR	0	9457	1/1	0.99	0.10	54,54,54,54	0
37	SR	1	9419	1/1	0.99	0.11	42,42,42,42	0
37	SR	0	9498	1/1	0.99	0.05	66,66,66,66	0
37	SR	A	9436	1/1	0.99	0.07	57,57,57,57	0
37	SR	R	9418	1/1	0.99	0.14	59,59,59,59	0
37	SR	0	9412	1/1	0.99	0.12	46,46,46,46	0
36	CL	0	9313	1/1	0.99	0.07	57,57,57,57	0
37	SR	0	9454	1/1	0.99	0.07	83,83,83,83	0
37	SR	0	9443	1/1	0.99	0.09	59,59,59,59	0
37	SR	0	9480	1/1	0.99	0.05	95,95,95,95	0
37	SR	0	9461	1/1	0.99	0.04	80,80,80,80	0
37	SR	0	9453	1/1	0.99	0.07	71,71,71,71	0
37	SR	0	9410	1/1	0.99	0.12	41,41,41,41	0
37	SR	0	9478	1/1	1.00	0.06	76,76,76,76	0
37	SR	0	9430	1/1	1.00	0.10	50,50,50,50	0
37	SR	0	9428	1/1	1.00	0.07	55,55,55,55	0
37	SR	0	9408	1/1	1.00	0.16	41,41,41,41	0
37	SR	0	9406	1/1	1.00	0.17	36,36,36,36	0
37	SR	L	9409	1/1	1.00	0.13	44,44,44,44	0
37	SR	0	9451	1/1	1.00	0.11	60,60,60,60	0
37	SR	9	9481	1/1	1.00	0.06	88,88,88,88	0
37	SR	0	9424	1/1	1.00	0.14	47,47,47,47	0
38	CD	1	9202	1/1	1.00	0.04	55,55,55,55	0
37	SR	0	9421	1/1	1.00	0.11	74,74,74,74	0
37	SR	0	9444	1/1	1.00	0.09	56,56,56,56	0

6.5 Other polymers ⓘ

There are no such residues in this entry.