



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2020 – 09:38 am BST

PDB ID : 1VQO  
Title : The structure of CCPMN bound to the large ribosomal subunit haloarcula marismortui  
Authors : Schmeing, T.M.; Steitz, T.A.  
Deposited on : 2004-12-16  
Resolution : 2.20 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

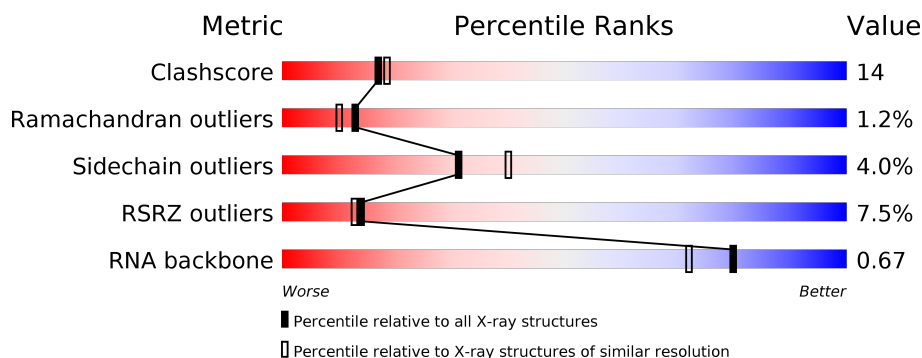
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)
RNA backbone	3102	1032 (2.60-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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>65%</div> <div>24%</div> <div>6%</div> </div> </div>
2	9	122	<div> <div>4%</div> <div> <div></div> <div>60%</div> <div>30%</div> <div>9%</div> </div> </div>
3	4	3	<div> <div></div> <div> <div>33%</div> <div>67%</div> </div> </div>
4	A	240	<div> <div>7%</div> <div> <div></div> <div>58%</div> <div>38%</div> </div> </div>
5	B	338	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>35%</div> </div> </div>
6	C	246	<div> <div>2%</div> <div> <div></div> <div>63%</div> <div>33%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
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	
31	3	92	

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Mol	Chain	Length	Quality of chain
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	8047	-	-	-	X
33	MG	0	8065	-	-	-	X
33	MG	0	8092	-	-	-	X
34	K	0	9001	-	-	-	X
35	NA	0	9179	-	-	-	X
35	NA	0	9184	-	-	-	X
37	SR	0	9547	-	-	-	X
37	SR	0	9601	-	-	-	X
37	SR	B	9521	-	-	-	X

## 2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99040 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))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

- 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	88	Total	Mg	0	0
			88	88		
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	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	64	Total Na 64 64	0	0
35	J	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	D	1	Total Na 1 1	0	0
35	B	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	R	3	Total Na 3 3	0	0
35	9	1	Total Na 1 1	0	0
35	S	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	9	Total Cl 9 9	0	0
36	J	3	Total Cl 3 3	0	0
36	K	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0
36	A	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0
36	O	1	Total Cl 1 1	0	0
36	R	1	Total Cl 1 1	0	0
36	Y	1	Total Cl 1 1	0	0
36	L	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	3	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0

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

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

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

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

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

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5780	Total	O	0	0
			5780	5780		
39	9	136	Total	O	0	0
			136	136		
39	4	4	Total	O	0	0
			4	4		
39	A	124	Total	O	0	0
			124	124		
39	B	141	Total	O	0	0
			141	141		
39	C	177	Total	O	0	0
			177	177		
39	D	46	Total	O	0	0
			46	46		
39	E	43	Total	O	0	0
			43	43		
39	F	25	Total	O	0	0
			25	25		
39	G	16	Total	O	0	0
			16	16		
39	H	71	Total	O	0	0
			71	71		
39	J	58	Total	O	0	0
			58	58		
39	K	60	Total	O	0	0
			60	60		
39	L	82	Total	O	0	0
			82	82		
39	M	125	Total	O	0	0
			125	125		
39	N	62	Total	O	0	0
			62	62		
39	O	40	Total	O	0	0
			40	40		
39	P	60	Total	O	0	0
			60	60		

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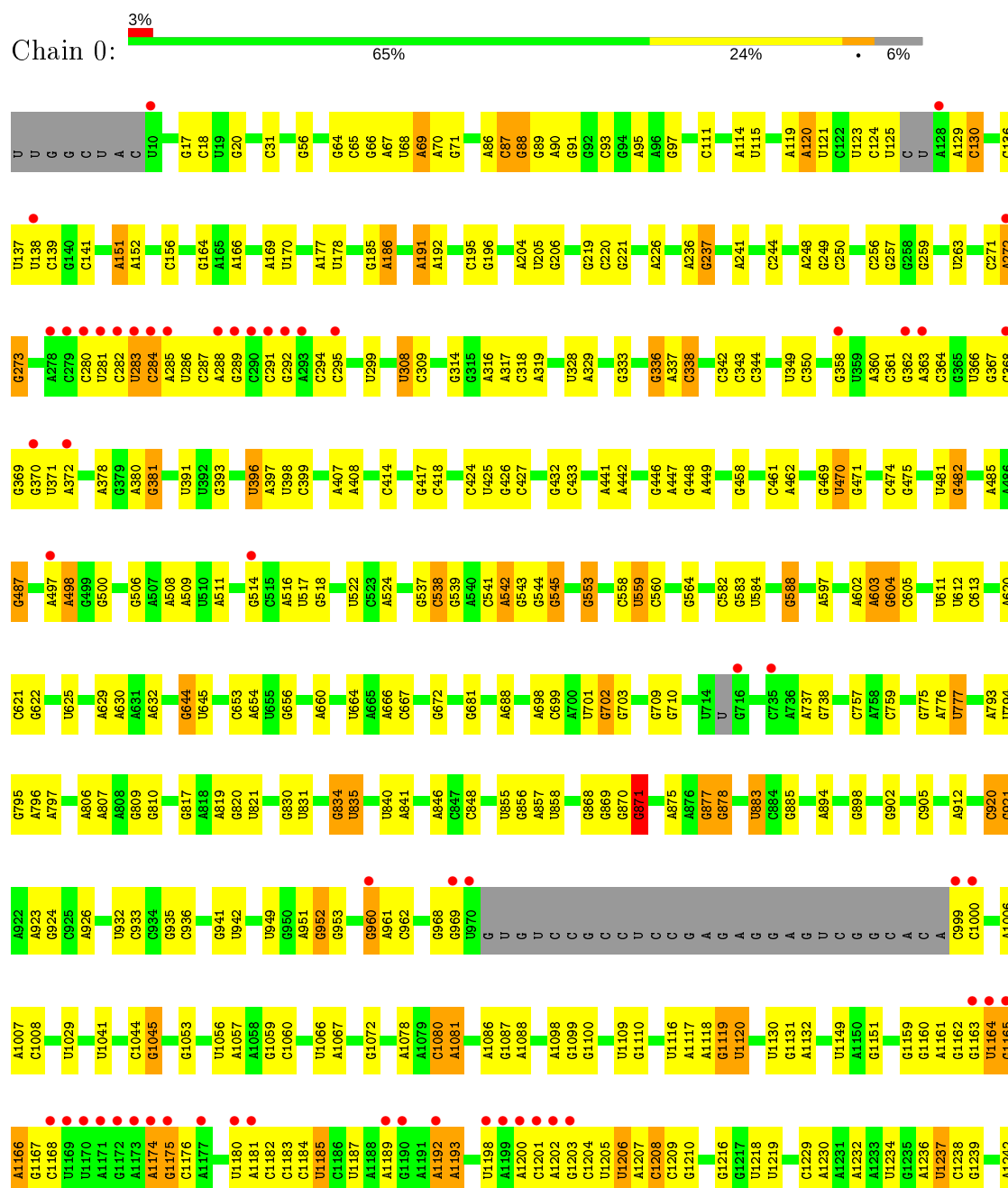
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	Q	49	Total 49	O 49	0	0
39	R	83	Total 83	O 83	0	0
39	S	30	Total 30	O 30	0	0
39	T	36	Total 36	O 36	0	0
39	U	28	Total 28	O 28	0	0
39	V	12	Total 12	O 12	0	0
39	W	68	Total 68	O 68	0	0
39	X	26	Total 26	O 26	0	0
39	Y	93	Total 93	O 93	0	0
39	Z	29	Total 29	O 29	0	0
39	1	52	Total 52	O 52	0	0
39	2	40	Total 40	O 40	0	0
39	3	66	Total 66	O 66	0	0
39	I	8	Total 8	O 8	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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

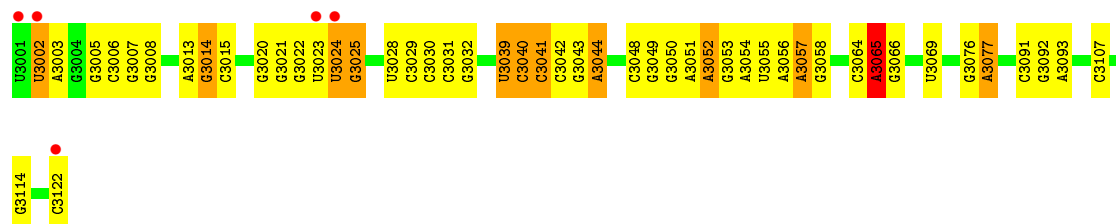


C2769	C2770	U2661	G2537	G2453	U2330	C	A	U2064	G1948	C1798	C1687	G1555	G1376	G1243
G2779	C2780	G2662	A2538	A2456	G2337	G	G	A2067	G1949	C1817	C1692	A1559	G1377	U1244
C2781	U2781	A2664	U2541	U2457	C2338	C	A	G2068	G1950	U1817	C1692	U	C1378	C1245
U2782	A2783	U	C2549	G2462	A	G	C	G2072	U	C1818	C1700	C1561	A1379	A1246
A2784	G2785	G2687	G2563	A2465	C2344	A	C	G2073	A	G1829	U1702	C1562	U1380	G1250
C2786	U2787	U2670	G2564	A2467	C2345	U	C	A2074	C	G1826	C1705	C1564	G1384	C1251
U2791	A2792	C2676	C2565	A2468	C2346	G	C	A2081	U	G1827	C1714	A1573	C1400	A1252
C2795	U2796	A2680	A2568	A2469	C2347	U	C	A2094	A	G1828	C1715	C1574	C1400	C1253
U2799	A2800	C2682	A2569	A2472	C2348	C	C	G2095	G	A1829	A1716	G1593	A1406	C1258
U2807	U2808	A2894	G2578	C2476	A2353	G2237	A	G2099	C	U1835	A1717	G1592	A1407	A1278
A2811	A2812	A2697	U2586	C2476	A2354	A2238	G	G2094	C	U1838	U1722	C1594	A1408	U1279
A2699	U2589	G2588	U2587	A2483	G2355	U2242	U	A2095	U1964	U1839	G1723	G1595	U1419	A1287
U2590	C2591	A2485	A2484	A2480	A2356	C2243	C	A	C1965	A1840	U1724	U1596	C1426	U1288
C2700	G2592	A2490	G2481	G2482	G2357	G2250	C	A2100	U1966	A1845	C1726	A1603	G1430	G1290
C2704	U2599	U2491	U2492	A2483	A2361	G2251	C	A2101	G1971	U1946	G1730	G1604	U1435	A1291
A2816	A2500	C2493	C2492	A2484	A2362	A2252	G	G2102	U1972	A1847	C1731	A1606	U1435	C1294
U2711	A2601	U2499	U2499	A2485	A2363	G2253	C	G2103	A1973	C1853	C1734	A1607	U1458	U1306
G2712	G2602	C2500	G2482	A2486	A2364	G2256	C	A2134	G1979	C1856	U1741	A1625	C1462	U1314
G2715	C2608	G2501	A2483	A2487	G2365	G2257	U	G2135	U1980	G1863	G1745	A1626	A1463	G1327
C2717	U2607	A2504	A2484	A2488	A2366	G2272	C	A2135	U1992	C1864	G1744	G1627	A1470	U1304
C2718	G2611	A2505	U2499	A2489	A2367	G2270	G	G2136	U1996	G1867	G1745	A1630	U1328	U1305
U2719	A2612	A2506	A2504	A2490	A2368	G2271	C	A	U2003	G1868	U1748	A1634	U1473	A1331
C2720	G2613	A2507	A2505	A2491	U2377	G2272	C	C	U2004	C1877	U1749	A1641	C1474	C1382
U2721	U2618	A2508	A2506	A2492	U2378	G2273	C	G	C2005	U1878	G1750	A1642	G1475	U1333
U2724	G2618	A2509	A2511	A2493	U2379	G2274	A	G	A2007	U1879	G1751	G1647	C1476	C1334
G2725	C2626	C2510	A2511	A2494	U2380	G2275	C	C	U2008	A1881	G1752	U1473	C1477	G1340
U2726	G2627	C2511	A2511	A2495	U2381	G2276	C	C	A2011	C1882	G1753	U1654	A1482	A1341
U2735	G2630	C2515	A2515	A2496	U2382	G2277	A	G	U2012	G1902	C1754	G1655	A1483	C1342
C2747	U2631	G2516	A2516	A2497	U2383	G2278	C	A	U2013	U1903	G1756	A1656	C1477	G1343
G2748	G2632	A2521	A2522	A2498	U2384	G2279	C	G	G2014	A1904	A1759	A1657	A1482	A1341
U2749	A2633	U2523	U2523	A2499	U2385	G2280	C	C	A2015	A1909	U1766	G1665	U1503	U1350
G2750	A2634	U2524	U2524	A2500	U2386	G2281	C	C	U2016	A1919	C1767	C1666	A1504	G1351
G2754	A2635	G2525	G2525	A2501	U2387	U2282	A	G	U2017	G1926	C1768	A1667	U1505	A1352
U2755	A2636	C2526	C2526	A2502	U2388	G2283	C	C	A2018	U1927	U1770	A1668	U1506	C1353
U2761	U2644	U2531	U2531	A2503	U2389	G2284	C	C	U2019	C1928	U1771	G1670	U1524	C1360
C2762	U2645	A2532	A2532	A2504	U2390	G2285	U	C	A2032	G1929	C1772	C1675	G1524	G1363
C2765	A2649	C2534	C2534	A2505	U2391	G2286	C	C	U2034	A1941	G1773	A1681	A1526	A1369
U2768	U2652	U2535	U2535	A2506	U2392	G2287	C	C	A2038	A1942	A1778	G1682	A1527	C1366
		C2536	C2536	A2507	U2393	G2288	U	C	A2039	A1943	A1779	G1683	A1528	U1372
		C2537	C2537	A2508	U2394	G2289	C	C	U2043	C1943	C1787	A1684	G1529	
		C2538	C2538	A2509	U2395	G2290	C	C	G2044	C1946	U1788	A1685	G1552	
		C2539	C2539	A2510	U2396	G2291	C	C	A2054	C1947	G1789	C1686		





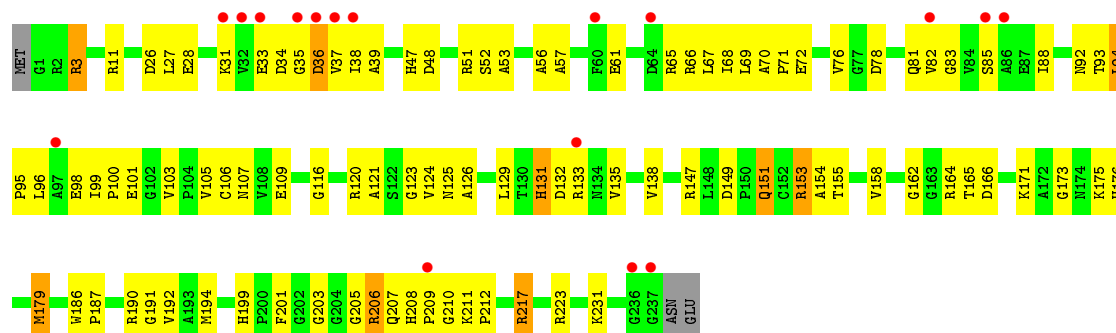
• Molecule 2: 5S ribosomal RNA



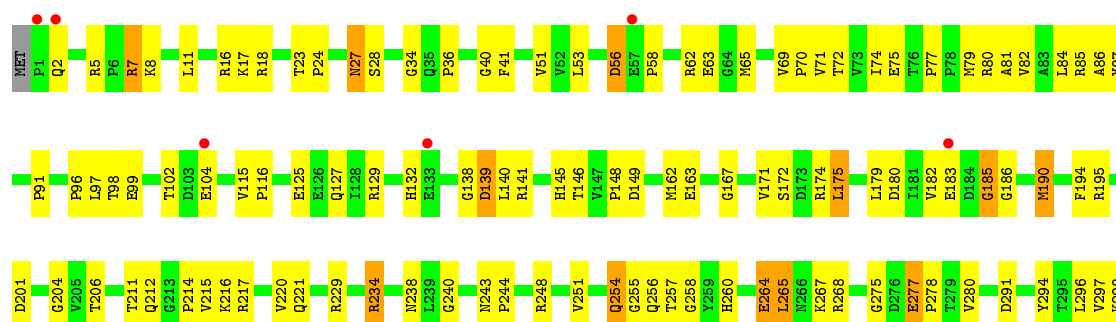
• Molecule 3: 5'-R(\*CP\*CP\*(PPU))-3'



• Molecule 4: 50S ribosomal protein L2P

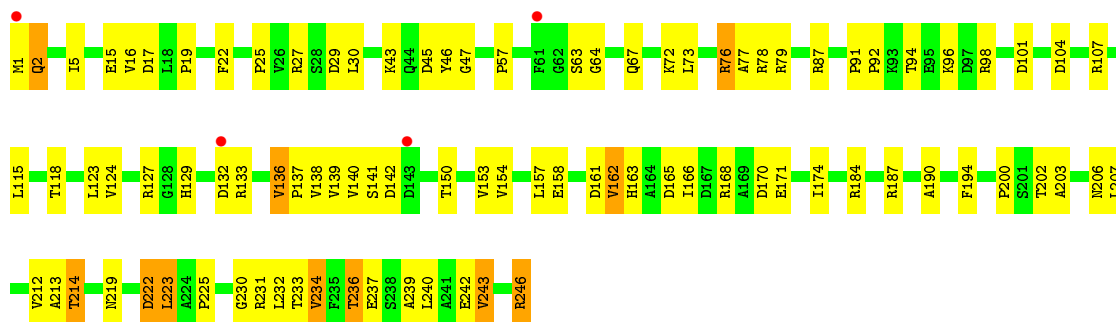


• Molecule 5: 50S ribosomal protein L3P

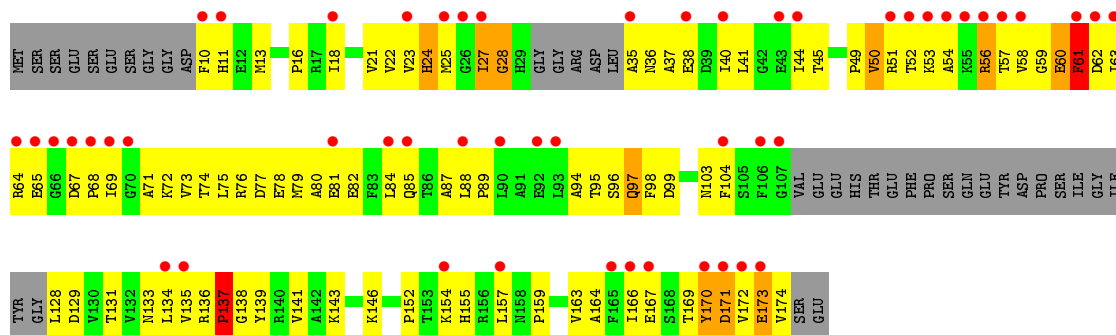




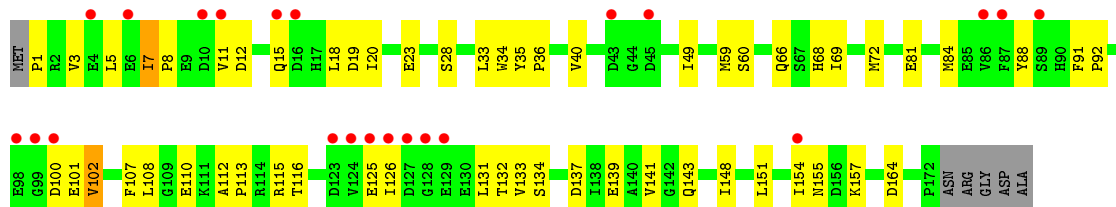
• Molecule 6: 50S ribosomal protein L4E



• Molecule 7: 50S ribosomal protein L5P

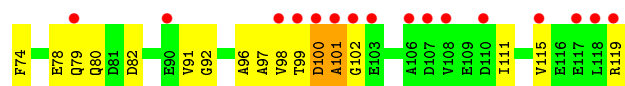


• Molecule 8: 50S ribosomal protein L6P

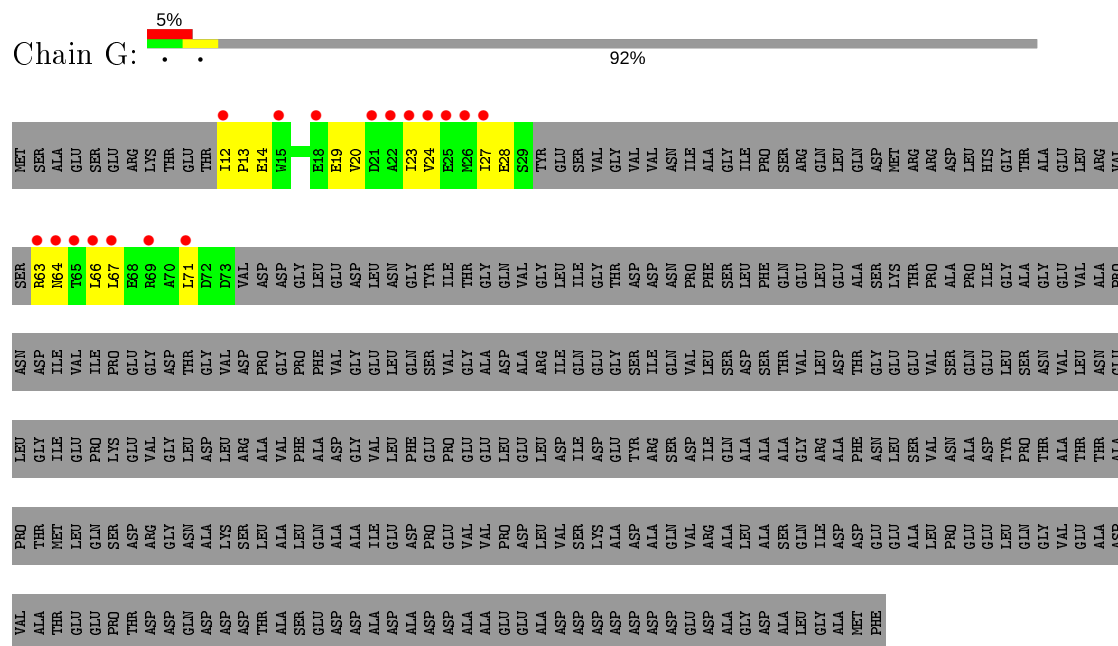


• Molecule 9: 50S ribosomal protein L7AE

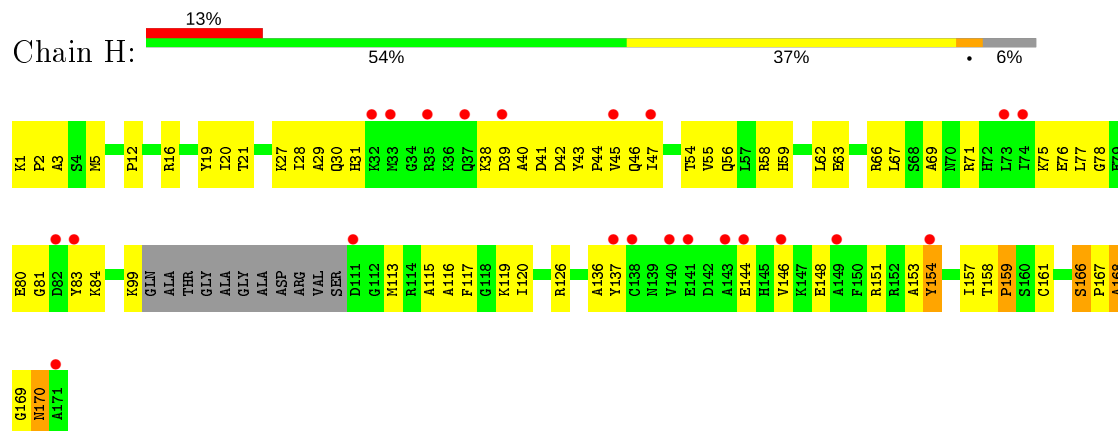




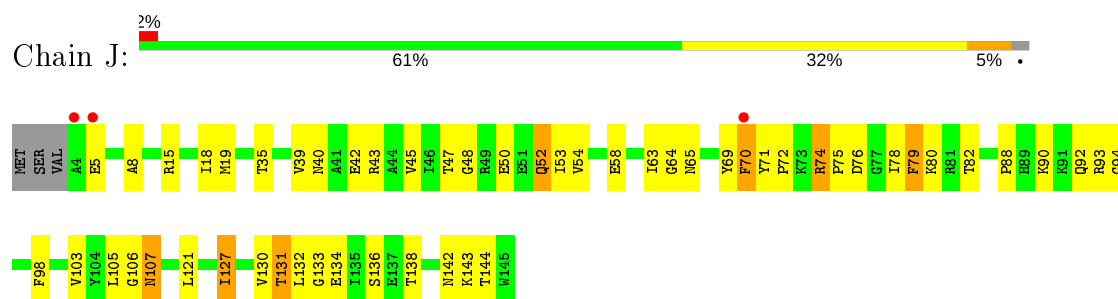
• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



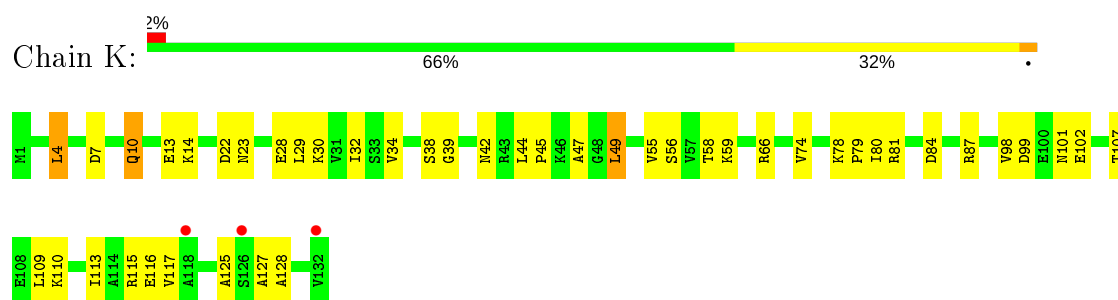
• Molecule 11: 50S RIBOSOMAL PROTEIN L10E



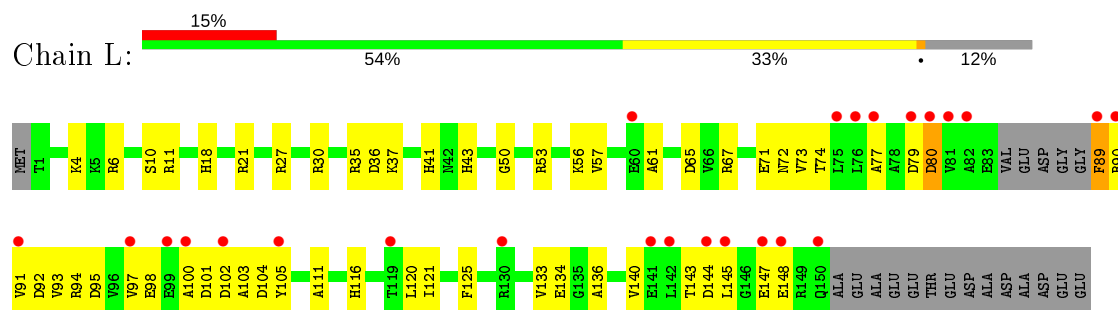
• Molecule 12: 50S ribosomal protein L13P



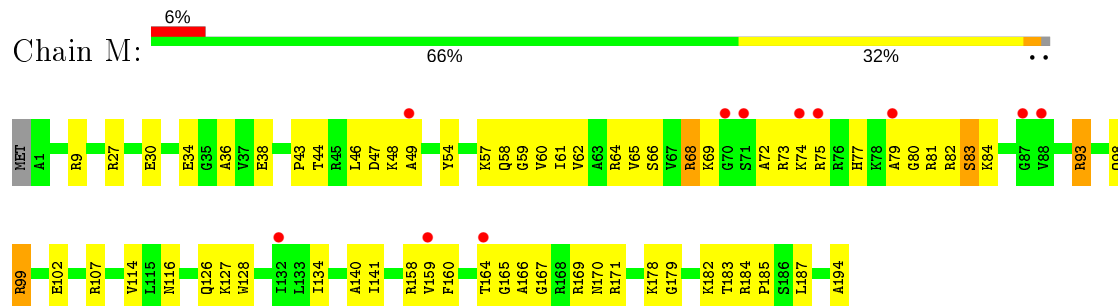
• Molecule 13: 50S ribosomal protein L14P



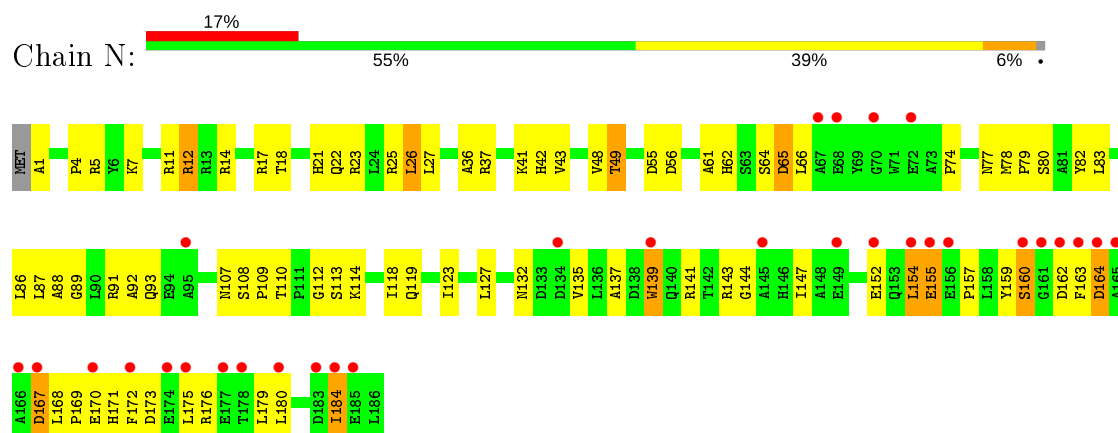
- Molecule 14: 50S ribosomal protein L15P



- Molecule 15: 50S Ribosomal Protein L15E



- Molecule 16: 50S ribosomal protein L18P

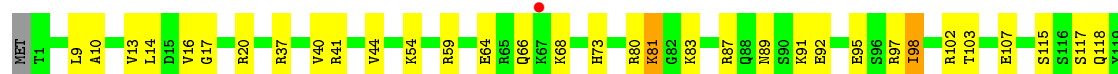


- Molecule 17: 50S ribosomal protein L18e

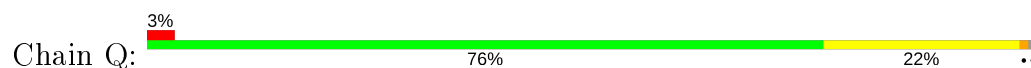




- Molecule 18: 50S ribosomal protein L19E



- Molecule 19: 50S ribosomal protein L21e



- Molecule 20: 50S ribosomal protein L22P

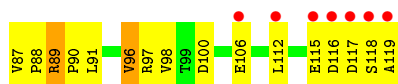


- Molecule 21: 50S ribosomal protein L23P



- Molecule 22: 50S ribosomal protein L24P

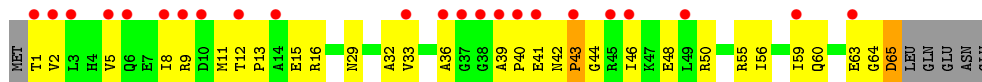




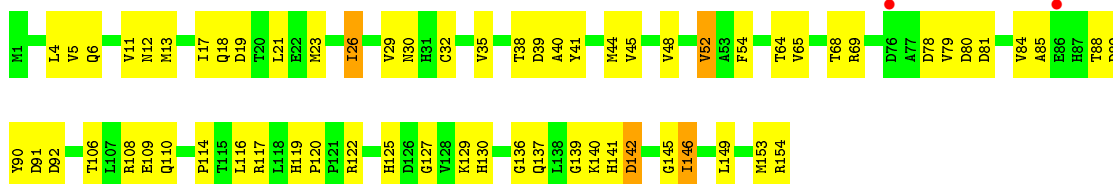
- Molecule 23: 50S ribosomal protein L24E



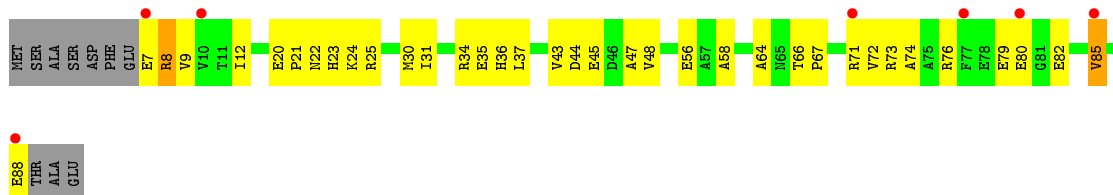
- Molecule 24: 50S ribosomal protein L29P



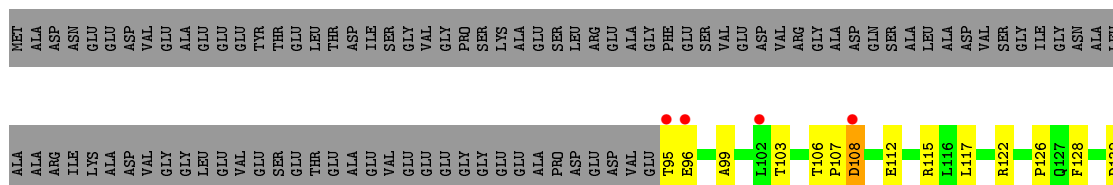
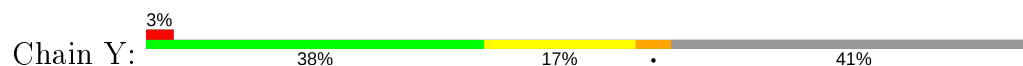
- Molecule 25: 50S ribosomal protein L30P

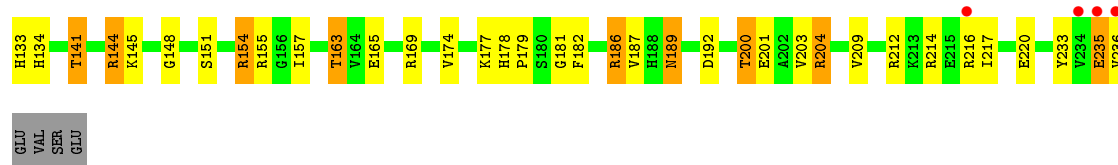


- Molecule 26: 50S ribosomal protein L31e



- Molecule 27: 50S ribosomal protein L32E





- Molecule 28: 50S ribosomal protein L37Ae



- Molecule 29: 50S ribosomal protein L37e



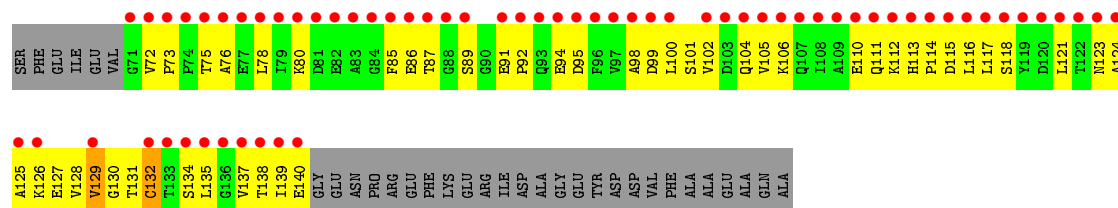
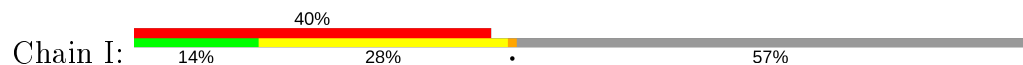
- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S ribosomal protein L44E



- Molecule 32: 50S RIBOSOMAL PROTEIN L11P



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.04Å 299.41Å 575.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 49.39 – 2.21	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-2.20) 88.8 (49.39-2.21)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.69 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.215 , 0.246 0.211 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.0	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 57.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	99040	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	0	0.37	0/65959	0.70	24/102870 (0.0%)
2	9	0.33	0/2905	0.71	1/4528 (0.0%)
3	4	0.43	0/40	0.63	0/60
4	A	0.32	0/1786	0.64	0/2408
5	B	0.35	0/2690	0.67	0/3652
6	C	0.37	0/1884	0.65	0/2551
7	D	0.29	0/1111	0.53	0/1498
8	E	0.32	0/1382	0.57	0/1880
9	F	0.32	0/901	0.53	0/1224
10	G	0.26	0/241	0.46	0/324
11	H	0.33	0/1287	0.64	0/1725
12	J	0.35	0/1136	0.61	0/1530
13	K	0.35	0/1001	0.67	0/1347
14	L	0.32	0/1130	0.66	0/1509
15	M	0.34	0/1584	0.60	0/2119
16	N	0.28	0/1474	0.59	0/1999
17	O	0.32	0/874	0.58	1/1181 (0.1%)
18	P	0.33	0/1147	0.54	0/1528
19	Q	0.34	0/749	0.69	1/1005 (0.1%)
20	R	0.35	0/1172	0.67	1/1578 (0.1%)
21	S	0.31	0/648	0.56	0/875
22	T	0.29	0/958	0.62	0/1289
23	U	0.34	0/417	0.56	0/562
24	V	0.25	0/502	0.51	0/675
25	W	0.34	0/1219	0.61	0/1655
26	X	0.32	0/664	0.59	0/895
27	Y	0.35	0/1146	0.66	0/1536
28	Z	0.32	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	0.49	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.36	0/98732	0.68	28/147637 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	1	40
2	9	0	1
All	All	1	41

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.80	131.06	109.50
1	0	871	G	C5'-C4'-O4'	-8.85	98.48	109.10
1	0	1942	A	C5'-C4'-C3'	8.20	129.12	116.00
1	0	777	U	O4'-C1'-N1	6.82	113.66	108.20
1	0	1819	G	C5'-C4'-C3'	6.76	126.81	116.00
1	0	1979	G	C2'-C3'-O3'	6.69	124.41	113.70
1	0	1819	G	C1'-O4'-C4'	-6.50	104.70	109.90
1	0	1592	G	N9-C1'-C2'	6.20	122.06	114.00
1	0	1504	A	C1'-O4'-C4'	-5.86	105.22	109.90
1	0	883	U	N1-C1'-C2'	5.84	121.59	114.00
1	0	2467	A	C1'-O4'-C4'	-5.83	105.24	109.90
2	9	3039	U	N1-C1'-C2'	5.69	121.39	114.00
1	0	1819	G	C4'-C3'-C2'	-5.58	97.02	102.60
1	0	206	G	C5'-C4'-C3'	-5.57	107.09	116.00
1	0	1120	U	C5'-C4'-C3'	-5.51	107.19	116.00
1	0	1504	A	N9-C1'-C2'	5.48	121.12	114.00
1	0	1829	A	N9-C1'-C2'	-5.46	105.99	112.00
1	0	1615	A	C5'-C4'-C3'	5.31	124.50	116.00
1	0	2313	C	C5'-C4'-O4'	5.30	115.46	109.10
1	0	1942	A	C4'-C3'-C2'	-5.20	97.40	102.60
19	Q	17	LYS	N-CA-C	-5.19	96.99	111.00
20	R	128	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	0	1942	A	C1'-O4'-C4'	-5.15	105.78	109.90
1	0	841	A	C1'-O4'-C4'	-5.14	105.78	109.90
1	0	1878	G	O4'-C1'-N9	5.12	112.30	108.20
1	0	2291	A	N9-C1'-C2'	5.06	120.58	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1352	A	OP1-P-O3'	5.04	116.28	105.20
17	O	66	GLY	N-CA-C	5.01	125.62	113.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1327	G	Sidechain
1	0	1340	G	Sidechain
1	0	1376	G	Sidechain
1	0	1430	G	Sidechain
1	0	1458	A	Sidechain
1	0	1592	G	Sidechain
1	0	1647	G	Sidechain
1	0	1726	G	Sidechain
1	0	1744	G	Sidechain
1	0	1819	G	Sidechain
1	0	1829	A	Sidechain
1	0	1845	A	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	191	A	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	2630	G	Sidechain
1	0	2679	G	Sidechain
1	0	2681	A	Sidechain
1	0	2842	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain

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Mol	Chain	Res	Type	Group
1	0	458	G	Sidechain
1	0	469	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	952	G	Sidechain
2	9	3065	A	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29812	718	0
2	9	2600	0	1326	56	0
3	4	74	0	51	2	0
4	A	1753	0	1766	117	0
5	B	2625	0	2532	131	0
6	C	1859	0	1816	111	0
7	D	1094	0	1085	101	0
8	E	1357	0	1266	53	0
9	F	890	0	843	52	0
10	G	240	0	231	15	0
11	H	1266	0	1268	68	0
12	J	1120	0	1098	68	0
13	K	992	0	1031	49	0
14	L	1118	0	1076	59	0
15	M	1560	0	1568	67	0
16	N	1445	0	1401	89	0
17	O	865	0	873	38	0
18	P	1136	0	1123	40	0
19	Q	735	0	728	18	0
20	R	1149	0	1122	46	0
21	S	641	0	605	17	0
22	T	950	0	924	53	0
23	U	410	0	364	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	V	499	0	511	37	0
25	W	1196	0	1137	76	0
26	X	654	0	653	42	0
27	Y	1130	0	1133	55	0
28	Z	578	0	539	33	0
29	1	431	0	426	24	0
30	2	396	0	413	23	0
31	3	755	0	728	23	0
32	I	519	0	500	54	0
33	0	88	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	64	0	0	0	0
35	9	1	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	D	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	9	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	2	0
36	K	1	0	0	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	9	3	0	0	0	0
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	5780	0	0	111	0
39	1	52	0	0	3	0
39	2	40	0	0	2	0
39	3	66	0	0	4	0
39	4	4	0	0	0	0
39	9	136	0	0	10	0
39	A	124	0	0	12	0
39	B	141	0	0	19	0
39	C	177	0	0	16	0
39	D	46	0	0	10	0
39	E	43	0	0	1	0
39	F	25	0	0	4	0
39	G	16	0	0	3	0
39	H	71	0	0	8	0
39	I	8	0	0	0	0
39	J	58	0	0	3	0
39	K	60	0	0	8	0
39	L	82	0	0	12	0
39	M	125	0	0	6	0
39	N	62	0	0	7	0
39	O	40	0	0	4	0
39	P	60	0	0	4	0
39	Q	49	0	0	3	0
39	R	83	0	0	5	0
39	S	30	0	0	0	0
39	T	36	0	0	4	0
39	U	28	0	0	4	0
39	V	12	0	0	1	0
39	W	68	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	X	26	0	0	6	0
39	Y	93	0	0	11	0
39	Z	29	0	0	2	0
All	All	99040	0	59949	2117	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 (2117) 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)
1:0:1160:G:H5'	1:0:1161:A:H5'	1.32	1.10
6:C:236:THR:HG22	6:C:239:ALA:H	1.10	1.10
26:X:74:ALA:HB2	26:X:85:VAL:HG13	1.34	1.10
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.32	1.08
2:9:3006:C:H5''	16:N:37:ARG:NH1	1.68	1.07
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.27	1.07
9:F:91:VAL:HG12	9:F:92:GLY:H	1.24	1.02
1:0:871:G:C8	1:0:871:G:H5'	1.95	1.01
5:B:264:GLU:HG2	5:B:267:LYS:HE2	1.40	1.00
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.24	0.99
12:J:93:ARG:HH11	12:J:93:ARG:HB3	1.23	0.99
1:0:156:C:H5''	15:M:171:ARG:HD3	1.40	0.99
5:B:86:ALA:HA	39:B:9580:HOH:O	1.64	0.96
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.44	0.96
21:S:51:GLN:HE21	21:S:53:ASN:HD21	1.13	0.95
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.48	0.95
2:9:3076:G:H3'	2:9:3077:A:H5''	1.49	0.95
1:0:2506:A:HO2'	1:0:2507:G:H8	0.97	0.94
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.11	0.94
7:D:25:MET:HE2	7:D:41:LEU:HG	1.50	0.94
1:0:871:G:H8	1:0:871:G:H5'	1.32	0.93
6:C:78:ARG:HG3	6:C:78:ARG:HH11	1.32	0.93
13:K:81:ARG:HB2	13:K:87:ARG:NH1	1.82	0.93
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.50	0.93
8:E:20:ILE:HD11	8:E:40:VAL:HG11	1.50	0.93
30:2:41:HIS:H	30:2:45:ASN:HD22	1.18	0.93
2:9:3006:C:H5''	16:N:37:ARG:HH12	1.29	0.92
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.48	0.92
1:0:1372:A:H3'	39:0:7690:HOH:O	1.70	0.92
29:1:25:LYS:HD2	30:2:49:GLU:H	1.31	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:211:LYS:HG2	4:A:212:PRO:HD2	1.52	0.92
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.52	0.92
13:K:10:GLN:H	13:K:10:GLN:NE2	1.66	0.91
16:N:144:GLY:O	16:N:147:ILE:HG22	1.71	0.91
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.50	0.91
13:K:39:GLY:HA2	39:K:4183:HOH:O	1.70	0.90
1:O:1242:A:H5'	12:J:82:THR:HG23	1.52	0.90
18:P:115:SER:H	18:P:118:GLN:HE21	1.19	0.90
5:B:140:LEU:HA	39:B:9580:HOH:O	1.71	0.90
6:C:104:ASP:HA	6:C:107:ARG:HH12	1.33	0.90
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.49	0.90
1:O:289:G:H22	1:O:363:A:H2	1.19	0.89
2:9:3056:A:H2'	2:9:3057:A:H5''	1.52	0.89
5:B:162:MET:SD	5:B:310:ARG:HD3	2.11	0.89
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.52	0.89
7:D:136:ARG:HH12	7:D:157:LEU:HA	1.36	0.89
13:K:10:GLN:H	13:K:10:GLN:HE21	0.89	0.89
26:X:25:ARG:HG2	39:X:5356:HOH:O	1.73	0.89
25:W:125:HIS:HD2	25:W:127:GLY:H	1.19	0.89
1:O:2524:G:H21	1:O:2526:C:H41	1.21	0.88
15:M:99:ARG:HH21	15:M:170:ASN:HD22	1.14	0.88
7:D:58:VAL:HB	7:D:62:ASP:HB3	1.54	0.88
13:K:10:GLN:N	13:K:10:GLN:HE21	1.71	0.88
11:H:29:ALA:HB3	11:H:66:ARG:HH12	1.39	0.88
5:B:5:ARG:HH11	5:B:8:LYS:HE2	1.39	0.87
5:B:238:ASN:HD22	5:B:240:GLY:H	1.22	0.87
7:D:57:THR:HG23	7:D:63:ILE:HA	1.56	0.87
1:O:288:A:H61	1:O:364:C:H42	1.20	0.87
6:C:1:MET:HG2	6:C:2:GLN:H	1.36	0.87
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.55	0.87
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.54	0.87
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.57	0.87
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.55	0.86
1:O:542:A:H5'	1:O:542:A:H8	1.38	0.86
6:C:236:THR:HG22	6:C:239:ALA:N	1.89	0.86
13:K:32:ILE:HD11	13:K:56:SER:HB3	1.57	0.86
1:O:1603:A:H5'	1:O:1605:G:O4'	1.76	0.86
1:O:870:G:H2'	1:O:871:G:H5''	1.57	0.86
8:E:36:PRO:HD3	12:J:127:ILE:HD12	1.56	0.85
12:J:19:MET:HE1	12:J:132:LEU:HD21	1.57	0.85
1:O:2812:A:H2	1:O:2814:A:H62	1.21	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1116:U:HO2'	1:0:1118:A:H2	0.86	0.84
18:P:115:SER:OG	18:P:118:GLN:HG3	1.77	0.84
1:0:2717:C:C2'	1:0:2718:C:H5''	2.07	0.84
4:A:192:VAL:HG12	4:A:207:GLN:HB3	1.59	0.84
5:B:51:VAL:HG23	5:B:329:TYR:O	1.78	0.84
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.60	0.84
27:Y:235:GLU:H	27:Y:235:GLU:CD	1.79	0.84
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.60	0.83
16:N:113:SER:HB2	39:N:9356:HOH:O	1.77	0.83
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.92	0.83
1:0:1593:C:OP1	18:P:117:SER:HB3	1.77	0.83
1:0:1474:C:H6	1:0:1474:C:H5'	1.44	0.83
5:B:307:ARG:HH11	5:B:307:ARG:HG3	1.44	0.83
1:0:1041:U:H5'	39:L:9490:HOH:O	1.78	0.83
1:0:506:G:H22	1:0:509:A:H5''	1.42	0.83
25:W:88:THR:HB	39:W:6679:HOH:O	1.78	0.83
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.60	0.83
25:W:88:THR:HG23	25:W:110:GLN:NE2	1.94	0.82
4:A:192:VAL:HB	39:A:9582:HOH:O	1.78	0.82
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.79	0.82
4:A:192:VAL:HG22	39:A:9621:HOH:O	1.78	0.82
1:0:1701:A:H4'	1:0:1702:U:H5''	1.61	0.82
1:0:560:C:H42	1:0:597:A:H61	1.23	0.82
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.61	0.82
1:0:1835:U:H5	1:0:1840:A:N7	1.77	0.82
1:0:2717:C:H2'	1:0:2718:C:H5''	1.62	0.82
39:O:5410:HOH:O	12:J:47:THR:HB	1.80	0.82
12:J:93:ARG:NH1	12:J:93:ARG:HB3	1.94	0.81
21:S:57:THR:HG22	21:S:59:ASP:H	1.45	0.81
4:A:153:ARG:HH11	4:A:153:ARG:HB2	1.46	0.81
24:V:1:THR:HG23	24:V:2:VAL:H	1.44	0.81
1:0:544:G:H2'	1:0:545:G:H5''	1.62	0.80
4:A:191:GLY:HA2	4:A:194:MET:HE2	1.61	0.80
27:Y:154:ARG:HH12	27:Y:155:ARG:HG2	1.46	0.80
5:B:179:LEU:O	5:B:183:GLU:HG2	1.82	0.80
11:H:27:LYS:H	11:H:59:HIS:HD2	1.29	0.80
1:0:1205:U:H2'	1:0:1206:U:H5''	1.62	0.80
6:C:115:LEU:HD13	6:C:223:LEU:HD21	1.62	0.80
6:C:5:ILE:HD11	6:C:16:VAL:HG23	1.62	0.80
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.63	0.80
25:W:13:MET:HE1	25:W:18:GLN:HA	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:199:HIS:HD2	4:A:201:PHE:H	1.27	0.79
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.00	0.79
1:O:559:U:H5'	1:O:559:U:H6	1.47	0.79
2:9:3039:U:H1'	2:9:3044:A:H61	1.48	0.79
4:A:191:GLY:HA2	4:A:194:MET:CE	2.12	0.79
6:C:107:ARG:NH1	6:C:107:ARG:HB3	1.98	0.79
39:O:6083:HOH:O	5:B:298:LYS:HG2	1.82	0.78
1:O:962:C:H1'	16:N:5:ARG:NH1	1.99	0.78
5:B:141:ARG:HD2	5:B:163:GLU:OE2	1.84	0.78
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.14	0.78
25:W:21:LEU:CD2	25:W:48:VAL:HG11	2.13	0.78
7:D:23:VAL:HG21	7:D:45:THR:HG21	1.65	0.78
1:O:645:U:OP2	14:L:4:LYS:HE2	1.84	0.78
7:D:25:MET:HE1	7:D:37:ALA:HB1	1.63	0.77
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.64	0.77
1:O:506:G:H22	1:O:509:A:C5'	1.97	0.77
6:C:246:ARG:NH1	6:C:246:ARG:HB3	1.99	0.77
1:O:1667:A:H8	1:O:1667:A:H5'	1.50	0.77
1:O:871:G:H8	1:O:871:G:C5'	1.97	0.77
9:F:53:ASP:OD1	9:F:80:GLN:HB2	1.84	0.77
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.19	0.77
1:O:2635:A:O2'	1:O:2636:C:H5'	1.85	0.77
1:O:2054:A:N3	20:R:128:ARG:NH2	2.33	0.77
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.14	0.77
1:O:1160:G:C5'	1:O:1161:A:H5'	2.13	0.77
5:B:56:ASP:HB3	5:B:322:ARG:HE	1.50	0.76
1:O:2748:G:H2'	39:O:8086:HOH:O	1.86	0.76
4:A:35:GLY:O	4:A:36:ASP:HB3	1.86	0.76
1:O:656:G:H5'	17:O:3:THR:HG22	1.67	0.76
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.67	0.75
1:O:553:G:P	27:Y:204:ARG:HH22	2.09	0.75
5:B:5:ARG:NH1	5:B:8:LYS:HE2	2.02	0.75
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.68	0.75
4:A:192:VAL:CG1	4:A:207:GLN:HB3	2.16	0.75
12:J:45:VAL:HG11	12:J:121:LEU:HD22	1.68	0.75
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.86	0.75
22:T:9:LYS:HE2	22:T:13:ARG:NH1	2.02	0.75
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.69	0.75
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.17	0.75
1:O:2840:A:OP1	5:B:211:THR:HG23	1.85	0.75
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:80:SER:HB2	39:N:9335:HOH:O	1.87	0.75
1:O:2506:A:O2'	1:O:2507:G:H8	1.68	0.75
1:O:871:G:C8	1:O:871:G:C5'	2.70	0.75
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.69	0.75
16:N:164:ASP:CG	16:N:167:ASP:HA	2.07	0.75
1:O:1160:G:H5'	1:O:1161:A:C5'	2.16	0.74
1:O:236:A:H4'	1:O:237:G:H5'	1.69	0.74
2:9:3014:G:H8	2:9:3014:G:H5'	1.52	0.74
1:O:1973:A:H5'	1:O:1973:A:H8	1.52	0.74
7:D:58:VAL:HG12	7:D:60:GLU:HG2	1.68	0.74
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.52	0.74
1:O:1116:U:O2'	1:O:1118:A:H2	1.68	0.74
1:O:545:G:H8	1:O:545:G:H5'	1.51	0.74
39:O:7941:HOH:O	5:B:211:THR:HG21	1.85	0.74
6:C:236:THR:CG2	6:C:239:ALA:H	1.96	0.74
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.01	0.73
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.71	0.73
1:O:2716:G:H5''	5:B:206:THR:HG21	1.70	0.73
6:C:115:LEU:HD21	6:C:243:VAL:HG13	1.68	0.73
1:O:2491:G:H1'	39:O:7383:HOH:O	1.88	0.73
6:C:132:ASP:HB3	39:C:9166:HOH:O	1.87	0.73
9:F:58:GLU:HA	9:F:61:MET:HE2	1.70	0.73
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.70	0.73
1:O:1377:C:H6	1:O:1377:C:H5'	1.52	0.73
8:E:15:GLN:HG2	8:E:19:ASP:O	1.89	0.73
5:B:195:ARG:HG2	5:B:323:LEU:HD22	1.68	0.73
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.54	0.73
20:R:99:ALA:HB1	20:R:109:MET:CE	2.19	0.73
1:O:2005:G:H3'	1:O:2005:G:OP2	1.89	0.73
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.70	0.73
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.69	0.72
5:B:16:ARG:NH1	39:B:9614:HOH:O	2.20	0.72
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.71	0.72
39:O:4356:HOH:O	22:T:9:LYS:HD2	1.89	0.72
26:X:71:ARG:HD3	39:X:2171:HOH:O	1.88	0.72
1:O:481:U:H5''	39:O:6210:HOH:O	1.90	0.72
6:C:246:ARG:HH11	6:C:246:ARG:HB3	1.52	0.72
11:H:99:LYS:HD3	11:H:119:LYS:HD3	1.72	0.72
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.70	0.72
1:O:1244:U:OP1	12:J:18:ILE:HD13	1.90	0.72
16:N:12:ARG:HD3	16:N:18:THR:OG1	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1183:C:N4	1:0:1184:C:H41	1.88	0.72
1:0:1206:U:H6	1:0:1206:U:H5'	1.54	0.72
1:0:281:U:H2'	1:0:282:C:O4'	1.89	0.71
1:0:1118:A:H62	1:0:1244:U:H3	1.38	0.71
1:0:870:G:C2'	1:0:871:G:H5''	2.20	0.71
5:B:221:GLN:HE22	13:K:42:ASN:HD22	1.39	0.71
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.18	0.71
1:0:2270:G:H4'	4:A:223:ARG:HH12	1.56	0.71
25:W:88:THR:HG22	25:W:89:ASP:N	2.05	0.71
1:0:796:A:HO2'	28:Z:10:ARG:N	1.87	0.71
11:H:170:ASN:N	11:H:170:ASN:HD22	1.86	0.71
1:0:2765:C:H4'	39:0:6083:HOH:O	1.91	0.71
14:L:73:VAL:HG23	14:L:74:THR:H	1.55	0.71
1:0:1299:G:O6	14:L:6:ARG:HD3	1.90	0.71
1:0:1166:A:H1'	1:0:1192:A:C2	2.26	0.70
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.73	0.70
12:J:74:ARG:O	12:J:78:ILE:HG12	1.92	0.70
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.18	0.70
31:3:70:ARG:HG3	31:3:77:ALA:HB2	1.74	0.70
2:9:3029:C:H2'	2:9:3030:C:H5'	1.73	0.70
6:C:78:ARG:HG3	6:C:78:ARG:NH1	2.03	0.70
18:P:115:SER:H	18:P:118:GLN:NE2	1.88	0.70
1:0:56:G:H5''	24:V:50:ARG:NH1	2.06	0.70
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.22	0.70
1:0:1166:A:H61	1:0:1180:U:H3	1.37	0.70
23:U:17:THR:HG22	23:U:18:GLY:N	2.07	0.70
1:0:1165:G:H4'	1:0:1174:A:O2'	1.91	0.70
1:0:1751:G:H2'	1:0:1752:G:H5''	1.74	0.70
1:0:542:A:H5'	1:0:542:A:C8	2.25	0.70
15:M:99:ARG:NH2	15:M:170:ASN:HD22	1.89	0.70
15:M:187:LEU:CD2	15:M:194:ALA:HB3	2.21	0.70
31:3:70:ARG:HG2	39:3:9501:HOH:O	1.91	0.70
24:V:12:THR:HG22	24:V:15:GLU:CG	2.20	0.70
25:W:125:HIS:CD2	25:W:127:GLY:H	2.07	0.70
1:0:2524:G:N2	1:0:2526:C:H41	1.90	0.70
24:V:39:ALA:N	24:V:40:PRO:HD2	2.07	0.70
1:0:1205:U:H2'	1:0:1206:U:C5'	2.21	0.69
1:0:2586:U:H3	1:0:2592:G:H22	1.37	0.69
1:0:1159:G:H21	1:0:1189:A:H8	1.40	0.69
8:E:20:ILE:CD1	8:E:40:VAL:HG11	2.22	0.69
6:C:162:VAL:HG22	6:C:232:LEU:HD21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:13:GLU:OE2	9:F:78:GLU:HG2	1.92	0.69
1:0:2749:U:H5'	39:0:8486:HOH:O	1.92	0.69
1:0:280:C:H2'	1:0:281:U:O4'	1.92	0.69
1:0:2851:G:C2'	1:0:2852:A:H5'	2.23	0.69
4:A:105:VAL:HG11	4:A:154:ALA:HB1	1.75	0.69
6:C:104:ASP:HA	6:C:107:ARG:NH1	2.06	0.69
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.56	0.69
1:0:902:G:N7	14:L:18:HIS:HD2	1.90	0.69
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.22	0.69
9:F:96:ALA:HA	39:F:3111:HOH:O	1.92	0.69
15:M:164:THR:HG22	15:M:166:ALA:H	1.58	0.69
26:X:71:ARG:HB3	26:X:88:GLU:OE1	1.93	0.69
1:0:1118:A:H3'	1:0:1118:A:H8	1.58	0.69
1:0:1641:A:H2'	1:0:1642:A:H5'	1.73	0.69
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.73	0.69
1:0:2524:G:H21	1:0:2526:C:N4	1.90	0.69
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.75	0.69
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.74	0.69
11:H:56:GLN:HE21	11:H:126:ARG:HE	1.38	0.69
14:L:67:ARG:O	14:L:71:GLU:HG3	1.93	0.69
25:W:88:THR:HG22	25:W:89:ASP:H	1.56	0.69
9:F:91:VAL:HG12	9:F:92:GLY:N	2.03	0.68
11:H:56:GLN:NE2	11:H:126:ARG:HE	1.91	0.68
2:9:3006:C:C5'	16:N:37:ARG:NH1	2.54	0.68
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.22	0.68
27:Y:115:ARG:HH11	27:Y:115:ARG:HB3	1.59	0.68
1:0:2676:C:H4'	12:J:70:PHE:CD1	2.27	0.68
17:O:96:VAL:HG13	17:O:100:GLN:HB2	1.75	0.68
1:0:1118:A:H3'	1:0:1118:A:C8	2.28	0.68
1:0:2533:C:H5'	1:0:2533:C:H6	1.58	0.68
1:0:282:C:O2'	1:0:283:U:H5'	1.92	0.68
4:A:199:HIS:CD2	4:A:201:PHE:H	2.10	0.68
1:0:2534:C:H1'	39:0:4100:HOH:O	1.93	0.68
2:9:3014:G:C8	2:9:3014:G:H5'	2.28	0.68
5:B:190:MET:HE2	5:B:194:PHE:HD1	1.57	0.68
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.75	0.68
6:C:140:VAL:HB	39:C:9254:HOH:O	1.93	0.68
8:E:23:GLU:HG2	8:E:28:SER:HB3	1.76	0.68
9:F:2:VAL:HG22	9:F:57:GLU:OE1	1.93	0.68
1:0:1119:G:N2	1:0:1246:A:C2	2.56	0.68
1:0:2820:A:OP1	5:B:98:THR:HG22	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:26:THR:HA	22:T:39:ASN:HB3	1.76	0.68
1:0:544:G:C2'	1:0:545:G:H5''	2.22	0.68
4:A:105:VAL:CG1	4:A:154:ALA:HB1	2.24	0.68
16:N:169:PRO:O	16:N:172:PHE:HB3	1.94	0.68
18:P:91:LYS:O	18:P:95:GLU:HG3	1.93	0.68
15:M:164:THR:HG22	15:M:166:ALA:N	2.09	0.68
1:0:1201:C:H2'	1:0:1202:A:H5'	1.74	0.67
5:B:102:THR:HG21	5:B:182:VAL:O	1.94	0.67
6:C:27:ARG:HG3	6:C:29:ASP:OD1	1.94	0.67
14:L:143:THR:HG22	14:L:144:ASP:H	1.57	0.67
27:Y:144:ARG:HH11	27:Y:144:ARG:CG	2.07	0.67
1:0:1116:U:O2'	1:0:1118:A:C2	2.46	0.67
1:0:1838:U:O2'	1:0:2644:C:H5'	1.94	0.67
1:0:1206:U:H2'	1:0:1207:A:O4'	1.94	0.67
9:F:37:THR:O	9:F:41:GLU:HG3	1.94	0.67
27:Y:144:ARG:HH11	27:Y:144:ARG:HG3	1.57	0.67
1:0:1189:A:H3'	39:0:8245:HOH:O	1.94	0.67
1:0:1979:G:H2'	39:0:3902:HOH:O	1.93	0.67
1:0:1119:G:H2'	12:J:52:GLN:NE2	2.09	0.67
16:N:23:ARG:NH1	16:N:27:LEU:HD11	2.09	0.67
1:0:1878:G:H1'	39:0:6661:HOH:O	1.94	0.67
29:1:25:LYS:HD2	30:2:49:GLU:N	2.07	0.67
4:A:51:ARG:HB2	39:A:9594:HOH:O	1.94	0.67
9:F:58:GLU:HG3	9:F:61:MET:HE1	1.75	0.67
32:I:75:THR:HA	32:I:112:LYS:HZ3	1.59	0.67
5:B:53:LEU:HD11	5:B:327:VAL:HG22	1.76	0.67
17:O:32:ARG:HD3	17:O:32:ARG:O	1.94	0.67
22:T:71:VAL:HG12	22:T:72:ILE:N	2.10	0.67
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.75	0.67
14:L:143:THR:HG22	14:L:144:ASP:N	2.10	0.67
1:0:797:A:H5'	28:Z:10:ARG:N	2.09	0.67
11:H:58:ARG:HG3	11:H:58:ARG:HH11	1.60	0.67
1:0:1205:U:C2'	1:0:1206:U:H5''	2.25	0.67
15:M:80:GLY:O	15:M:81:ARG:HD2	1.93	0.67
1:0:1666:C:H2'	1:0:1667:A:H5'	1.77	0.66
2:9:3039:U:H1'	2:9:3044:A:N6	2.09	0.66
2:9:3056:A:C2'	2:9:3057:A:H5''	2.23	0.66
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.77	0.66
6:C:118:THR:HG22	6:C:137:PRO:HB3	1.77	0.66
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.31	0.66
10:G:12:ILE:N	10:G:13:PRO:HD3	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.30	0.66
1:0:2270:G:H4'	4:A:223:ARG:NH1	2.10	0.66
2:9:3051:A:H5'	16:N:160:SER:HB3	1.77	0.66
4:A:48:ASP:HB3	39:A:9594:HOH:O	1.95	0.66
1:0:1474:C:C6	1:0:1474:C:H5'	2.31	0.66
1:0:2420:G:O2'	1:0:2421:G:H5'	1.96	0.66
1:0:396:U:O2'	1:0:418:C:H4'	1.96	0.66
2:9:3013:A:O2'	2:9:3014:G:H5''	1.95	0.66
15:M:107:ARG:HH11	15:M:107:ARG:HG3	1.60	0.66
25:W:48:VAL:HG12	25:W:48:VAL:O	1.95	0.66
1:0:797:A:C4'	28:Z:10:ARG:N	2.59	0.66
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.16	0.66
29:1:25:LYS:HE2	39:2:7213:HOH:O	1.95	0.66
27:Y:151:SER:O	27:Y:155:ARG:HG3	1.96	0.66
32:I:106:LYS:O	32:I:110:GLU:HG3	1.96	0.66
14:L:80:ASP:HB2	14:L:90:ARG:O	1.95	0.66
17:O:45:LEU:CD1	17:O:88:LYS:HD2	2.26	0.66
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.95	0.66
11:H:166:SER:HB3	11:H:167:PRO:HD3	1.76	0.65
26:X:9:VAL:HG22	26:X:88:GLU:OE2	1.97	0.65
1:0:1701:A:H4'	1:0:1702:U:C5'	2.26	0.65
1:0:2291:A:C8	1:0:2309:C:H5'	2.31	0.65
5:B:102:THR:HG23	5:B:182:VAL:HG12	1.77	0.65
14:L:133:VAL:HA	39:L:9471:HOH:O	1.97	0.65
2:9:3014:G:O2'	16:N:1:ALA:HB2	1.97	0.65
25:W:13:MET:CE	25:W:17:ILE:HG22	2.26	0.65
5:B:102:THR:CG2	5:B:182:VAL:HG12	2.27	0.65
5:B:62:ARG:HA	5:B:65:MET:HE3	1.78	0.65
6:C:1:MET:HG2	6:C:2:GLN:N	2.11	0.65
1:0:558:C:C2'	1:0:559:U:H5''	2.27	0.65
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.12	0.65
17:O:42:GLU:HB2	39:O:2176:HOH:O	1.96	0.65
21:S:57:THR:HG22	21:S:59:ASP:N	2.12	0.65
11:H:166:SER:CB	11:H:167:PRO:CD	2.75	0.65
32:I:99:ASP:OD1	32:I:138:THR:HB	1.96	0.65
5:B:125:GLU:O	5:B:129:ARG:HG3	1.97	0.65
5:B:238:ASN:HD22	5:B:240:GLY:N	1.95	0.65
11:H:30:GLN:H	11:H:66:ARG:NH1	1.95	0.65
13:K:55:VAL:HG12	13:K:56:SER:N	2.11	0.65
1:0:2578:G:H5'	1:0:2578:G:H8	1.61	0.65
8:E:7:ILE:HD11	8:E:12:ASP:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.78	0.64
4:A:153:ARG:CB	4:A:153:ARG:HH11	2.11	0.64
5:B:307:ARG:NH1	5:B:307:ARG:HG3	2.06	0.64
1:O:2364:A:H5''	19:Q:15:LYS:HD3	1.79	0.64
1:O:2505:G:O2'	1:O:2506:A:H5'	1.98	0.64
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.79	0.64
32:I:102:VAL:O	32:I:106:LYS:HG3	1.97	0.64
24:V:56:ILE:O	24:V:60:GLN:HG3	1.96	0.64
1:O:470:U:O2'	29:1:16:HIS:HD2	1.81	0.64
27:Y:154:ARG:HH11	27:Y:154:ARG:HB3	1.61	0.64
1:O:541:C:H2'	1:O:542:A:C5'	2.27	0.64
14:L:36:ASP:HB2	39:L:9431:HOH:O	1.98	0.64
1:O:282:C:H1'	1:O:368:C:N4	2.12	0.64
5:B:254:GLN:HG2	5:B:255:GLY:N	2.10	0.64
6:C:163:HIS:HD2	39:C:9241:HOH:O	1.80	0.64
32:I:110:GLU:HA	32:I:113:HIS:CE1	2.33	0.64
2:9:3051:A:H5'	16:N:160:SER:CB	2.27	0.64
27:Y:165:GLU:HB3	39:Y:9391:HOH:O	1.96	0.64
29:1:8:GLN:HE22	29:1:11:LYS:NZ	1.96	0.64
2:9:3006:C:OP1	16:N:37:ARG:NH1	2.31	0.64
5:B:62:ARG:HA	5:B:65:MET:CE	2.28	0.64
15:M:69:LYS:O	15:M:73:ARG:NH2	2.31	0.64
21:S:51:GLN:HE21	21:S:53:ASN:ND2	1.93	0.64
6:C:45:ASP:OD2	6:C:98:ARG:HD2	1.98	0.63
12:J:19:MET:CE	12:J:132:LEU:HD11	2.27	0.63
27:Y:144:ARG:CZ	39:Y:9409:HOH:O	2.45	0.63
4:A:36:ASP:HA	4:A:83:GLY:HA3	1.79	0.63
6:C:236:THR:HG21	39:C:9178:HOH:O	1.98	0.63
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.28	0.63
1:O:949:U:H4'	19:Q:95:GLU:HA	1.78	0.63
4:A:179:MET:HG2	4:A:186:TRP:CB	2.28	0.63
1:O:962:C:H1'	16:N:5:ARG:HH12	1.63	0.63
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.61	0.63
1:O:2346:C:O2'	7:D:52:THR:HG21	1.98	0.63
1:O:2481:G:H5''	39:O:5130:HOH:O	1.97	0.63
1:O:541:C:C2'	1:O:542:A:H5''	2.28	0.63
16:N:154:LEU:O	16:N:155:GLU:HB3	1.98	0.63
1:O:681:G:N3	1:O:681:G:H5'	2.14	0.63
1:O:111:C:O2'	29:1:20:ARG:HG2	1.99	0.63
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.29	0.63
7:D:65:GLU:HA	39:D:6752:HOH:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:25:ARG:HD3	26:X:64:ALA:O	1.98	0.63
29:1:25:LYS:CD	30:2:49:GLU:H	2.06	0.63
1:0:1766:U:O2	1:0:1778:A:H5'	1.99	0.63
1:0:877:G:H5'	1:0:878:G:OP1	1.98	0.63
8:E:68:HIS:O	8:E:72:MET:HG3	1.99	0.63
9:F:60:VAL:HG12	9:F:60:VAL:O	1.99	0.63
22:T:115:GLU:HG3	22:T:116:ASP:N	2.13	0.63
1:0:1119:G:H22	1:0:1246:A:H2	1.39	0.62
1:0:289:G:N2	1:0:363:A:H2	1.94	0.62
6:C:139:VAL:HG13	39:C:9251:HOH:O	1.99	0.62
9:F:48:VAL:HG23	9:F:74:PHE:HB3	1.81	0.62
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.79	0.62
39:0:7132:HOH:O	27:Y:155:ARG:HD2	1.98	0.62
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.28	0.62
5:B:215:VAL:HB	5:B:234:ARG:HH12	1.64	0.62
1:0:2769:C:C2'	1:0:2770:G:H5'	2.29	0.62
4:A:179:MET:HA	4:A:179:MET:CE	2.30	0.62
5:B:98:THR:HG21	5:B:127:GLN:OE1	1.99	0.62
1:0:2426:G:H1'	39:0:6634:HOH:O	1.98	0.62
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.30	0.62
1:0:1119:G:H8	12:J:52:GLN:HE22	1.46	0.62
1:0:2896:A:N3	1:0:2896:A:H2'	2.15	0.62
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.80	0.62
7:D:170:TYR:O	7:D:171:ASP:HB3	1.99	0.62
1:0:1700:C:H5''	1:0:1701:A:OP2	1.99	0.62
1:0:2827:A:H2'	1:0:2828:G:O4'	1.99	0.62
14:L:91:VAL:HG13	14:L:120:LEU:HD23	1.81	0.62
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.98	0.62
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.81	0.62
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.80	0.62
22:T:38:ARG:NH1	39:T:6217:HOH:O	2.33	0.62
1:0:1183:C:H2'	39:0:6785:HOH:O	2.00	0.62
1:0:2769:C:O2'	1:0:2770:G:H5'	2.00	0.62
9:F:21:GLU:O	9:F:24:ARG:HG3	2.00	0.62
7:D:146:LYS:NZ	16:N:107:ASN:HD21	1.98	0.62
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.63	0.62
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.79	0.62
1:0:1426:C:H2'	39:0:3214:HOH:O	1.98	0.62
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.82	0.62
29:1:10:LYS:HG3	39:1:9488:HOH:O	1.99	0.61
7:D:136:ARG:NH1	7:D:157:LEU:HA	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2064:U:H5'	1:0:2652:U:H4'	1.81	0.61
1:0:1181:A:H5'	32:I:94:GLU:OE2	1.99	0.61
15:M:59:GLY:HA3	15:M:141:ILE:HD12	1.82	0.61
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.35	0.61
1:0:757:C:OP1	14:L:27:ARG:HD2	2.00	0.61
17:O:87:THR:O	17:O:91:GLN:HG3	2.00	0.61
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.81	0.61
1:0:1377:C:H5'	1:0:1377:C:C6	2.36	0.61
39:9:4350:HOH:O	19:Q:25:PRO:HB2	1.99	0.61
1:0:1528:A:H2'	1:0:1529:G:O4'	2.01	0.61
5:B:275:GLY:O	5:B:291:ASP:HA	2.01	0.61
1:0:1209:C:H2'	1:0:1210:G:H8	1.65	0.61
1:0:1666:C:O2'	1:0:1667:A:H5''	1.99	0.61
1:0:2468:A:H61	31:3:48:ASN:HD21	1.46	0.61
1:0:381:G:H5''	39:0:4905:HOH:O	1.99	0.61
8:E:100:ASP:HB2	39:E:2789:HOH:O	2.01	0.61
15:M:79:ALA:HB3	15:M:81:ARG:NH1	2.15	0.61
6:C:194:PHE:CD2	6:C:234:VAL:HG11	2.34	0.61
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.30	0.61
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.16	0.61
15:M:27:ARG:HH12	15:M:44:THR:CG2	2.14	0.61
18:P:64:GLU:HG2	39:P:163:HOH:O	2.00	0.61
1:0:1268:C:O2'	27:Y:169:ARG:HB2	2.00	0.61
1:0:343:C:O2'	1:0:344:C:H5'	1.99	0.61
6:C:79:ARG:O	6:C:87:ARG:HG2	2.00	0.61
1:0:2003:U:H4'	1:0:2004:U:H5	1.65	0.61
1:0:2769:C:H2'	1:0:2770:G:O4'	2.00	0.61
1:0:380:A:OP2	15:M:9:ARG:HD2	2.01	0.61
7:D:159:PRO:O	7:D:163:VAL:HG23	1.99	0.61
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.30	0.61
7:D:84:LEU:HA	7:D:87:ALA:HB3	1.83	0.61
1:0:2507:G:H2'	1:0:2510:C:H42	1.66	0.60
6:C:246:ARG:CB	6:C:246:ARG:HH11	2.13	0.60
9:F:48:VAL:HG23	9:F:74:PHE:CB	2.31	0.60
17:O:59:VAL:HG23	17:O:111:VAL:HG22	1.83	0.60
18:P:115:SER:N	18:P:118:GLN:HE21	1.93	0.60
18:P:89:ASN:OD1	18:P:92:GLU:HB2	2.00	0.60
39:0:5188:HOH:O	4:A:206:ARG:HD3	1.99	0.60
39:0:7025:HOH:O	27:Y:141:THR:HG23	2.01	0.60
1:0:1184:C:H1'	39:0:7950:HOH:O	2.00	0.60
1:0:221:G:H5''	39:0:6299:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:129:VAL:O	32:I:129:VAL:HG12	2.00	0.60
17:O:53:GLN:HG2	17:O:56:GLU:OE1	2.01	0.60
1:O:1116:U:H3	1:O:1246:A:H62	1.49	0.60
1:O:541:C:H2'	1:O:542:A:H5''	1.83	0.60
39:O:9975:HOH:O	29:1:1:THR:HA	2.00	0.60
11:H:27:LYS:N	11:H:59:HIS:HD2	1.99	0.60
1:O:56:G:H5''	24:V:50:ARG:HH12	1.64	0.60
1:O:1175:G:H1'	1:O:1193:A:H2'	1.83	0.60
16:N:164:ASP:OD1	16:N:167:ASP:HA	2.00	0.60
7:D:138:GLY:N	39:D:7597:HOH:O	2.35	0.60
26:X:31:ILE:O	26:X:35:GLU:HG3	2.02	0.60
6:C:107:ARG:HH11	6:C:107:ARG:HB3	1.64	0.60
9:F:58:GLU:HG3	9:F:61:MET:CE	2.32	0.60
21:S:51:GLN:NE2	21:S:53:ASN:HD21	1.92	0.60
1:O:308:U:H5'	22:T:97:ARG:NH2	2.16	0.60
1:O:138:U:H5''	1:O:139:C:OP2	2.02	0.60
15:M:27:ARG:NH1	15:M:44:THR:CG2	2.64	0.60
24:V:55:ARG:O	24:V:59:ILE:HG12	2.02	0.60
5:B:40:GLY:HA3	39:B:9642:HOH:O	2.01	0.60
1:O:338:C:H4'	6:C:174:ILE:CD1	2.31	0.60
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.31	0.60
23:U:45:GLU:HB2	23:U:48:ASN:ND2	2.16	0.60
8:E:34:TRP:O	12:J:127:ILE:HD11	2.02	0.60
1:O:1119:G:H2'	12:J:52:GLN:HE22	1.65	0.60
5:B:307:ARG:HB3	39:B:9647:HOH:O	2.01	0.59
6:C:77:ALA:O	6:C:78:ARG:HG3	2.01	0.59
11:H:21:THR:O	11:H:120:ILE:HD12	2.02	0.59
32:I:116:LEU:HD22	32:I:127:GLU:OE1	2.02	0.59
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.84	0.59
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.32	0.59
28:Z:22:SER:O	28:Z:26:VAL:HG23	2.02	0.59
1:O:1681:G:H5''	1:O:1682:A:H5'	1.82	0.59
1:O:272:A:H5'	1:O:273:G:OP2	2.02	0.59
1:O:1118:A:H8	1:O:1119:G:H5''	1.67	0.59
1:O:883:U:H2'	1:O:883:U:O2	2.02	0.59
9:F:46:GLU:OE1	9:F:100:ASP:HA	2.02	0.59
25:W:139:GLY:O	25:W:141:HIS:HD2	1.85	0.59
1:O:2073:G:OP2	1:O:2490:A:H5'	2.02	0.59
1:O:2718:C:H6	1:O:2718:C:H5'	1.68	0.59
6:C:2:GLN:HB3	39:C:9189:HOH:O	2.02	0.59
25:W:141:HIS:HB2	25:W:146:ILE:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:211:LYS:CG	4:A:212:PRO:HD2	2.29	0.59
4:A:95:PRO:HG2	4:A:98:GLU:HG2	1.84	0.59
1:0:474:C:O3'	6:C:73:LEU:HD21	2.03	0.59
13:K:30:LYS:O	13:K:55:VAL:HG13	2.02	0.59
22:T:49:GLU:OE2	22:T:97:ARG:HD2	2.03	0.59
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.84	0.59
17:O:45:LEU:HD11	17:O:88:LYS:HD2	1.84	0.59
31:3:6:ARG:NH1	31:3:21:GLU:HG3	2.17	0.59
4:A:209:PRO:O	4:A:211:LYS:N	2.34	0.59
8:E:81:GLU:HG2	8:E:134:SER:CB	2.33	0.59
1:0:447:A:P	22:T:1:SER:HB2	2.43	0.59
23:U:39:ASN:ND2	23:U:44:ARG:HH11	2.00	0.59
1:0:524:A:H5''	20:R:29:LYS:HD3	1.84	0.59
4:A:94:LEU:HD12	4:A:98:GLU:HB2	1.85	0.59
8:E:107:PHE:O	8:E:110:GLU:HG3	2.03	0.59
5:B:305:ASP:O	5:B:306:LYS:HB2	2.03	0.59
18:P:9:LEU:O	18:P:13:VAL:HG12	2.03	0.59
22:T:49:GLU:CB	22:T:59:GLU:HG2	2.33	0.59
1:0:558:C:H2'	1:0:559:U:C5'	2.32	0.59
6:C:236:THR:H	6:C:239:ALA:HB3	1.68	0.59
15:M:27:ARG:NH1	15:M:44:THR:HG21	2.17	0.59
17:O:32:ARG:NE	17:O:35:LYS:HD2	2.18	0.59
1:0:95:A:H5''	1:0:97:G:O4'	2.03	0.58
31:3:38:ARG:HB3	31:3:42:ARG:HH12	1.68	0.58
9:F:48:VAL:HG12	9:F:97:ALA:HB2	1.85	0.58
1:0:538:C:OP2	27:Y:134:HIS:HE1	1.86	0.58
1:0:475:G:C5'	6:C:73:LEU:HD23	2.33	0.58
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.85	0.58
1:0:2563:U:H2'	1:0:2565:C:O5'	2.02	0.58
5:B:212:GLN:HB2	5:B:257:THR:CG2	2.28	0.58
17:O:97:SER:OG	17:O:100:GLN:HG3	2.03	0.58
1:0:1352:A:O2'	1:0:1353:C:OP1	2.20	0.58
4:A:66:ARG:HH11	4:A:66:ARG:HB2	1.68	0.58
1:0:2521:A:OP2	11:H:3:ALA:HB3	2.03	0.58
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.19	0.58
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.85	0.58
24:V:8:ILE:HA	24:V:11:MET:CE	2.33	0.58
1:0:1182:C:H1'	1:0:1192:A:H8	1.67	0.58
1:0:69:A:H5'	1:0:69:A:C8	2.39	0.58
5:B:217:ARG:HG3	5:B:257:THR:HG22	1.85	0.58
32:I:125:ALA:O	32:I:129:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:O:7389:HOH:O	15:M:178:LYS:HB2	2.03	0.58
15:M:60:VAL:C	15:M:61:ILE:HD12	2.22	0.58
5:B:145:HIS:HD2	5:B:146:THR:O	1.86	0.58
7:D:75:LEU:HD22	7:D:79:MET:HB3	1.85	0.58
14:L:104:ASP:HB2	39:L:9461:HOH:O	2.04	0.58
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.86	0.58
24:V:8:ILE:HG21	24:V:59:ILE:HG13	1.85	0.58
25:W:64:THR:O	25:W:68:THR:HG22	2.04	0.58
8:E:84:MET:HE1	8:E:148:ILE:HD12	1.86	0.58
14:L:80:ASP:CB	14:L:90:ARG:HB3	2.32	0.58
16:N:176:ARG:HG3	16:N:180:LEU:HD13	1.86	0.58
1:O:1218:U:H2'	1:O:1219:U:C6	2.39	0.58
2:9:3054:A:H2	39:9:3535:HOH:O	1.85	0.58
20:R:39:THR:HB	20:R:42:GLU:HG3	1.84	0.58
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.19	0.58
26:X:37:LEU:HD13	26:X:85:VAL:CG2	2.30	0.58
1:O:558:C:O2'	1:O:559:U:H5''	2.04	0.58
1:O:248:A:H5'	1:O:249:G:OP2	2.04	0.58
1:O:2878:U:H2'	1:O:2879:A:O4'	2.04	0.58
10:G:20:VAL:O	10:G:24:VAL:HG23	2.03	0.58
39:O:8128:HOH:O	31:3:60:LYS:HG3	2.03	0.57
4:A:206:ARG:HD3	4:A:206:ARG:H	1.67	0.57
7:D:57:THR:HG23	7:D:63:ILE:CA	2.33	0.57
8:E:88:TYR:CE1	8:E:92:PRO:HA	2.39	0.57
12:J:130:VAL:HG12	12:J:131:THR:N	2.19	0.57
15:M:164:THR:HG22	15:M:167:GLY:H	1.69	0.57
1:O:1979:G:O2'	1:O:1980:U:OP1	2.20	0.57
1:O:2676:C:H4'	12:J:70:PHE:CE1	2.39	0.57
31:3:62:THR:HB	39:3:9481:HOH:O	2.03	0.57
4:A:153:ARG:NH1	4:A:153:ARG:HB2	2.18	0.57
10:G:12:ILE:HD12	39:G:692:HOH:O	2.04	0.57
11:H:154:TYR:HB2	39:H:9557:HOH:O	2.04	0.57
7:D:13:MET:HA	7:D:137:PRO:HG2	1.86	0.57
7:D:24:HIS:HB2	7:D:72:LYS:CB	2.33	0.57
11:H:166:SER:CB	11:H:167:PRO:HD3	2.35	0.57
24:V:64:GLY:O	24:V:65:ASP:HB2	2.03	0.57
1:O:1625:U:H4'	39:O:5245:HOH:O	2.05	0.57
5:B:185:GLY:HA2	39:B:9631:HOH:O	2.03	0.57
15:M:182:LYS:O	15:M:194:ALA:HB2	2.05	0.57
1:O:960:G:H4'	39:O:7917:HOH:O	2.03	0.57
5:B:41:PHE:CD1	5:B:79:MET:HE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:91:VAL:CG1	9:F:92:GLY:H	2.07	0.57
4:A:125:ASN:HB3	4:A:158:VAL:HG12	1.87	0.57
5:B:72:THR:HB	39:B:9603:HOH:O	2.04	0.57
13:K:58:THR:HG22	13:K:59:LYS:HG3	1.85	0.57
14:L:80:ASP:HB3	14:L:90:ARG:HB3	1.87	0.57
21:S:77:VAL:O	21:S:80:ARG:HG2	2.05	0.57
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.31	0.57
1:O:2866:U:H4'	1:O:2867:G:H5'	1.85	0.57
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.69	0.57
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.34	0.57
1:O:1878:G:O2'	1:O:1879:U:OP2	2.22	0.57
2:9:3069:U:OP1	16:N:4:PRO:HG3	2.05	0.57
7:D:23:VAL:HG21	7:D:45:THR:CG2	2.35	0.57
32:I:134:SER:O	32:I:135:LEU:HD23	2.05	0.57
1:O:2726:U:O2'	26:X:22:ASN:ND2	2.38	0.57
1:O:475:G:H5'	6:C:73:LEU:HD23	1.86	0.57
32:I:110:GLU:HA	32:I:113:HIS:NE2	2.19	0.57
1:O:1185:U:H4'	32:I:123:ASN:HB3	1.87	0.57
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.87	0.57
1:O:1819:G:H2'	1:O:1820:G:H4'	1.86	0.57
1:O:241:A:C2	1:O:378:A:H4'	2.40	0.57
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.34	0.57
7:D:25:MET:SD	7:D:40:ILE:HD11	2.44	0.57
23:U:52:THR:HG22	23:U:54:THR:N	2.20	0.57
27:Y:115:ARG:NE	39:Y:9353:HOH:O	2.38	0.57
1:O:121:U:OP2	30:2:10:ARG:NH2	2.32	0.56
5:B:310:ARG:HD2	39:B:9590:HOH:O	2.04	0.56
11:H:158:THR:HB	11:H:159:PRO:HD3	1.87	0.56
11:H:20:ILE:HG23	11:H:120:ILE:HD11	1.86	0.56
1:O:1594:C:OP2	18:P:120:ARG:HD2	2.05	0.56
39:O:3159:HOH:O	18:P:81:LYS:HG2	2.04	0.56
28:Z:17:ARG:HD3	39:Z:9218:HOH:O	2.05	0.56
1:O:2644:C:O2'	1:O:2645:U:H5'	2.05	0.56
1:O:2717:C:O2'	1:O:2718:C:H5''	2.03	0.56
1:O:545:G:C8	1:O:545:G:H5'	2.36	0.56
1:O:1853:C:OP1	4:A:231:LYS:HG3	2.05	0.56
5:B:74:ILE:HD13	5:B:309:VAL:HG21	1.86	0.56
7:D:136:ARG:HB3	7:D:137:PRO:HD2	1.88	0.56
7:D:135:VAL:HG22	7:D:136:ARG:H	1.70	0.56
32:I:113:HIS:N	32:I:114:PRO:HD2	2.21	0.56
15:M:57:LYS:HE2	15:M:140:ALA:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2781:U:H1'	8:E:139:GLU:OE2	2.04	0.56
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.86	0.56
1:O:2851:G:O2'	1:O:2852:A:H5'	2.06	0.56
4:A:26:ASP:O	4:A:28:GLU:N	2.38	0.56
32:I:89:SER:HB2	32:I:95:ASP:HB2	1.88	0.56
1:O:164:G:H4'	14:L:30:ARG:HD3	1.87	0.56
18:P:40:VAL:O	18:P:44:VAL:HG23	2.05	0.56
24:V:39:ALA:N	24:V:40:PRO:CD	2.68	0.56
25:W:88:THR:HG22	25:W:90:TYR:HD1	1.69	0.56
1:O:1328:A:OP1	27:Y:169:ARG:HD2	2.06	0.56
15:M:107:ARG:NH1	15:M:107:ARG:HG3	2.21	0.56
15:M:99:ARG:HH21	15:M:170:ASN:ND2	1.96	0.56
5:B:80:ARG:HB2	5:B:145:HIS:CE1	2.41	0.56
8:E:101:GLU:HB2	8:E:116:THR:O	2.04	0.56
11:H:166:SER:HB2	11:H:167:PRO:CD	2.36	0.56
11:H:170:ASN:N	11:H:170:ASN:ND2	2.54	0.56
27:Y:154:ARG:HH12	27:Y:155:ARG:CG	2.16	0.56
1:O:926:A:O2'	14:L:41:HIS:HD2	1.89	0.56
5:B:85:ARG:NH1	39:B:9632:HOH:O	2.38	0.56
8:E:11:VAL:HG12	8:E:12:ASP:N	2.20	0.56
14:L:136:ALA:HB3	39:L:9471:HOH:O	2.05	0.56
16:N:154:LEU:HG	16:N:155:GLU:H	1.70	0.56
5:B:234:ARG:HH11	5:B:234:ARG:HB3	1.69	0.56
6:C:16:VAL:HG12	6:C:17:ASP:H	1.70	0.56
8:E:154:ILE:HD11	8:E:157:LYS:HB2	1.88	0.56
2:9:3007:G:H5'	39:9:5071:HOH:O	2.06	0.56
5:B:96:PRO:HG3	39:B:9632:HOH:O	2.05	0.56
9:F:46:GLU:O	9:F:73:PRO:HD2	2.05	0.56
12:J:39:VAL:HG11	12:J:107:ASN:CG	2.27	0.56
5:B:91:PRO:O	12:J:144:THR:HG21	2.06	0.56
16:N:22:GLN:HG2	16:N:26:LEU:HD22	1.88	0.56
23:U:17:THR:CG2	23:U:18:GLY:N	2.69	0.56
39:K:7438:HOH:O	23:U:20:MET:HE1	2.05	0.56
1:O:625:U:H5''	1:O:1044:C:N4	2.21	0.56
1:O:2812:A:C2	1:O:2814:A:N6	2.65	0.56
2:9:3002:U:OP2	2:9:3003:A:H5'	2.06	0.56
4:A:105:VAL:HG11	4:A:154:ALA:CB	2.35	0.56
13:K:4:LEU:HD22	13:K:116:GLU:HB3	1.88	0.56
16:N:176:ARG:O	16:N:180:LEU:HD13	2.05	0.56
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.69	0.56
6:C:236:THR:HA	39:C:9254:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:1:PRO:H3	9:F:4:VAL:HG23	1.71	0.56
16:N:82:TYR:OH	16:N:176:ARG:NH1	2.39	0.56
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.41	0.56
39:O:5303:HOH:O	16:N:21:HIS:HD2	1.90	0.55
1:O:2748:G:H1'	39:O:8464:HOH:O	2.04	0.55
1:O:2780:C:H1'	8:E:143:GLN:HE21	1.72	0.55
1:O:797:A:H4'	28:Z:10:ARG:N	2.21	0.55
1:O:93:C:H5''	24:V:1:THR:HB	1.88	0.55
14:L:148:GLU:HB2	39:L:9487:HOH:O	2.05	0.55
18:P:143:ALA:HA	39:P:162:HOH:O	2.07	0.55
1:O:1165:G:H1'	1:O:1174:A:H1'	1.87	0.55
1:O:2502:C:C2'	1:O:2503:A:H5'	2.36	0.55
1:O:2265:U:H2'	1:O:2266:A:C8	2.42	0.55
19:Q:11:ARG:HD3	39:Q:5620:HOH:O	2.06	0.55
1:O:1787:C:OP1	18:P:68:LYS:HE2	2.06	0.55
1:O:2670:G:O2'	1:O:2671:U:H5'	2.06	0.55
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.70	0.55
1:O:1244:U:H2'	12:J:47:THR:HG21	1.88	0.55
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.37	0.55
1:O:447:A:OP2	22:T:1:SER:HB2	2.07	0.55
5:B:138:GLY:O	5:B:139:ASP:O	2.24	0.55
5:B:297:VAL:HB	39:B:9603:HOH:O	2.06	0.55
1:O:1946:C:H2'	1:O:1971:G:C8	2.42	0.55
1:O:949:U:O2'	19:Q:40:HIS:HE1	1.89	0.55
1:O:960:G:H3'	1:O:960:G:N3	2.22	0.55
7:D:59:GLY:O	7:D:61:PHE:N	2.40	0.55
11:H:167:PRO:O	11:H:168:ALA:HB2	2.07	0.55
32:I:138:THR:HG22	32:I:139:ILE:N	2.22	0.55
16:N:143:ARG:NH2	16:N:169:PRO:HB2	2.21	0.55
1:O:516:A:H5'	39:O:6210:HOH:O	2.06	0.55
2:9:3020:G:O2'	2:9:3021:G:H5'	2.06	0.55
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.89	0.55
5:B:5:ARG:HH11	5:B:8:LYS:CE	2.17	0.55
6:C:170:ASP:O	6:C:171:GLU:HG3	2.07	0.55
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.22	0.55
22:T:89:ARG:HG3	22:T:89:ARG:O	2.07	0.55
1:O:1299:G:H5'	39:O:4667:HOH:O	2.06	0.55
1:O:1462:C:H2'	1:O:1463:A:C8	2.42	0.55
1:O:2406:U:H1'	39:O:7222:HOH:O	2.06	0.55
22:T:40:VAL:HG22	22:T:41:ARG:N	2.22	0.55
1:O:119:A:H2'	1:O:120:A:H5''	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1552:G:N2	1:0:1634:G:H1'	2.23	0.54
1:0:2252:A:H2'	1:0:2253:G:O4'	2.06	0.54
5:B:58:PRO:HA	5:B:63:GLU:OE1	2.06	0.54
13:K:109:LEU:HD13	13:K:113:ILE:CD1	2.36	0.54
25:W:88:THR:CG2	25:W:89:ASP:H	2.20	0.54
27:Y:133:HIS:HD2	39:Y:9380:HOH:O	1.90	0.54
1:0:2073:G:H3'	39:0:4424:HOH:O	2.07	0.54
1:0:2419:U:H5''	1:0:2420:G:H5'	1.88	0.54
15:M:187:LEU:HD23	15:M:194:ALA:HB3	1.89	0.54
16:N:154:LEU:O	16:N:155:GLU:CB	2.55	0.54
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.08	0.54
1:0:1384:C:H5'	26:X:30:MET:HG2	1.88	0.54
1:0:475:G:OP1	6:C:73:LEU:HD22	2.07	0.54
2:9:3048:C:H4'	16:N:141:ARG:HH21	1.73	0.54
39:0:5272:HOH:O	28:Z:13:ARG:HD3	2.07	0.54
1:0:151:A:H2'	1:0:152:A:O4'	2.07	0.54
1:0:69:A:H5'	1:0:69:A:H8	1.73	0.54
6:C:129:HIS:HD2	6:C:165:ASP:OD2	1.90	0.54
17:O:25:VAL:HG23	17:O:26:TRP:H	1.72	0.54
1:0:156:C:H5''	15:M:171:ARG:CD	2.28	0.54
30:2:48:ASP:O	30:2:49:GLU:HB2	2.06	0.54
6:C:107:ARG:HH11	6:C:107:ARG:CB	2.20	0.54
25:W:149:LEU:HG	25:W:153:MET:CE	2.38	0.54
28:Z:30:GLU:HA	28:Z:33:MET:HE3	1.89	0.54
1:0:1187:U:O2'	1:0:1189:A:H2	1.91	0.54
1:0:2533:C:C6	1:0:2533:C:H5'	2.42	0.54
5:B:258:GLY:H	5:B:260:HIS:CE1	2.25	0.54
11:H:136:ALA:HB3	11:H:146:VAL:HG21	1.88	0.54
13:K:87:ARG:CZ	39:K:4854:HOH:O	2.54	0.54
1:0:1278:A:H4'	1:0:1279:U:C4	2.42	0.54
1:0:2362:A:H2'	1:0:2363:G:C8	2.43	0.54
1:0:969:G:H1	1:0:999:C:H42	1.54	0.54
5:B:140:LEU:HD23	39:B:9580:HOH:O	2.08	0.54
5:B:195:ARG:HD2	5:B:324:ASP:OD1	2.07	0.54
9:F:12:LEU:HD21	9:F:111:ILE:HG23	1.89	0.54
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.90	0.54
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.22	0.54
28:Z:72:GLU:OE1	28:Z:77:LYS:HE2	2.07	0.54
29:1:25:LYS:HD2	30:2:48:ASP:HA	1.90	0.54
2:9:3029:C:C2'	2:9:3030:C:H5'	2.37	0.54
6:C:118:THR:CG2	6:C:137:PRO:HB3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:64:ARG:NE	7:D:67:ASP:HB3	2.22	0.54
10:G:67:LEU:O	10:G:71:LEU:HG	2.07	0.54
20:R:29:LYS:NZ	39:R:9449:HOH:O	2.39	0.54
1:0:1595:G:O2'	1:0:1596:U:H5'	2.08	0.54
1:0:185:G:H4'	1:0:186:A:H4'	1.90	0.54
1:0:2851:G:H2'	1:0:2852:A:H5'	1.90	0.54
4:A:94:LEU:N	4:A:94:LEU:HD23	2.22	0.54
5:B:18:ARG:HE	5:B:256:GLN:NE2	2.06	0.54
9:F:57:GLU:O	9:F:61:MET:HG3	2.07	0.54
22:T:75:GLU:O	22:T:76:ASP:HB2	2.08	0.54
1:0:1778:A:H2'	1:0:1779:A:H5'	1.89	0.54
12:J:45:VAL:HG11	12:J:121:LEU:CD2	2.38	0.54
16:N:110:THR:HB	16:N:113:SER:OG	2.08	0.54
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.37	0.54
25:W:106:THR:OG1	25:W:109:GLU:HG3	2.08	0.54
1:0:1789:G:O6	18:P:73:HIS:HE1	1.91	0.53
1:0:2908:A:H2'	1:0:2909:G:O4'	2.06	0.53
5:B:268:ARG:NH2	5:B:325:PRO:HG3	2.23	0.53
7:D:23:VAL:HG22	7:D:73:VAL:HB	1.89	0.53
15:M:164:THR:CG2	15:M:166:ALA:H	2.21	0.53
15:M:27:ARG:NH2	15:M:44:THR:HG23	2.22	0.53
16:N:114:LYS:O	16:N:118:ILE:HG13	2.07	0.53
1:0:1189:A:H1'	1:0:1209:C:O4'	2.08	0.53
31:3:55:VAL:HG22	39:3:9444:HOH:O	2.07	0.53
4:A:107:ASN:OD1	4:A:120:ARG:HD2	2.07	0.53
6:C:214:THR:HG23	39:C:9240:HOH:O	2.08	0.53
1:0:2346:C:H4'	7:D:52:THR:CG2	2.38	0.53
11:H:27:LYS:H	11:H:59:HIS:CD2	2.18	0.53
32:I:92:PRO:C	32:I:94:GLU:H	2.11	0.53
18:P:103:THR:O	18:P:107:GLU:HG3	2.08	0.53
1:0:2890:A:H1'	23:U:56:ARG:NH2	2.22	0.53
27:Y:99:ALA:HB2	27:Y:233:TYR:CE2	2.43	0.53
1:0:1201:C:H5"	39:0:6774:HOH:O	2.08	0.53
4:A:191:GLY:HA2	4:A:194:MET:HE3	1.90	0.53
6:C:127:ARG:HD3	6:C:129:HIS:HE1	1.74	0.53
6:C:98:ARG:NH1	39:C:9160:HOH:O	2.41	0.53
8:E:81:GLU:HG2	8:E:134:SER:HB3	1.90	0.53
19:Q:75:ILE:HD13	19:Q:84:ILE:HD11	1.90	0.53
1:0:2817:G:P	39:0:8491:HOH:O	2.67	0.53
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.09	0.53
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:64:ARG:HD2	39:M:9386:HOH:O	2.08	0.53
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.37	0.53
1:0:2645:U:OP2	1:0:2645:U:C6	2.62	0.53
1:0:500:G:H21	20:R:98:ASN:HD21	1.55	0.53
30:2:5:LYS:O	30:2:9:LYS:HG3	2.08	0.53
4:A:33:GLU:CD	4:A:33:GLU:H	2.10	0.53
7:D:23:VAL:CG2	7:D:73:VAL:HB	2.38	0.53
13:K:99:ASP:OD1	13:K:101:ASN:N	2.41	0.53
27:Y:96:GLU:O	27:Y:235:GLU:HA	2.09	0.53
1:0:1053:G:OP1	11:H:12:PRO:HG3	2.08	0.53
1:0:2783:A:H5''	39:0:5797:HOH:O	2.07	0.53
1:0:558:C:H2'	1:0:559:U:H5''	1.89	0.53
32:I:100:LEU:O	32:I:139:ILE:HG23	2.09	0.53
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.39	0.53
25:W:4:LEU:O	25:W:32:CYS:HA	2.09	0.53
4:A:132:ASP:OD1	4:A:133:ARG:N	2.41	0.53
5:B:264:GLU:HG2	5:B:267:LYS:CE	2.26	0.53
7:D:35:ALA:O	7:D:38:GLU:HG3	2.08	0.53
11:H:30:GLN:H	11:H:66:ARG:HH11	1.57	0.53
32:I:118:SER:HB2	32:I:123:ASN:HB2	1.91	0.53
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.38	0.53
1:0:1119:G:N2	1:0:1246:A:N1	2.57	0.53
1:0:656:G:H5'	17:O:3:THR:CG2	2.37	0.53
5:B:41:PHE:CG	5:B:79:MET:HE2	2.44	0.53
2:9:3029:C:O3'	7:D:138:GLY:HA2	2.09	0.53
11:H:40:ALA:HB1	11:H:137:TYR:CE2	2.44	0.53
15:M:183:THR:HG22	15:M:194:ALA:HB1	1.91	0.53
1:0:2807:U:P	5:B:27:ASN:HD21	2.32	0.53
1:0:299:U:H5'	39:0:7830:HOH:O	2.09	0.53
1:0:1943:C:H4'	4:A:211:LYS:O	2.09	0.53
5:B:214:PRO:HD2	39:B:9524:HOH:O	2.09	0.53
16:N:152:GLU:C	16:N:154:LEU:H	2.12	0.53
1:0:1400:C:H4'	26:X:56:GLU:HG2	1.90	0.53
1:0:775:G:OP1	29:1:16:HIS:HE1	1.92	0.53
31:3:48:ASN:ND2	31:3:50:GLY:H	2.07	0.53
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.08	0.53
26:X:43:VAL:HG12	26:X:44:ASP:N	2.23	0.53
1:0:1641:A:C2'	1:0:1642:A:H5'	2.38	0.52
1:0:2472:C:O2'	1:0:2634:G:H4'	2.08	0.52
1:0:2661:U:H3	1:0:2812:A:H62	1.57	0.52
1:0:541:C:H2'	1:0:542:A:H5'	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:8:ALA:HA	12:J:35:THR:HG22	1.90	0.52
15:M:79:ALA:HB3	15:M:81:ARG:HH12	1.74	0.52
22:T:32:ARG:NH1	22:T:38:ARG:HH12	2.06	0.52
4:A:76:VAL:HG23	28:Z:63:LYS:HB3	1.91	0.52
1:O:2100:A:H4'	6:C:64:GLY:O	2.08	0.52
17:O:22:GLY:HA2	39:O:2823:HOH:O	2.08	0.52
1:O:441:A:H1'	1:O:442:A:N7	2.23	0.52
5:B:190:MET:CE	5:B:194:PHE:HD1	2.22	0.52
14:L:97:VAL:HG12	14:L:98:GLU:O	2.09	0.52
1:O:447:A:OP1	22:T:2:LYS:HG2	2.09	0.52
8:E:133:VAL:HG12	8:E:141:VAL:HG13	1.92	0.52
11:H:28:ILE:HG23	39:H:9546:HOH:O	2.09	0.52
22:T:40:VAL:HG22	22:T:41:ARG:H	1.74	0.52
25:W:130:HIS:O	25:W:136:GLY:HA3	2.09	0.52
26:X:22:ASN:O	26:X:25:ARG:HG3	2.09	0.52
1:O:1328:A:C8	27:Y:169:ARG:HD3	2.45	0.52
1:O:291:C:H2'	1:O:292:G:O4'	2.10	0.52
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.57	0.52
30:2:36:ASN:HB3	30:2:39:ARG:HG3	1.91	0.52
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.44	0.52
2:9:3050:G:H5''	16:N:159:TYR:HE1	1.74	0.52
15:M:30:GLU:O	15:M:34:GLU:HG3	2.09	0.52
24:V:5:VAL:HG23	39:V:2271:HOH:O	2.09	0.52
1:O:1167:G:H4'	32:I:135:LEU:CD2	2.40	0.52
6:C:107:ARG:NE	39:C:9263:HOH:O	2.36	0.52
13:K:87:ARG:NH1	39:K:4066:HOH:O	2.43	0.52
23:U:9:CYS:O	23:U:52:THR:HG23	2.10	0.52
25:W:29:VAL:O	25:W:30:ASN:HB2	2.10	0.52
1:O:446:G:OP2	22:T:6:LYS:NZ	2.39	0.52
30:2:20:ARG:HD2	30:2:39:ARG:NH2	2.24	0.52
2:9:3076:G:C3'	2:9:3077:A:H5''	2.32	0.52
5:B:8:LYS:HG3	5:B:220:VAL:HG12	1.92	0.52
39:O:4582:HOH:O	22:T:82:THR:HA	2.09	0.52
24:V:1:THR:HG22	24:V:48:GLU:OE1	2.10	0.52
1:O:1189:A:O2'	1:O:1208:C:H2'	2.10	0.52
16:N:37:ARG:NE	39:N:9333:HOH:O	2.42	0.52
17:O:38:ARG:NH1	39:O:7674:HOH:O	2.43	0.52
1:O:1080:C:H4'	1:O:1081:A:OP1	2.09	0.52
1:O:1555:G:H4'	1:O:1630:A:H2	1.75	0.52
1:O:2064:U:H5'	1:O:2652:U:O3'	2.10	0.52
1:O:407:A:H5'	39:O:6572:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:407:A:H2'	1:0:408:A:C8	2.45	0.52
1:0:848:C:H5'	39:0:7771:HOH:O	2.10	0.52
8:E:35:TYR:HA	12:J:127:ILE:HD12	1.92	0.52
13:K:55:VAL:CG1	13:K:56:SER:N	2.72	0.52
16:N:163:PHE:HZ	16:N:171:HIS:HD1	1.57	0.52
18:P:14:LEU:O	18:P:16:VAL:HG23	2.10	0.52
18:P:16:VAL:HG13	18:P:20:ARG:NH1	2.24	0.52
24:V:1:THR:HG23	24:V:2:VAL:N	2.19	0.52
1:0:2636:C:H3'	1:0:2637:A:C5'	2.40	0.51
17:O:25:VAL:HG11	17:O:111:VAL:HG11	1.93	0.51
19:Q:75:ILE:CD1	19:Q:84:ILE:HD11	2.40	0.51
1:0:1451:C:H5'	1:0:1505:U:C5	2.45	0.51
1:0:1626:A:H2'	1:0:1627:G:O4'	2.10	0.51
1:0:2133:U:H4'	1:0:2134:G:H5'	1.91	0.51
1:0:2748:G:H8	39:0:8086:HOH:O	1.92	0.51
1:0:1363:G:OP1	6:C:76:ARG:NH2	2.43	0.51
8:E:5:LEU:HD21	8:E:66:GLN:HG3	1.92	0.51
8:E:69:ILE:HA	8:E:72:MET:CE	2.40	0.51
10:G:64:ASN:N	10:G:64:ASN:HD22	2.07	0.51
11:H:2:PRO:HD2	11:H:5:MET:SD	2.49	0.51
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.76	0.51
28:Z:37:HIS:O	28:Z:45:ASP:HA	2.10	0.51
1:0:1189:A:H1'	1:0:1209:C:C1'	2.40	0.51
1:0:622:G:P	27:Y:148:GLY:HA3	2.49	0.51
4:A:149:ASP:OD1	4:A:151:GLN:HB2	2.09	0.51
1:0:2250:G:OP1	4:A:31:LYS:HD3	2.10	0.51
1:0:2694:A:H4'	8:E:91:PHE:CE1	2.46	0.51
1:0:1771:U:H5'	28:Z:20:ARG:HH21	1.76	0.51
1:0:1218:U:H2'	1:0:1219:U:H6	1.74	0.51
1:0:2717:C:H2'	1:0:2718:C:C5'	2.37	0.51
1:0:2795:C:O2'	1:0:2796:U:H5'	2.10	0.51
1:0:316:A:H5'	22:T:54:ASP:OD2	2.09	0.51
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.91	0.51
5:B:267:LYS:HE3	5:B:300:SER:O	2.10	0.51
6:C:142:ASP:OD1	6:C:237:GLU:HB3	2.11	0.51
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.91	0.51
10:G:12:ILE:N	10:G:13:PRO:CD	2.74	0.51
32:I:131:THR:O	32:I:135:LEU:HG	2.10	0.51
12:J:131:THR:HG22	12:J:133:GLY:N	2.26	0.51
22:T:61:GLU:HG3	39:T:3851:HOH:O	2.09	0.51
22:T:71:VAL:HG13	22:T:91:LEU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:5:VAL:O	25:W:52:VAL:HG22	2.10	0.51
1:0:1882:C:OP1	4:A:192:VAL:HG23	2.09	0.51
1:0:2502:C:H2'	1:0:2503:A:H5'	1.91	0.51
4:A:100:PRO:HG2	4:A:103:VAL:CG2	2.40	0.51
5:B:53:LEU:CD1	5:B:327:VAL:HG22	2.41	0.51
7:D:81:GLU:O	7:D:85:GLN:HG3	2.10	0.51
1:0:1118:A:C8	1:0:1119:G:H5''	2.45	0.51
1:0:602:A:O2'	1:0:605:C:H4'	2.10	0.51
11:H:45:VAL:HA	11:H:167:PRO:O	2.10	0.51
16:N:143:ARG:NH1	16:N:173:ASP:OD2	2.43	0.51
20:R:106:GLY:HA2	20:R:109:MET:CE	2.41	0.51
1:0:2769:C:H2'	1:0:2770:G:C5'	2.40	0.51
1:0:485:A:N3	1:0:487:G:H5''	2.25	0.51
1:0:65:C:O2'	1:0:66:G:H5'	2.10	0.51
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.39	0.51
1:0:2632:G:H5''	4:A:210:GLY:HA3	1.92	0.51
6:C:242:GLU:HG3	39:C:9186:HOH:O	2.10	0.51
9:F:48:VAL:CG2	9:F:74:PHE:HB3	2.40	0.51
18:P:16:VAL:HG12	18:P:17:GLY:N	2.25	0.51
39:0:5855:HOH:O	25:W:122:ARG:NH2	2.36	0.51
25:W:80:ASP:O	25:W:84:VAL:HG23	2.09	0.51
1:0:2747:C:H4'	39:0:8486:HOH:O	2.10	0.51
1:0:621:C:H5'	27:Y:132:ASP:OD2	2.11	0.51
4:A:125:ASN:CB	4:A:158:VAL:HG12	2.40	0.51
6:C:16:VAL:HG12	6:C:17:ASP:N	2.26	0.51
6:C:46:TYR:CE2	6:C:98:ARG:NH1	2.79	0.51
32:I:78:LEU:HD12	32:I:112:LYS:NZ	2.26	0.51
12:J:131:THR:HG22	12:J:134:GLU:H	1.74	0.51
13:K:115:ARG:HG3	13:K:116:GLU:N	2.26	0.51
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.92	0.51
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.25	0.51
25:W:38:THR:HG22	25:W:39:ASP:N	2.25	0.51
1:0:797:A:C5'	28:Z:10:ARG:N	2.72	0.51
1:0:1972:U:H2'	1:0:1973:A:C5'	2.41	0.51
1:0:709:G:O2'	17:O:25:VAL:HG12	2.09	0.51
1:0:120:A:H5'	29:1:20:ARG:HH21	1.76	0.51
13:K:49:LEU:HD22	13:K:117:VAL:CG2	2.41	0.51
39:0:4127:HOH:O	18:P:91:LYS:HD3	2.11	0.51
27:Y:216:ARG:HD2	39:Y:9367:HOH:O	2.10	0.51
1:0:2416:G:O2'	16:N:25:ARG:HG2	2.10	0.51
1:0:644:G:O2'	14:L:4:LYS:HE3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:41:HIS:HD2	30:2:44:ARG:H	1.58	0.51
6:C:129:HIS:HE1	6:C:231:ARG:HA	1.75	0.51
11:H:58:ARG:HG3	11:H:58:ARG:NH1	2.26	0.51
14:L:125:PHE:CZ	14:L:140:VAL:HG13	2.46	0.51
14:L:57:VAL:HG12	14:L:57:VAL:O	2.10	0.51
25:W:5:VAL:O	25:W:52:VAL:CG2	2.59	0.51
1:0:371:U:H2'	1:0:372:A:C8	2.46	0.50
1:0:564:G:H1'	39:0:6848:HOH:O	2.09	0.50
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.92	0.50
7:D:36:ASN:HA	39:D:7500:HOH:O	2.11	0.50
8:E:49:ILE:HD11	8:E:69:ILE:HD12	1.92	0.50
13:K:13:GLU:OE1	13:K:44:LEU:HD12	2.10	0.50
16:N:162:ASP:HA	39:N:9330:HOH:O	2.11	0.50
23:U:9:CYS:HA	23:U:52:THR:HG23	1.92	0.50
1:0:1506:U:H6	1:0:1506:U:H5'	1.76	0.50
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.51	0.50
2:9:3050:G:H5''	16:N:159:TYR:CE1	2.47	0.50
6:C:118:THR:O	6:C:136:VAL:HG13	2.10	0.50
7:D:51:ARG:HD3	39:D:7636:HOH:O	2.11	0.50
8:E:69:ILE:HA	8:E:72:MET:HE3	1.93	0.50
28:Z:42:CYS:SG	28:Z:43:GLY:N	2.85	0.50
1:0:1687:C:O2	29:1:9:GLY:HA2	2.11	0.50
1:0:2480:G:H3'	39:0:4777:HOH:O	2.11	0.50
4:A:101:GLU:OE2	4:A:131:HIS:HB2	2.12	0.50
32:I:102:VAL:HG12	32:I:106:LYS:HE3	1.93	0.50
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.41	0.50
1:0:20:G:H21	20:R:117:HIS:HD2	1.58	0.50
1:0:2704:C:O2	8:E:110:GLU:HB3	2.11	0.50
1:0:2825:C:H4'	1:0:2826:G:O5'	2.12	0.50
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.45	0.50
2:9:3049:G:O2'	2:9:3050:G:H5'	2.11	0.50
8:E:20:ILE:CD1	8:E:33:LEU:HD12	2.42	0.50
1:0:1184:C:H4'	32:I:126:LYS:HB3	1.92	0.50
12:J:54:VAL:O	12:J:58:GLU:HG3	2.11	0.50
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.25	0.50
27:Y:209:VAL:HG12	27:Y:214:ARG:HG3	1.93	0.50
1:0:2912:C:H2'	1:0:2913:A:O4'	2.12	0.50
5:B:312:ARG:HD3	5:B:315:VAL:HG13	1.94	0.50
6:C:142:ASP:OD1	6:C:236:THR:HG23	2.11	0.50
25:W:65:VAL:HA	25:W:68:THR:HG22	1.92	0.50
1:0:2726:U:O2	1:0:2749:U:O5'	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:36:ASP:O	4:A:38:ILE:N	2.42	0.50
5:B:264:GLU:CG	5:B:267:LYS:HE2	2.28	0.50
7:D:50:VAL:O	7:D:71:ALA:HA	2.11	0.50
11:H:148:GLU:HA	11:H:148:GLU:OE1	2.12	0.50
32:I:91:GLU:HB2	32:I:95:ASP:OD2	2.12	0.50
15:M:68:ARG:HD3	15:M:68:ARG:O	2.11	0.50
1:0:1406:A:H4'	1:0:1407:A:H5''	1.94	0.50
1:0:2816:A:H2'	39:0:8491:HOH:O	2.12	0.50
1:0:558:C:H2'	1:0:559:U:H5'	1.94	0.50
1:0:625:U:H5'	39:0:3793:HOH:O	2.12	0.50
1:0:894:A:N1	6:C:87:ARG:NH2	2.59	0.50
8:E:7:ILE:HD11	8:E:11:VAL:O	2.11	0.50
12:J:71:TYR:CD1	12:J:72:PRO:HD2	2.47	0.50
15:M:107:ARG:NH1	39:M:9378:HOH:O	2.44	0.50
1:0:2032:U:H2'	1:0:2033:G:H5'	1.92	0.50
31:3:35:TRP:HD1	39:3:9487:HOH:O	1.94	0.50
7:D:37:ALA:O	7:D:40:ILE:HG12	2.11	0.50
1:0:1701:A:H5'	39:0:6821:HOH:O	2.11	0.49
1:0:1926:G:H2'	1:0:1927:A:C8	2.47	0.49
1:0:2032:U:H2'	1:0:2033:G:C5'	2.42	0.49
4:A:72:GLU:HG3	28:Z:66:GLY:HA2	1.92	0.49
11:H:157:ILE:HD11	11:H:161:CYS:SG	2.52	0.49
12:J:70:PHE:CG	12:J:70:PHE:O	2.65	0.49
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.32	0.49
17:O:25:VAL:HG11	17:O:111:VAL:CG1	2.42	0.49
27:Y:144:ARG:CG	27:Y:144:ARG:NH1	2.69	0.49
28:Z:53:GLY:HA2	28:Z:67:GLY:O	2.12	0.49
1:0:136:C:H2'	1:0:137:U:O4'	2.12	0.49
1:0:1435:U:H5'	39:0:3214:HOH:O	2.12	0.49
1:0:329:A:OP2	6:C:206:ASN:HB2	2.13	0.49
1:0:870:G:OP2	4:A:3:ARG:HD3	2.12	0.49
5:B:81:ALA:O	5:B:186:GLY:HA3	2.11	0.49
13:K:14:LYS:HG3	13:K:32:ILE:O	2.12	0.49
15:M:98:GLN:O	15:M:102:GLU:HG3	2.11	0.49
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.43	0.49
18:P:125:LYS:HB3	18:P:130:GLU:HG3	1.93	0.49
19:Q:30:VAL:O	19:Q:30:VAL:HG12	2.12	0.49
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.11	0.49
1:0:1118:A:C8	1:0:1118:A:C3'	2.91	0.49
1:0:1667:A:C8	1:0:1667:A:H5'	2.38	0.49
1:0:1736:A:H1'	39:0:8155:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:170:TYR:O	7:D:171:ASP:CB	2.60	0.49
9:F:16:ALA:HA	9:F:111:ILE:HD13	1.94	0.49
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.41	0.49
1:0:1773:G:C8	28:Z:16:ALA:HA	2.47	0.49
1:0:1666:C:H2'	1:0:1667:A:C5'	2.42	0.49
1:0:666:A:H2'	1:0:667:C:O4'	2.13	0.49
31:3:3:MET:O	31:3:90:PHE:HA	2.12	0.49
4:A:105:VAL:HG12	4:A:106:CYS:N	2.27	0.49
6:C:19:PRO:HG2	6:C:22:PHE:CE1	2.48	0.49
6:C:246:ARG:NH1	39:C:9174:HOH:O	2.44	0.49
7:D:135:VAL:HG22	7:D:136:ARG:N	2.27	0.49
32:I:105:VAL:HG11	32:I:129:VAL:CG2	2.42	0.49
12:J:39:VAL:HG13	12:J:106:GLY:O	2.12	0.49
22:T:88:PRO:HB3	39:T:6320:HOH:O	2.13	0.49
26:X:66:THR:HG23	26:X:67:PRO:HD2	1.94	0.49
27:Y:235:GLU:CD	27:Y:235:GLU:N	2.53	0.49
1:0:2748:G:OP1	1:0:2749:U:H5''	2.12	0.49
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.94	0.49
32:I:129:VAL:HG13	32:I:139:ILE:HD11	1.95	0.49
12:J:15:ARG:NH1	12:J:43:ARG:NH1	2.61	0.49
13:K:49:LEU:HD12	13:K:80:ILE:HD13	1.94	0.49
1:0:2895:C:H4'	39:X:4132:HOH:O	2.12	0.49
1:0:653:C:H2'	1:0:654:A:C8	2.48	0.49
6:C:25:PRO:HG2	39:C:9123:HOH:O	2.12	0.49
24:V:8:ILE:HA	24:V:11:MET:HE2	1.95	0.49
25:W:137:GLN:NE2	25:W:141:HIS:HE1	1.95	0.49
27:Y:117:LEU:HA	27:Y:174:VAL:HG11	1.94	0.49
1:0:2365:G:H5''	39:Q:6597:HOH:O	2.10	0.49
1:0:2443:C:O3'	14:L:56:LYS:HE3	2.11	0.49
1:0:399:C:H5'	15:M:179:GLY:O	2.12	0.49
2:9:3057:A:C8	7:D:141:VAL:HG21	2.47	0.49
7:D:23:VAL:O	7:D:23:VAL:HG23	2.13	0.49
9:F:48:VAL:HG12	9:F:97:ALA:CB	2.41	0.49
1:0:1573:A:H2'	1:0:1574:C:O4'	2.12	0.49
1:0:328:U:O4'	6:C:202:THR:HG22	2.13	0.49
6:C:153:VAL:O	6:C:157:LEU:HG	2.13	0.49
6:C:194:PHE:CE2	6:C:234:VAL:HG11	2.48	0.49
13:K:23:ASN:HD21	13:K:107:THR:HB	1.77	0.49
15:M:69:LYS:HG3	15:M:126:GLN:CA	2.42	0.49
20:R:39:THR:HG23	20:R:107:GLU:O	2.13	0.49
27:Y:145:LYS:HE2	39:Y:9403:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:14:GLU:HB3	39:G:4173:HOH:O	2.13	0.49
11:H:78:GLY:C	11:H:80:GLU:H	2.16	0.49
12:J:142:ASN:O	12:J:144:THR:N	2.46	0.49
14:L:89:PHE:CD1	14:L:89:PHE:N	2.81	0.49
1:0:1853:C:O2'	4:A:217:ARG:NH2	2.46	0.49
1:0:2456:A:H2'	1:0:2457:U:C6	2.48	0.49
1:0:2626:C:H2'	1:0:2627:G:C8	2.48	0.49
5:B:190:MET:CE	5:B:194:PHE:CD1	2.96	0.49
7:D:104:PHE:CE2	7:D:166:ILE:HD13	2.48	0.49
9:F:29:VAL:HG12	9:F:98:VAL:HA	1.94	0.49
15:M:61:ILE:N	15:M:61:ILE:HD12	2.27	0.49
21:S:57:THR:CG2	21:S:58:MET:N	2.75	0.49
22:T:69:LYS:O	22:T:71:VAL:HG23	2.13	0.49
24:V:64:GLY:O	24:V:65:ASP:CB	2.60	0.49
25:W:84:VAL:HG12	39:W:6679:HOH:O	2.11	0.49
39:0:3561:HOH:O	26:X:23:HIS:HD2	1.95	0.49
1:0:1165:G:O3'	1:0:1174:A:H4'	2.13	0.48
1:0:2908:A:C2'	1:0:2909:G:H5'	2.42	0.48
1:0:449:A:C8	6:C:43:LYS:HG2	2.48	0.48
4:A:81:GLN:HB2	4:A:92:ASN:ND2	2.28	0.48
5:B:17:LYS:O	5:B:260:HIS:HD2	1.95	0.48
5:B:62:ARG:CA	5:B:65:MET:HE3	2.43	0.48
1:0:2694:A:H4'	8:E:91:PHE:HE1	1.77	0.48
12:J:50:GLU:O	12:J:54:VAL:HG23	2.13	0.48
13:K:125:ALA:C	13:K:127:ALA:H	2.15	0.48
15:M:169:ARG:NH2	39:M:9352:HOH:O	2.46	0.48
18:P:121:ASP:O	18:P:125:LYS:HG3	2.13	0.48
22:T:41:ARG:NH1	22:T:41:ARG:HG2	2.27	0.48
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.48	0.48
1:0:1209:C:H2'	1:0:1210:G:C8	2.48	0.48
1:0:737:A:H2'	1:0:738:G:O4'	2.13	0.48
4:A:39:ALA:HB3	4:A:61:GLU:OE2	2.14	0.48
7:D:24:HIS:HB2	7:D:72:LYS:HB3	1.94	0.48
32:I:139:ILE:HG22	32:I:140:GLU:N	2.29	0.48
13:K:87:ARG:NE	39:K:4854:HOH:O	2.46	0.48
25:W:21:LEU:HD22	25:W:26:ILE:HD13	1.93	0.48
1:0:1198:U:H2'	1:0:1200:A:OP2	2.13	0.48
1:0:1675:C:H5''	30:2:5:LYS:HD2	1.95	0.48
1:0:371:U:H2'	1:0:372:A:H8	1.77	0.48
1:0:558:C:C2'	1:0:559:U:C5'	2.91	0.48
5:B:7:ARG:HG2	5:B:7:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:140:VAL:HG12	6:C:141:SER:N	2.28	0.48
8:E:3:VAL:HG22	8:E:49:ILE:HB	1.94	0.48
10:G:12:ILE:HG13	39:G:6833:HOH:O	2.12	0.48
14:L:91:VAL:CG1	14:L:120:LEU:HD23	2.43	0.48
39:0:4965:HOH:O	15:M:83:SER:HB3	2.13	0.48
1:0:656:G:C5'	17:O:3:THR:HG22	2.40	0.48
20:R:96:VAL:HG13	20:R:106:GLY:HA3	1.95	0.48
24:V:43:PRO:O	24:V:46:ILE:HG22	2.12	0.48
1:0:1603:A:H5''	1:0:1605:G:H5'	1.95	0.48
1:0:1972:U:H2'	1:0:1973:A:H5'	1.96	0.48
1:0:951:A:C2'	1:0:952:G:H5'	2.43	0.48
4:A:135:VAL:HG21	4:A:147:ARG:NH1	2.28	0.48
14:L:145:LEU:O	14:L:148:GLU:HG3	2.13	0.48
14:L:72:ASN:HB2	39:L:9480:HOH:O	2.13	0.48
14:L:97:VAL:O	14:L:100:ALA:HB2	2.13	0.48
23:U:20:MET:CG	23:U:28:THR:HG23	2.44	0.48
24:V:5:VAL:CG1	24:V:9:ARG:NH1	2.77	0.48
26:X:72:VAL:CG2	26:X:85:VAL:HG12	2.37	0.48
1:0:204:A:C2'	1:0:205:U:H5'	2.44	0.48
5:B:294:TYR:HE2	39:B:9644:HOH:O	1.95	0.48
11:H:75:LYS:O	11:H:75:LYS:HG2	2.13	0.48
26:X:43:VAL:CG1	26:X:44:ASP:N	2.76	0.48
1:0:2837:U:H2'	39:0:7353:HOH:O	2.13	0.48
1:0:776:A:OP1	29:1:28:HIS:HE1	1.96	0.48
1:0:820:G:O2'	1:0:856:G:H4'	2.14	0.48
6:C:107:ARG:NH1	39:C:9235:HOH:O	2.47	0.48
11:H:29:ALA:C	11:H:30:GLN:HG3	2.33	0.48
32:I:128:VAL:C	32:I:130:GLY:H	2.16	0.48
1:0:1242:A:C5'	12:J:82:THR:HG23	2.36	0.48
18:P:16:VAL:HG13	18:P:20:ARG:CZ	2.43	0.48
1:0:1056:U:H2'	1:0:1057:A:O4'	2.13	0.48
1:0:1462:C:H2'	1:0:1463:A:H8	1.78	0.48
1:0:1717:A:H5''	18:P:54:LYS:HB2	1.95	0.48
31:3:11:CYS:HB2	31:3:20:HIS:CE1	2.49	0.48
2:9:3092:G:H2'	2:9:3093:A:C8	2.49	0.48
5:B:75:GLU:C	5:B:77:PRO:HD3	2.33	0.48
6:C:133:ARG:NE	6:C:138:VAL:HG22	2.29	0.48
7:D:82:GLU:HA	7:D:85:GLN:HE21	1.78	0.48
11:H:116:ALA:O	11:H:117:PHE:C	2.52	0.48
12:J:52:GLN:HG3	12:J:53:ILE:N	2.28	0.48
39:9:5071:HOH:O	16:N:18:THR:HG21	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1159:G:H1	1:0:1208:C:H42	1.62	0.48
1:0:249:G:O2'	1:0:250:C:H5'	2.14	0.48
1:0:2820:A:H2'	1:0:2821:C:C6	2.47	0.48
1:0:482:G:H4'	1:0:508:A:N1	2.29	0.48
31:3:65:THR:CG2	31:3:67:LEU:HG	2.42	0.48
4:A:88:ILE:HG22	4:A:88:ILE:O	2.13	0.48
7:D:25:MET:CE	7:D:37:ALA:HB1	2.40	0.48
11:H:1:LYS:HE2	11:H:1:LYS:HA	1.95	0.48
32:I:78:LEU:HD12	32:I:112:LYS:HZ2	1.77	0.48
15:M:187:LEU:HD22	15:M:194:ALA:HB3	1.95	0.48
19:Q:3:SER:HB3	39:Q:5998:HOH:O	2.13	0.48
1:0:2072:G:H3'	1:0:2073:G:C5'	2.44	0.48
1:0:2421:G:H2'	39:0:4671:HOH:O	2.12	0.48
1:0:90:A:H2'	1:0:91:G:O4'	2.14	0.48
2:9:3024:U:H3'	2:9:3025:G:H5'	1.95	0.48
5:B:84:LEU:HB2	5:B:182:VAL:HG21	1.96	0.48
1:0:2348:C:H1'	7:D:131:THR:HG21	1.96	0.48
13:K:28:GLU:OE2	13:K:58:THR:HG21	2.14	0.48
20:R:132:ARG:NH2	39:R:9492:HOH:O	2.47	0.48
23:U:47:ARG:HG2	39:U:4381:HOH:O	2.14	0.48
25:W:142:ASP:HB3	25:W:145:GLY:H	1.79	0.48
1:0:1634:G:H3'	39:0:4492:HOH:O	2.13	0.48
1:0:1942:A:H3'	39:0:7839:HOH:O	2.14	0.48
1:0:2414:A:H2'	1:0:2415:A:C8	2.49	0.48
1:0:834:G:H4'	1:0:835:U:OP2	2.14	0.48
31:3:17:HIS:O	31:3:18:GLN:HG3	2.14	0.48
4:A:223:ARG:NE	39:A:9560:HOH:O	2.46	0.48
12:J:103:VAL:HG12	39:J:5907:HOH:O	2.14	0.48
14:L:10:SER:O	14:L:11:ARG:HB3	2.13	0.48
14:L:21:ARG:N	39:L:9424:HOH:O	2.46	0.48
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.96	0.48
17:O:57:THR:HB	17:O:111:VAL:HG23	1.96	0.48
20:R:18:LEU:HB2	20:R:143:VAL:HG13	1.95	0.48
25:W:88:THR:HG22	25:W:90:TYR:CD1	2.49	0.48
1:0:2363:G:O2'	19:Q:11:ARG:HG3	2.14	0.47
4:A:51:ARG:NH1	4:A:120:ARG:O	2.47	0.47
32:I:72:VAL:HG11	32:I:111:GLN:O	2.13	0.47
13:K:81:ARG:HD3	13:K:87:ARG:CZ	2.44	0.47
1:0:1236:A:H2'	1:0:1237:U:O4'	2.14	0.47
1:0:1290:G:H3'	39:0:5735:HOH:O	2.13	0.47
1:0:1333:U:H2'	1:0:1334:C:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1477:C:H5'	1:0:1868:G:C5'	2.44	0.47
1:0:1750:C:H4'	39:0:7969:HOH:O	2.15	0.47
1:0:2587:OMU:H6	1:0:2587:OMU:O5'	2.13	0.47
4:A:194:MET:CE	4:A:199:HIS:HB2	2.44	0.47
7:D:172:VAL:HG12	7:D:173:GLU:N	2.28	0.47
17:O:80:ASP:OD1	17:O:81:PHE:N	2.47	0.47
20:R:113:HIS:HE1	20:R:144:GLU:CD	2.17	0.47
22:T:38:ARG:HG3	22:T:38:ARG:NH1	2.29	0.47
27:Y:122:ARG:NH2	39:Y:9333:HOH:O	2.47	0.47
1:0:1044:C:H5''	39:0:9647:HOH:O	2.13	0.47
1:0:2911:C:O2'	1:0:2912:C:H5'	2.14	0.47
4:A:179:MET:HA	4:A:179:MET:HE3	1.97	0.47
5:B:254:GLN:HG2	5:B:255:GLY:H	1.79	0.47
7:D:99:ASP:O	7:D:159:PRO:HG3	2.14	0.47
12:J:88:PRO:O	12:J:94:GLY:HA3	2.15	0.47
17:O:98:LEU:O	17:O:102:ILE:HG13	2.15	0.47
25:W:110:GLN:HE21	25:W:110:GLN:HA	1.77	0.47
1:0:2505:G:C2'	1:0:2506:A:H5'	2.45	0.47
3:4:75:C:H2'	3:4:76:PPU:C8	2.44	0.47
4:A:36:ASP:HB2	4:A:85:SER:H	1.80	0.47
8:E:125:GLU:HB2	8:E:132:THR:HG23	1.97	0.47
32:I:113:HIS:N	32:I:114:PRO:CD	2.78	0.47
22:T:71:VAL:CG1	22:T:72:ILE:N	2.77	0.47
1:0:1973:A:H5'	1:0:1973:A:C8	2.40	0.47
1:0:2711:U:H1'	39:0:4046:HOH:O	2.13	0.47
1:0:317:A:H5''	22:T:52:ARG:HD2	1.96	0.47
1:0:449:A:N7	6:C:43:LYS:HG2	2.29	0.47
2:9:3008:G:O6	16:N:11:ARG:NH1	2.43	0.47
4:A:26:ASP:CG	4:A:26:ASP:O	2.53	0.47
5:B:41:PHE:CG	5:B:190:MET:HE3	2.49	0.47
7:D:44:ILE:HG23	7:D:45:THR:HG23	1.97	0.47
10:G:24:VAL:O	10:G:28:GLU:HB2	2.14	0.47
1:0:926:A:O2'	14:L:41:HIS:CD2	2.67	0.47
39:0:4783:HOH:O	27:Y:186:ARG:HD2	2.15	0.47
28:Z:26:VAL:O	28:Z:30:GLU:HG3	2.14	0.47
1:0:1181:A:N1	1:0:1192:A:O2'	2.47	0.47
1:0:1351:G:OP1	6:C:96:LYS:NZ	2.45	0.47
6:C:236:THR:HG22	6:C:239:ALA:CB	2.45	0.47
7:D:76:ARG:O	7:D:77:ASP:HB2	2.14	0.47
9:F:101:ALA:HA	39:F:5413:HOH:O	2.15	0.47
1:0:1167:G:H4'	32:I:135:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:170:GLU:HA	16:N:173:ASP:OD2	2.15	0.47
17:O:39:THR:O	17:O:115:ARG:NH2	2.47	0.47
21:S:57:THR:HG22	21:S:58:MET:N	2.29	0.47
1:O:1119:G:H8	12:J:52:GLN:NE2	2.09	0.47
1:O:1482:A:O2'	1:O:1483:C:H5'	2.15	0.47
7:D:166:ILE:HB	39:D:6326:HOH:O	2.14	0.47
8:E:20:ILE:HD12	8:E:33:LEU:HD12	1.95	0.47
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.44	0.47
14:L:145:LEU:O	14:L:145:LEU:HD23	2.15	0.47
1:O:709:G:O2'	17:O:25:VAL:CG1	2.62	0.47
17:O:25:VAL:HG23	17:O:26:TRP:N	2.29	0.47
22:T:96:VAL:HG13	22:T:97:ARG:N	2.29	0.47
24:V:8:ILE:HA	24:V:11:MET:HE3	1.96	0.47
26:X:34:ARG:NH1	26:X:48:VAL:O	2.45	0.47
1:O:1066:U:H2'	1:O:1067:A:C8	2.49	0.47
1:O:1234:U:N3	5:B:244:PRO:HB3	2.30	0.47
1:O:2456:A:H2'	1:O:2457:U:H6	1.80	0.47
1:O:2541:U:H3	1:O:2618:G:H1	1.61	0.47
1:O:396:U:H1'	39:O:8194:HOH:O	2.15	0.47
4:A:121:ALA:O	4:A:124:VAL:HG22	2.14	0.47
5:B:280:VAL:HG13	5:B:333:GLU:O	2.14	0.47
7:D:27:ILE:HD11	7:D:37:ALA:HB3	1.96	0.47
8:E:1:PRO:HG2	8:E:59:MET:SD	2.55	0.47
14:L:73:VAL:HG23	14:L:74:THR:N	2.24	0.47
20:R:119:VAL:CG1	20:R:119:VAL:O	2.62	0.47
28:Z:60:CYS:O	28:Z:61:ASP:HB2	2.15	0.47
1:O:1503:U:H2'	1:O:1504:A:O4'	2.15	0.47
4:A:131:HIS:O	4:A:132:ASP:HB2	2.14	0.47
5:B:171:VAL:HG23	5:B:172:SER:N	2.30	0.47
16:N:93:GLN:HE21	16:N:127:LEU:CD1	2.27	0.47
17:O:47:ARG:HG3	17:O:47:ARG:HH11	1.80	0.47
25:W:4:LEU:HD11	25:W:45:VAL:HG12	1.97	0.47
1:O:1342:C:C2'	1:O:1343:C:H5'	2.45	0.47
1:O:2890:A:H1'	23:U:56:ARG:CZ	2.45	0.47
1:O:68:U:H4'	39:O:7269:HOH:O	2.14	0.47
1:O:920:C:H4'	1:O:921:G:C2	2.50	0.47
1:O:1684:A:H1'	30:2:43:ARG:HH22	1.79	0.47
2:9:3041:C:O4'	7:D:50:VAL:HG22	2.14	0.47
4:A:109:GLU:HG2	4:A:116:GLY:N	2.30	0.47
6:C:154:VAL:O	6:C:158:GLU:HG3	2.15	0.47
6:C:168:ARG:NH2	6:C:190:ALA:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:41:LEU:HA	7:D:44:ILE:HG22	1.96	0.47
8:E:23:GLU:HG2	8:E:28:SER:CB	2.44	0.47
9:F:36:THR:HG23	9:F:97:ALA:HB2	1.97	0.47
11:H:169:GLY:HA3	39:H:9555:HOH:O	2.13	0.47
15:M:164:THR:CG2	15:M:165:GLY:N	2.78	0.47
24:V:39:ALA:C	24:V:41:GLU:H	2.19	0.47
26:X:7:GLU:HA	26:X:74:ALA:O	2.14	0.47
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.96	0.47
1:O:1350:U:H2'	1:O:1351:G:O4'	2.15	0.47
1:O:2531:U:O2'	1:O:2532:A:H5'	2.14	0.47
4:A:39:ALA:O	4:A:61:GLU:HG3	2.14	0.47
7:D:128:LEU:HB2	39:D:6007:HOH:O	2.14	0.47
11:H:28:ILE:HG21	11:H:31:HIS:CE1	2.50	0.47
39:9:5537:HOH:O	16:N:110:THR:HG22	2.16	0.47
1:O:2299:G:O6	19:Q:1:PRO:HA	2.15	0.47
20:R:46:TYR:O	20:R:50:VAL:HG23	2.14	0.47
25:W:88:THR:CG2	25:W:89:ASP:N	2.72	0.47
1:O:1098:A:H2'	1:O:1099:G:O4'	2.15	0.46
1:O:1714:C:O2'	1:O:1715:C:H5'	2.15	0.46
1:O:2353:A:H4'	1:O:2354:A:O5'	2.15	0.46
1:O:541:C:C2'	1:O:542:A:C5'	2.92	0.46
1:O:88:G:H2'	1:O:89:G:C8	2.49	0.46
2:9:3039:U:C2'	2:9:3040:C:OP1	2.63	0.46
2:9:3107:C:H5	39:9:3167:HOH:O	1.97	0.46
6:C:136:VAL:HG22	6:C:137:PRO:HA	1.96	0.46
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.97	0.46
22:T:96:VAL:CG1	22:T:97:ARG:N	2.78	0.46
26:X:9:VAL:HG13	26:X:88:GLU:OE1	2.16	0.46
6:C:219:ASN:O	6:C:222:ASP:OD1	2.33	0.46
9:F:31:LYS:HE3	39:F:2623:HOH:O	2.15	0.46
1:O:244:C:OP2	9:F:38:LYS:HE3	2.15	0.46
10:G:19:GLU:HG2	10:G:66:LEU:HD13	1.98	0.46
11:H:59:HIS:HA	11:H:62:LEU:HD23	1.95	0.46
32:I:124:ALA:O	32:I:128:VAL:HG23	2.15	0.46
14:L:101:ASP:C	14:L:103:ALA:H	2.19	0.46
16:N:89:GLY:O	16:N:92:ALA:HB3	2.15	0.46
18:P:59:ARG:HH22	18:P:66:GLN:HE22	1.62	0.46
20:R:132:ARG:CZ	39:R:9492:HOH:O	2.63	0.46
20:R:114:VAL:HA	20:R:144:GLU:O	2.15	0.46
20:R:61:GLN:NE2	39:R:9449:HOH:O	2.48	0.46
23:U:17:THR:CG2	23:U:18:GLY:H	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:45:GLU:HG3	39:X:6178:HOH:O	2.14	0.46
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.50	0.46
1:0:1067:A:H5'	39:0:4933:HOH:O	2.15	0.46
1:0:2769:C:H2'	1:0:2770:G:H5'	1.96	0.46
1:0:794:U:H3	1:0:819:A:H61	1.62	0.46
30:2:36:ASN:HB3	30:2:39:ARG:NE	2.30	0.46
5:B:41:PHE:HA	5:B:79:MET:HE2	1.97	0.46
11:H:38:LYS:HE2	11:H:42:ASP:HB2	1.97	0.46
2:9:3051:A:H5'	16:N:160:SER:HB2	1.96	0.46
20:R:69:LYS:HB2	20:R:72:VAL:HG23	1.97	0.46
20:R:84:ALA:O	20:R:88:PHE:HD1	1.98	0.46
24:V:56:ILE:HG22	24:V:60:GLN:NE2	2.31	0.46
1:0:1669:A:H2'	1:0:1670:G:C8	2.51	0.46
1:0:2338:G:H2'	7:D:129:ASP:OD1	2.16	0.46
1:0:259:G:H21	15:M:58:GLN:NE2	2.14	0.46
1:0:2712:G:H5'	39:K:4183:HOH:O	2.16	0.46
1:0:2824:C:H5''	1:0:2825:C:H5'	1.97	0.46
1:0:316:A:N3	1:0:336:G:O2'	2.43	0.46
1:0:497:A:H2'	1:0:498:A:C5'	2.45	0.46
4:A:203:GLY:HA2	39:A:9534:HOH:O	2.14	0.46
4:A:34:ASP:OD1	4:A:35:GLY:N	2.49	0.46
5:B:36:PRO:HA	5:B:167:GLY:O	2.16	0.46
6:C:5:ILE:HG13	6:C:15:GLU:HA	1.97	0.46
8:E:81:GLU:HG2	8:E:134:SER:HB2	1.97	0.46
14:L:145:LEU:C	14:L:145:LEU:HD23	2.35	0.46
22:T:20:HIS:HB3	22:T:41:ARG:HD2	1.96	0.46
24:V:42:ASN:O	24:V:44:GLY:N	2.48	0.46
1:0:1940:C:H4'	39:0:7839:HOH:O	2.15	0.46
1:0:2591:C:H2'	1:0:2592:G:O4'	2.15	0.46
1:0:2676:C:H6	1:0:2676:C:H5''	1.81	0.46
1:0:2779:G:H21	8:E:143:GLN:NE2	2.13	0.46
1:0:2831:C:O3'	20:R:71:LYS:HE2	2.16	0.46
1:0:2852:A:H5''	39:0:5799:HOH:O	2.15	0.46
1:0:2906:A:H5'	1:0:2907:C:O4'	2.15	0.46
1:0:368:C:H2'	1:0:369:G:H5'	1.97	0.46
1:0:952:G:N3	1:0:2302:A:H2'	2.31	0.46
2:9:3057:A:O2'	7:D:152:PRO:HD2	2.15	0.46
7:D:21:VAL:HG23	7:D:80:ALA:HB1	1.97	0.46
7:D:96:SER:C	7:D:98:PHE:H	2.18	0.46
9:F:65:GLU:O	9:F:69:GLU:HG2	2.16	0.46
11:H:47:ILE:HD12	11:H:146:VAL:CG1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:43:VAL:CG1	16:N:118:ILE:HD11	2.46	0.46
39:9:4707:HOH:O	16:N:147:ILE:HD12	2.15	0.46
16:N:87:LEU:HD21	16:N:91:ARG:NH2	2.30	0.46
20:R:122:GLN:HB3	20:R:138:SER:HB2	1.95	0.46
1:0:1666:C:C2'	1:0:1667:A:C5'	2.94	0.46
1:0:1748:U:H4'	39:0:8016:HOH:O	2.15	0.46
1:0:2346:C:O5'	1:0:2346:C:H6	1.98	0.46
1:0:2401:A:H2'	1:0:2402:A:C8	2.51	0.46
2:9:3054:A:O2'	2:9:3055:U:H5'	2.15	0.46
5:B:175:LEU:O	5:B:175:LEU:HD23	2.16	0.46
7:D:27:ILE:HG22	7:D:28:GLY:N	2.29	0.46
12:J:92:GLN:HB3	39:J:1405:HOH:O	2.15	0.46
21:S:2:TRP:CH2	21:S:31:ARG:HB2	2.51	0.46
23:U:17:THR:HG22	23:U:18:GLY:H	1.79	0.46
39:0:3175:HOH:O	25:W:119:HIS:HE1	1.98	0.46
1:0:1007:A:H2'	11:H:19:TYR:CZ	2.51	0.46
39:0:7645:HOH:O	29:1:1:THR:HB	2.15	0.46
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.51	0.46
30:2:22:PRO:HG2	30:2:25:VAL:HG21	1.97	0.46
5:B:307:ARG:CG	5:B:307:ARG:HH11	2.21	0.46
5:B:41:PHE:HA	5:B:79:MET:CE	2.45	0.46
9:F:12:LEU:CD2	9:F:111:ILE:HG23	2.46	0.46
12:J:76:ASP:HA	39:J:5907:HOH:O	2.14	0.46
23:U:49:LEU:HG	39:U:3805:HOH:O	2.15	0.46
27:Y:212:ARG:HD2	39:Y:9399:HOH:O	2.15	0.46
1:0:1120:U:H5''	1:0:1120:U:C6	2.51	0.46
1:0:137:U:H2'	1:0:139:C:C5	2.51	0.46
1:0:2320:U:H4'	1:0:2321:A:O4'	2.15	0.46
4:A:123:GLY:HA3	4:A:162:GLY:HA2	1.98	0.46
9:F:39:SER:HB3	9:F:45:ALA:HB2	1.97	0.46
1:0:1185:U:OP1	32:I:126:LYS:HD3	2.15	0.46
13:K:7:ASP:OD2	13:K:81:ARG:NH2	2.48	0.46
14:L:134:GLU:HG3	39:L:9454:HOH:O	2.15	0.46
39:0:7912:HOH:O	22:T:9:LYS:HG3	2.14	0.46
1:0:1667:A:H2'	1:0:1668:U:C6	2.51	0.46
1:0:2453:G:H5''	39:L:9437:HOH:O	2.15	0.46
1:0:424:C:H2'	1:0:425:U:C6	2.50	0.46
4:A:126:ALA:HB1	4:A:138:VAL:CG1	2.46	0.46
5:B:51:VAL:HG21	5:B:327:VAL:HG13	1.97	0.46
7:D:154:LYS:HD2	7:D:154:LYS:N	2.31	0.46
11:H:119:LYS:HB2	11:H:119:LYS:HE3	1.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:43:TYR:HA	11:H:44:PRO:HD3	1.78	0.46
1:0:1168:C:H5''	32:I:87:THR:HG23	1.98	0.46
8:E:35:TYR:HA	12:J:127:ILE:CD1	2.46	0.46
1:0:2515:C:H2'	1:0:2516:G:O4'	2.15	0.46
1:0:432:G:O2'	1:0:433:C:H5'	2.16	0.46
1:0:999:C:H2'	1:0:1000:C:O4'	2.16	0.46
1:0:470:U:O2'	29:1:16:HIS:CD2	2.65	0.46
30:2:49:GLU:HB2	39:2:131:HOH:O	2.15	0.46
31:3:65:THR:HG23	31:3:67:LEU:HG	1.98	0.46
4:A:105:VAL:HG13	4:A:155:THR:O	2.15	0.46
5:B:97:LEU:O	5:B:98:THR:HG23	2.16	0.46
6:C:78:ARG:CG	6:C:78:ARG:NH1	2.75	0.46
7:D:95:THR:OG1	7:D:174:VAL:HG22	2.16	0.46
32:I:75:THR:CA	32:I:112:LYS:HZ3	2.28	0.46
15:M:47:ASP:CG	15:M:48:LYS:N	2.70	0.46
16:N:132:ASN:O	16:N:135:VAL:HG12	2.15	0.46
16:N:74:PRO:HG2	16:N:159:TYR:CE1	2.51	0.46
22:T:47:THR:HB	22:T:100:ASP:HB3	1.97	0.46
25:W:139:GLY:O	25:W:141:HIS:CD2	2.68	0.46
27:Y:108:ASP:N	27:Y:108:ASP:OD1	2.49	0.46
1:0:2329:C:O2'	1:0:2330:U:H5'	2.16	0.45
1:0:2635:A:C2'	1:0:2636:C:H5'	2.46	0.45
1:0:2649:A:H5'	1:0:2649:A:H8	1.81	0.45
1:0:588:G:O6	25:W:154:ARG:NH1	2.50	0.45
2:9:3049:G:H2'	2:9:3050:G:O4'	2.17	0.45
4:A:33:GLU:OE1	4:A:33:GLU:N	2.31	0.45
7:D:167:GLU:C	7:D:169:THR:H	2.20	0.45
11:H:69:ALA:HB2	11:H:153:ALA:HB2	1.98	0.45
15:M:43:PRO:HG3	15:M:62:VAL:HG21	1.97	0.45
1:0:1306:U:OP1	6:C:184:ARG:HD2	2.17	0.45
1:0:1342:C:O2'	1:0:1343:C:H5'	2.16	0.45
1:0:256:C:H2'	1:0:257:G:O4'	2.16	0.45
1:0:2612:A:H4'	39:0:4284:HOH:O	2.15	0.45
1:0:263:U:O4'	9:F:59:ILE:HD13	2.16	0.45
1:0:834:G:H3'	1:0:835:U:H4'	1.99	0.45
5:B:36:PRO:HB3	5:B:174:ARG:CB	2.47	0.45
9:F:70:LYS:C	9:F:72:VAL:H	2.20	0.45
14:L:120:LEU:HD12	14:L:133:VAL:HG21	1.98	0.45
15:M:72:ALA:HB2	15:M:93:ARG:HG2	1.98	0.45
15:M:74:LYS:HG2	15:M:75:ARG:N	2.30	0.45
23:U:11:THR:HG22	23:U:53:ASP:OD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:48:VAL:CG1	25:W:48:VAL:O	2.64	0.45
25:W:85:ALA:HB2	25:W:91:ASP:O	2.16	0.45
25:W:88:THR:CG2	25:W:90:TYR:HD1	2.27	0.45
27:Y:154:ARG:NH1	27:Y:155:ARG:HG2	2.24	0.45
1:0:1151:G:OP1	10:G:63:ARG:NH1	2.49	0.45
1:0:120:A:H2'	1:0:120:A:N3	2.32	0.45
1:0:286:U:H2'	1:0:287:C:C6	2.52	0.45
4:A:65:ARG:C	4:A:66:ARG:HG3	2.36	0.45
6:C:19:PRO:HG2	6:C:22:PHE:CD1	2.51	0.45
12:J:47:THR:HG22	12:J:48:GLY:N	2.32	0.45
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.98	0.45
21:S:10:VAL:HG11	24:V:36:ALA:CA	2.45	0.45
1:0:1441:G:O2'	1:0:1442:A:H5'	2.17	0.45
1:0:1751:G:C2'	1:0:1752:G:H5''	2.43	0.45
1:0:426:G:H2'	1:0:427:C:O4'	2.16	0.45
1:0:702:G:O2'	1:0:703:G:H5'	2.17	0.45
4:A:207:GLN:O	4:A:208:HIS:HB3	2.16	0.45
15:M:184:ARG:HG3	15:M:185:PRO:HA	1.99	0.45
20:R:119:VAL:HG12	20:R:119:VAL:O	2.17	0.45
23:U:4:ARG:HH11	23:U:4:ARG:HG2	1.81	0.45
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.49	0.45
1:0:1131:G:H5'	2:9:3091:C:O4'	2.16	0.45
1:0:284:C:H4'	1:0:285:A:H8	1.82	0.45
1:0:288:A:H2'	1:0:289:G:C8	2.50	0.45
1:0:319:A:H4'	1:0:338:C:C5	2.51	0.45
1:0:64:G:H2'	1:0:65:C:O4'	2.17	0.45
39:0:4996:HOH:O	4:A:11:ARG:CZ	2.64	0.45
5:B:146:THR:C	5:B:148:PRO:HD3	2.37	0.45
9:F:60:VAL:HG13	9:F:63:ILE:HG13	1.97	0.45
24:V:39:ALA:O	24:V:41:GLU:N	2.42	0.45
1:0:2415:A:H2'	1:0:2416:G:H5'	1.98	0.45
1:0:338:C:H4'	6:C:174:ILE:HD12	1.98	0.45
1:0:363:A:H1'	39:0:5847:HOH:O	2.15	0.45
5:B:41:PHE:CD2	5:B:190:MET:HE3	2.52	0.45
7:D:10:PHE:CG	7:D:11:HIS:N	2.84	0.45
9:F:99:THR:HG23	9:F:99:THR:O	2.17	0.45
11:H:40:ALA:HB1	11:H:137:TYR:CD2	2.52	0.45
13:K:98:VAL:CG2	13:K:102:GLU:C	2.85	0.45
15:M:114:VAL:O	15:M:158:ARG:HD3	2.17	0.45
16:N:64:SER:C	16:N:66:LEU:H	2.20	0.45
26:X:76:ARG:NH1	26:X:76:ARG:HG3	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1167:G:H2'	1:0:1168:C:O4'	2.16	0.45
1:0:1203:G:O2'	1:0:1204:C:H5'	2.17	0.45
1:0:1252:A:H2'	1:0:1253:C:O4'	2.16	0.45
1:0:2019:A:H5'	39:0:5123:HOH:O	2.16	0.45
1:0:2402:A:O2'	1:0:2403:C:H5'	2.17	0.45
29:1:25:LYS:HD2	30:2:48:ASP:CA	2.46	0.45
7:D:170:TYR:CD1	7:D:170:TYR:N	2.85	0.45
32:I:101:SER:OG	32:I:104:GLN:HG3	2.16	0.45
12:J:75:PRO:HD3	12:J:136:SER:OG	2.16	0.45
24:V:12:THR:OG1	24:V:13:PRO:HD2	2.16	0.45
28:Z:42:CYS:SG	28:Z:59:TYR:HD2	2.40	0.45
1:0:432:G:H2'	1:0:433:C:H6	1.82	0.45
1:0:506:G:N2	1:0:509:A:H5''	2.21	0.45
4:A:101:GLU:HB3	4:A:129:LEU:O	2.15	0.45
7:D:10:PHE:CD1	7:D:11:HIS:N	2.85	0.45
8:E:101:GLU:OE2	8:E:115:ARG:HD3	2.17	0.45
14:L:67:ARG:HG2	14:L:67:ARG:HH11	1.81	0.45
25:W:125:HIS:HE1	39:W:3071:HOH:O	1.99	0.45
25:W:78:ASP:OD2	25:W:79:VAL:N	2.50	0.45
27:Y:144:ARG:NH1	39:Y:9374:HOH:O	2.50	0.45
1:0:1484:G:H2'	39:0:9723:HOH:O	2.16	0.45
1:0:1592:G:O2'	1:0:1593:C:O4'	2.32	0.45
1:0:2072:G:C6	1:0:2533:C:H1'	2.52	0.45
1:0:1734:C:OP1	5:B:234:ARG:NH1	2.50	0.45
6:C:150:THR:HA	6:C:203:ALA:O	2.17	0.45
7:D:82:GLU:HA	7:D:85:GLN:NE2	2.32	0.45
14:L:143:THR:CG2	14:L:144:ASP:N	2.80	0.45
16:N:83:LEU:HD13	16:N:175:LEU:CD2	2.41	0.45
1:0:1086:A:C6	25:W:11:VAL:HG11	2.52	0.45
1:0:1724:U:H5''	39:0:4333:HOH:O	2.16	0.45
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.16	0.45
1:0:2102:G:H5''	1:0:2538:A:C2	2.51	0.45
1:0:2724:U:H2'	1:0:2725:G:O4'	2.17	0.45
1:0:2883:A:H2'	1:0:2884:G:O4'	2.17	0.45
1:0:542:A:H2'	1:0:543:G:O4'	2.17	0.45
39:0:4690:HOH:O	5:B:216:LYS:HE2	2.16	0.45
24:V:56:ILE:HG22	24:V:60:GLN:HE21	1.80	0.45
25:W:11:VAL:O	25:W:12:ASN:HB2	2.17	0.45
25:W:65:VAL:HG12	25:W:116:LEU:HD13	1.98	0.45
1:0:1175:G:H2'	1:0:1176:C:O4'	2.17	0.44
1:0:1527:A:H1'	1:0:1528:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2541:U:H1'	3:4:76:PPU:O2'	2.17	0.44
1:0:362:G:H2'	1:0:363:A:C8	2.52	0.44
1:0:366:U:H2'	1:0:367:G:O4'	2.17	0.44
1:0:407:A:H8	39:0:5045:HOH:O	2.00	0.44
2:9:3028:U:H2'	2:9:3029:C:C6	2.52	0.44
2:9:3044:A:O4'	7:D:76:ARG:NE	2.50	0.44
39:0:9836:HOH:O	4:A:11:ARG:HD3	2.17	0.44
4:A:57:ALA:HB1	4:A:65:ARG:HE	1.82	0.44
6:C:72:LYS:HG2	6:C:77:ALA:HA	1.99	0.44
9:F:14:ASP:O	9:F:18:GLU:HG3	2.17	0.44
25:W:13:MET:HE1	25:W:18:GLN:CA	2.41	0.44
25:W:19:ASP:O	25:W:23:MET:HG3	2.17	0.44
1:0:1189:A:H1'	1:0:1209:C:H1'	1.99	0.44
1:0:1380:U:O4	1:0:2043:U:H4'	2.17	0.44
1:0:220:C:H1'	39:0:6313:HOH:O	2.17	0.44
30:2:48:ASP:O	30:2:49:GLU:CB	2.65	0.44
5:B:321:PRO:HA	39:B:9653:HOH:O	2.17	0.44
7:D:25:MET:HE1	7:D:37:ALA:O	2.17	0.44
10:G:19:GLU:HG2	10:G:66:LEU:CD1	2.47	0.44
16:N:86:LEU:HD21	16:N:180:LEU:HD12	1.99	0.44
39:9:3472:HOH:O	16:N:41:LYS:HD3	2.16	0.44
1:0:317:A:OP1	22:T:52:ARG:O	2.35	0.44
22:T:64:ASN:HB3	22:T:73:HIS:HB2	1.98	0.44
28:Z:32:GLU:HA	28:Z:35:GLU:HG3	1.99	0.44
1:0:2243:C:H5''	39:0:4351:HOH:O	2.18	0.44
1:0:2894:C:O2'	1:0:2895:C:H5'	2.17	0.44
4:A:56:ALA:O	4:A:68:ILE:HG22	2.17	0.44
4:A:70:ALA:HA	4:A:71:PRO:HD3	1.81	0.44
5:B:321:PRO:HG3	39:B:9599:HOH:O	2.17	0.44
7:D:78:GLU:O	7:D:82:GLU:HG3	2.18	0.44
13:K:49:LEU:HD22	13:K:117:VAL:HG21	2.00	0.44
14:L:143:THR:O	14:L:147:GLU:HG3	2.18	0.44
20:R:113:HIS:HE1	20:R:144:GLU:OE1	1.99	0.44
26:X:37:LEU:HD11	26:X:85:VAL:HG11	1.99	0.44
26:X:30:MET:CE	26:X:58:ALA:HB3	2.43	0.44
26:X:74:ALA:CB	26:X:85:VAL:HG13	2.25	0.44
1:0:1202:A:H2'	1:0:1203:G:O4'	2.18	0.44
39:M:9334:HOH:O	31:3:46:ILE:HB	2.17	0.44
39:0:9728:HOH:O	5:B:229:ARG:HD2	2.16	0.44
5:B:243:ASN:HA	5:B:244:PRO:C	2.37	0.44
12:J:74:ARG:HH12	12:J:76:ASP:CB	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:125:PHE:CE1	14:L:140:VAL:HG13	2.53	0.44
15:M:49:ALA:C	15:M:54:TYR:HB3	2.38	0.44
16:N:171:HIS:CE1	39:N:9363:HOH:O	2.70	0.44
24:V:8:ILE:CG2	24:V:59:ILE:HG13	2.46	0.44
1:0:806:A:H2'	1:0:807:A:O4'	2.17	0.44
1:0:870:G:C3'	1:0:871:G:H5''	2.48	0.44
7:D:51:ARG:HH11	7:D:68:PRO:HB3	1.83	0.44
10:G:27:ILE:HD13	10:G:71:LEU:HD23	1.98	0.44
18:P:97:ARG:HD2	39:P:159:HOH:O	2.17	0.44
23:U:52:THR:HG22	23:U:54:THR:H	1.80	0.44
26:X:20:GLU:HG3	26:X:21:PRO:CD	2.48	0.44
28:Z:10:ARG:HA	39:Z:9214:HOH:O	2.16	0.44
28:Z:11:SER:O	28:Z:14:PHE:HB2	2.17	0.44
1:0:1200:A:H3'	39:0:6312:HOH:O	2.18	0.44
1:0:1902:G:H2'	1:0:1903:U:O4'	2.17	0.44
1:0:2649:A:C8	1:0:2649:A:H5'	2.53	0.44
1:0:664:U:O4	1:0:681:G:H5''	2.18	0.44
6:C:233:THR:HG22	6:C:234:VAL:N	2.32	0.44
8:E:15:GLN:NE2	8:E:40:VAL:O	2.51	0.44
9:F:60:VAL:HG13	9:F:63:ILE:CG1	2.48	0.44
32:I:105:VAL:HG11	32:I:129:VAL:HG22	1.99	0.44
1:0:1180:U:O2'	32:I:92:PRO:HD2	2.18	0.44
32:I:85:PHE:CD1	32:I:98:ALA:HB2	2.53	0.44
17:O:78:ALA:C	17:O:98:LEU:HD13	2.38	0.44
23:U:44:ARG:HB3	39:U:3805:HOH:O	2.17	0.44
1:0:1878:G:O2'	1:0:1879:U:P	2.75	0.44
1:0:2104:C:O2	1:0:2485:A:N1	2.50	0.44
1:0:2663:U:O2	39:0:8491:HOH:O	2.21	0.44
1:0:308:U:C4	1:0:342:C:H1'	2.53	0.44
1:0:398:U:H2'	1:0:399:C:C6	2.53	0.44
4:A:96:LEU:O	4:A:131:HIS:HE1	2.00	0.44
7:D:154:LYS:HD2	7:D:154:LYS:H	1.83	0.44
8:E:7:ILE:HA	8:E:8:PRO:HD3	1.92	0.44
32:I:113:HIS:HE1	32:I:121:LEU:HD22	1.83	0.44
12:J:42:GLU:O	12:J:131:THR:HG23	2.18	0.44
1:0:56:G:C5'	24:V:50:ARG:HH12	2.30	0.44
25:W:108:ARG:HG3	25:W:114:PRO:HG3	1.99	0.44
1:0:1295:G:H4'	39:L:9490:HOH:O	2.18	0.44
1:0:475:G:H5'	6:C:73:LEU:CD2	2.48	0.44
1:0:968:G:O2'	1:0:969:G:H5'	2.17	0.44
2:9:3052:A:H2'	2:9:3053:G:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:36:ASP:O	4:A:36:ASP:CG	2.55	0.44
1:0:2549:C:H1'	5:B:248:ARG:NH2	2.33	0.44
18:P:13:VAL:HG21	18:P:41:ARG:HG2	2.00	0.44
23:U:14:GLU:OE1	23:U:15:PRO:HD2	2.17	0.44
25:W:149:LEU:HG	25:W:153:MET:HE2	1.99	0.44
1:0:1201:C:C2'	1:0:1202:A:H5'	2.42	0.44
1:0:125:U:H2'	39:0:4367:HOH:O	2.18	0.44
6:C:27:ARG:HG2	6:C:30:LEU:HG	1.98	0.44
7:D:167:GLU:OE2	7:D:173:GLU:HG2	2.18	0.44
11:H:67:LEU:O	11:H:71:ARG:HB2	2.18	0.44
15:M:69:LYS:HG2	15:M:127:LYS:HG3	2.00	0.44
21:S:33:SER:OG	21:S:36:GLU:HG3	2.18	0.44
1:0:1163:G:H2'	1:0:1164:U:C5	2.53	0.43
1:0:1741:U:H3'	39:0:3379:HOH:O	2.18	0.43
1:0:2044:G:OP1	26:X:23:HIS:HE1	2.01	0.43
1:0:710:G:H5'	17:O:25:VAL:HG13	1.99	0.43
4:A:36:ASP:C	4:A:38:ILE:H	2.21	0.43
5:B:238:ASN:ND2	5:B:240:GLY:H	2.03	0.43
5:B:23:THR:HA	5:B:24:PRO:HD3	1.87	0.43
6:C:115:LEU:O	6:C:118:THR:HB	2.18	0.43
6:C:127:ARG:CZ	6:C:225:PRO:HG2	2.46	0.43
11:H:54:THR:O	11:H:55:VAL:HG13	2.17	0.43
14:L:80:ASP:HB2	14:L:90:ARG:HB3	2.00	0.43
7:D:146:LYS:HZ3	16:N:107:ASN:HD21	1.66	0.43
16:N:154:LEU:HD11	16:N:157:PRO:HA	2.00	0.43
1:0:1299:G:N2	39:0:5261:HOH:O	2.51	0.43
1:0:1314:U:H2'	39:0:6429:HOH:O	2.17	0.43
1:0:1406:A:H4'	1:0:1407:A:C5'	2.48	0.43
5:B:85:ARG:HB2	5:B:99:GLU:HG2	1.99	0.43
7:D:94:ALA:HA	7:D:174:VAL:O	2.17	0.43
20:R:114:VAL:HG13	20:R:114:VAL:O	2.18	0.43
1:0:2435:U:H1'	39:0:5996:HOH:O	2.18	0.43
1:0:603:A:H5''	1:0:604:G:OP1	2.17	0.43
4:A:217:ARG:CG	4:A:217:ARG:HH11	2.32	0.43
5:B:115:VAL:HA	5:B:116:PRO:HD3	1.92	0.43
5:B:16:ARG:NE	39:B:9556:HOH:O	2.39	0.43
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.47	0.43
11:H:154:TYR:HA	11:H:157:ILE:HG12	2.00	0.43
1:0:1817:U:O2	18:P:81:LYS:NZ	2.47	0.43
1:0:1878:G:H5''	39:0:3406:HOH:O	2.18	0.43
1:0:1966:U:H2'	1:0:1967:U:H2'	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2090:G:H2'	1:0:2091:G:C8	2.53	0.43
2:9:3014:G:H2'	2:9:3015:C:H5'	2.00	0.43
2:9:3058:G:H1'	39:9:3839:HOH:O	2.17	0.43
4:A:179:MET:HG2	4:A:186:TRP:HB2	1.99	0.43
4:A:223:ARG:CZ	39:A:9560:HOH:O	2.66	0.43
1:0:1654:U:H2'	4:A:47:HIS:CD2	2.54	0.43
7:D:128:LEU:C	7:D:128:LEU:HD23	2.39	0.43
7:D:88:LEU:N	7:D:89:PRO:CD	2.80	0.43
18:P:121:ASP:OD1	18:P:125:LYS:HE3	2.17	0.43
18:P:143:ALA:HB2	39:P:186:HOH:O	2.18	0.43
20:R:39:THR:HB	20:R:42:GLU:CG	2.47	0.43
1:0:1250:C:O2'	1:0:1251:C:H5'	2.19	0.43
1:0:1473:U:O2'	1:0:1474:C:H5''	2.19	0.43
1:0:2506:A:O2'	1:0:2507:G:O5'	2.37	0.43
39:K:1387:HOH:O	23:U:20:MET:HE3	2.19	0.43
24:V:16:ARG:NH2	24:V:63:GLU:HG3	2.33	0.43
1:0:1291:A:H2	39:0:5858:HOH:O	2.01	0.43
1:0:1603:A:H5'	1:0:1605:G:C4'	2.48	0.43
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.99	0.43
2:9:3039:U:HO2'	2:9:3042:C:H5	1.61	0.43
4:A:53:ALA:HB3	39:A:9594:HOH:O	2.17	0.43
5:B:277:GLU:N	5:B:278:PRO:HD2	2.33	0.43
11:H:47:ILE:HD12	11:H:146:VAL:HG13	2.00	0.43
11:H:169:GLY:C	11:H:170:ASN:HD22	2.21	0.43
13:K:113:ILE:HD12	13:K:128:ALA:HB2	1.99	0.43
1:0:1119:G:C8	12:J:52:GLN:NE2	2.87	0.43
1:0:1470:A:OP1	15:M:93:ARG:HD2	2.17	0.43
1:0:2252:A:C5	1:0:2253:G:H1'	2.53	0.43
1:0:2300:A:H4'	1:0:2301:A:O5'	2.19	0.43
4:A:82:VAL:HG13	4:A:93:THR:HB	1.99	0.43
5:B:132:HIS:CE1	5:B:171:VAL:HG21	2.54	0.43
6:C:157:LEU:HD22	6:C:162:VAL:CG1	2.49	0.43
6:C:246:ARG:NE	39:C:9228:HOH:O	2.43	0.43
7:D:173:GLU:O	7:D:174:VAL:C	2.57	0.43
8:E:84:MET:HE3	8:E:131:LEU:HD13	2.00	0.43
11:H:146:VAL:HG22	39:H:9543:HOH:O	2.18	0.43
14:L:144:ASP:HA	14:L:147:GLU:OE1	2.19	0.43
1:0:2453:G:H4'	14:L:50:GLY:C	2.38	0.43
1:0:793:A:H5''	18:P:83:LYS:HG2	2.01	0.43
21:S:8:PRO:HD2	24:V:32:ALA:HA	2.00	0.43
25:W:54:PHE:CZ	25:W:140:LYS:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1131:G:C6	1:0:1230:A:C4	3.06	0.43
5:B:71:VAL:HG11	5:B:296:LEU:HD22	2.00	0.43
9:F:26:THR:HG21	9:F:102:GLY:C	2.39	0.43
12:J:90:LYS:HB2	36:J:9302:CL:CL	2.55	0.43
13:K:22:ASP:O	13:K:110:LYS:HE3	2.18	0.43
17:O:73:ASP:HA	17:O:92:VAL:O	2.19	0.43
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.18	0.43
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.59	0.43
1:0:123:U:O2'	1:0:124:C:H5'	2.18	0.43
1:0:1594:C:O2'	1:0:1607:A:H4'	2.18	0.43
1:0:2256:G:C2'	1:0:2257:G:H5'	2.49	0.43
1:0:2791:U:H1'	1:0:2792:A:H5''	2.01	0.43
1:0:391:U:OP2	15:M:84:LYS:NZ	2.48	0.43
1:0:447:A:O2'	1:0:448:G:H5'	2.19	0.43
1:0:810:G:H1'	39:0:7750:HOH:O	2.19	0.43
1:0:920:C:H5''	1:0:921:G:O5'	2.19	0.43
2:9:3031:C:H2'	2:9:3032:G:O4'	2.19	0.43
7:D:99:ASP:HB3	7:D:103:ASN:H	1.83	0.43
7:D:57:THR:HA	39:D:5728:HOH:O	2.19	0.43
8:E:8:PRO:HB2	8:E:11:VAL:HG23	2.01	0.43
12:J:39:VAL:CG1	12:J:40:ASN:N	2.82	0.43
14:L:6:ARG:NH2	39:L:9444:HOH:O	2.51	0.43
15:M:58:GLN:HG3	39:M:9404:HOH:O	2.18	0.43
20:R:104:PHE:CB	20:R:109:MET:HE1	2.49	0.43
22:T:71:VAL:HG12	22:T:72:ILE:H	1.79	0.43
28:Z:56:GLN:HA	28:Z:62:TYR:O	2.19	0.43
1:0:2016:U:H2'	1:0:2017:U:O4'	2.19	0.43
1:0:2540:G:O2'	1:0:2541:U:H5''	2.19	0.43
30:2:20:ARG:HG3	30:2:21:VAL:N	2.34	0.43
4:A:33:GLU:O	4:A:34:ASP:HB2	2.18	0.43
6:C:200:PRO:HB3	6:C:212:VAL:HG23	2.01	0.43
6:C:46:TYR:CE1	6:C:92:PRO:HB3	2.54	0.43
7:D:60:GLU:O	7:D:60:GLU:HG3	2.19	0.43
7:D:18:ILE:HD13	7:D:84:LEU:CD1	2.49	0.43
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.33	0.43
32:I:101:SER:H	32:I:104:GLN:NE2	2.17	0.43
15:M:77:HIS:HD2	15:M:79:ALA:O	2.01	0.43
16:N:167:ASP:C	16:N:168:LEU:HG	2.39	0.43
16:N:36:ALA:N	39:N:9333:HOH:O	2.52	0.43
17:O:26:TRP:HB2	39:O:3062:HOH:O	2.19	0.43
18:P:13:VAL:HG11	18:P:40:VAL:CG1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:949:U:C4'	19:Q:95:GLU:HA	2.46	0.43
20:R:18:LEU:HG	20:R:91:LEU:HD13	2.01	0.43
1:0:1878:G:H4'	39:0:4709:HOH:O	2.19	0.42
1:0:2645:U:OP2	1:0:2645:U:H6	2.02	0.42
1:0:2831:C:H2'	1:0:2832:C:H5'	2.00	0.42
1:0:360:A:H2'	1:0:361:C:O4'	2.19	0.42
1:0:497:A:H2'	1:0:498:A:H5'	2.01	0.42
29:1:10:LYS:N	39:1:9488:HOH:O	2.49	0.42
5:B:265:LEU:HD21	5:B:316:ARG:HD3	2.01	0.42
1:0:672:G:O6	6:C:213:ALA:HB1	2.19	0.42
6:C:57:PRO:HG2	6:C:73:LEU:HD13	2.01	0.42
7:D:37:ALA:HA	39:D:5583:HOH:O	2.19	0.42
8:E:112:ALA:HA	8:E:113:PRO:HD3	1.89	0.42
9:F:80:GLN:HB3	39:F:2563:HOH:O	2.17	0.42
14:L:92:ASP:HA	14:L:121:ILE:HB	2.00	0.42
15:M:169:ARG:NH1	39:M:9372:HOH:O	2.52	0.42
16:N:119:GLN:O	16:N:123:ILE:HG13	2.18	0.42
18:P:141:ILE:C	18:P:143:ALA:H	2.22	0.42
1:0:195:C:H2'	1:0:196:G:H5'	2.01	0.42
1:0:2256:G:O2'	1:0:2257:G:H5'	2.20	0.42
1:0:2356:A:H2'	1:0:2357:G:O4'	2.18	0.42
1:0:263:U:C2	9:F:59:ILE:CD1	3.02	0.42
31:3:73:GLU:O	31:3:73:GLU:HG2	2.18	0.42
4:A:179:MET:HG2	4:A:186:TRP:HB3	2.01	0.42
5:B:41:PHE:CB	5:B:190:MET:HE3	2.50	0.42
1:0:2310:G:OP2	11:H:115:ALA:HA	2.18	0.42
11:H:151:ARG:HA	11:H:154:TYR:CE2	2.54	0.42
12:J:74:ARG:NH1	12:J:105:LEU:HD11	2.33	0.42
16:N:36:ALA:HB1	16:N:118:ILE:HD12	2.01	0.42
16:N:37:ARG:CZ	39:N:9333:HOH:O	2.67	0.42
1:0:935:G:H4'	17:O:38:ARG:HH12	1.84	0.42
26:X:8:ARG:NH1	39:X:2479:HOH:O	2.51	0.42
27:Y:115:ARG:CZ	39:Y:9353:HOH:O	2.67	0.42
27:Y:107:PRO:HB3	27:Y:182:PHE:CE2	2.54	0.42
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	2.01	0.42
1:0:1701:A:P	39:0:4968:HOH:O	2.77	0.42
1:0:1826:C:O2'	1:0:1827:G:H5'	2.19	0.42
1:0:2715:G:N2	5:B:264:GLU:OE1	2.53	0.42
2:9:3040:C:N4	7:D:53:LYS:HE3	2.34	0.42
1:0:2270:G:C4'	4:A:223:ARG:HH12	2.28	0.42
8:E:18:LEU:HD13	8:E:34:TRP:CG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:63:ILE:CG2	12:J:64:GLY:N	2.82	0.42
13:K:98:VAL:HG22	13:K:102:GLU:C	2.39	0.42
15:M:36:ALA:O	15:M:65:VAL:HA	2.19	0.42
16:N:137:ALA:HB1	16:N:141:ARG:HD3	2.01	0.42
22:T:117:ASP:OD1	22:T:118:SER:N	2.51	0.42
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.90	0.42
1:0:2067:A:H2'	1:0:2068:G:O4'	2.19	0.42
1:0:2241:C:O2'	1:0:2242:U:H5'	2.19	0.42
1:0:2636:C:C3'	1:0:2637:A:C5'	2.96	0.42
1:0:2718:C:H5'	1:0:2718:C:C6	2.51	0.42
1:0:612:U:H2'	1:0:613:C:C6	2.55	0.42
4:A:164:ARG:CZ	39:A:9575:HOH:O	2.67	0.42
4:A:94:LEU:HB2	4:A:95:PRO:HD2	2.00	0.42
5:B:333:GLU:HB2	39:U:3564:HOH:O	2.18	0.42
6:C:236:THR:O	6:C:237:GLU:C	2.57	0.42
9:F:5:ASP:O	9:F:119:ARG:NH1	2.52	0.42
32:I:72:VAL:HG13	32:I:73:PRO:HD2	2.01	0.42
16:N:108:SER:HA	16:N:109:PRO:HD3	1.82	0.42
1:0:1369:A:H4'	20:R:64:SER:OG	2.19	0.42
1:0:2821:C:H4'	5:B:116:PRO:HG3	2.01	0.42
1:0:522:U:O2'	1:0:1366:C:H5'	2.18	0.42
2:9:3052:A:O2'	2:9:3053:G:H5'	2.20	0.42
4:A:201:PHE:HB3	39:A:9621:HOH:O	2.19	0.42
6:C:1:MET:HG2	6:C:2:GLN:HE21	1.84	0.42
39:0:5543:HOH:O	11:H:58:ARG:HG3	2.18	0.42
12:J:47:THR:CG2	12:J:48:GLY:N	2.83	0.42
21:S:29:ASP:OD2	21:S:31:ARG:NH1	2.51	0.42
26:X:20:GLU:HG3	26:X:21:PRO:HD2	2.00	0.42
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.55	0.42
1:0:130:C:H2'	39:0:3769:HOH:O	2.18	0.42
1:0:2324:G:N2	1:0:2377:U:H1'	2.34	0.42
1:0:2704:C:H2'	1:0:2705:U:O4'	2.20	0.42
1:0:1705:C:O2	1:0:2735:U:H5''	2.20	0.42
1:0:2838:A:H2'	1:0:2839:C:C6	2.55	0.42
1:0:424:C:H2'	1:0:425:U:H6	1.84	0.42
2:9:3024:U:H3'	2:9:3025:G:C5'	2.50	0.42
5:B:69:VAL:HA	5:B:70:PRO:HD3	1.86	0.42
6:C:124:VAL:HA	6:C:230:GLY:O	2.18	0.42
32:I:76:ALA:O	32:I:80:LYS:HG3	2.20	0.42
39:0:9737:HOH:O	15:M:82:ARG:HD2	2.19	0.42
26:X:73:ARG:HH12	26:X:88:GLU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:115:ARG:HH11	27:Y:115:ARG:CB	2.29	0.42
1:0:1298:U:H2'	1:0:1299:G:C8	2.53	0.42
1:0:1603:A:H5''	1:0:1604:G:H3'	2.01	0.42
1:0:1759:A:N3	1:0:1818:C:H2'	2.35	0.42
1:0:185:G:C4'	1:0:186:A:H4'	2.49	0.42
1:0:1878:G:O2'	1:0:1879:U:C6	2.70	0.42
1:0:2880:A:H2'	1:0:2881:C:H5'	2.02	0.42
6:C:194:PHE:CD2	6:C:234:VAL:CG1	3.01	0.42
7:D:18:ILE:HG12	7:D:134:LEU:CD2	2.49	0.42
11:H:76:GLU:C	11:H:77:LEU:HD23	2.40	0.42
14:L:61:ALA:HB2	14:L:105:TYR:CZ	2.54	0.42
17:O:14:LEU:HG	17:O:102:ILE:HD11	2.01	0.42
25:W:110:GLN:NE2	25:W:110:GLN:CA	2.82	0.42
26:X:23:HIS:CD2	26:X:24:LYS:HG3	2.55	0.42
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	2.02	0.42
27:Y:163:THR:HB	39:Y:9398:HOH:O	2.20	0.42
1:0:1419:U:H2'	1:0:1685:A:C2	2.54	0.42
1:0:2676:C:H4'	12:J:70:PHE:HD1	1.78	0.42
1:0:1654:U:H2'	4:A:47:HIS:HD2	1.83	0.42
5:B:87:TYR:OH	5:B:163:GLU:OE2	2.30	0.42
5:B:24:PRO:HG3	5:B:204:GLY:HA2	2.00	0.42
6:C:194:PHE:HA	6:C:234:VAL:HG13	2.02	0.42
7:D:18:ILE:HD13	7:D:84:LEU:HD12	2.01	0.42
1:0:1992:U:OP2	13:K:66:ARG:HD2	2.19	0.42
14:L:94:ARG:NH1	14:L:143:THR:HG21	2.35	0.42
19:Q:33:PHE:HE2	19:Q:93:ARG:HG3	1.85	0.42
1:0:1244:U:C6	12:J:47:THR:HG22	2.54	0.42
1:0:1287:A:O4'	25:W:117:ARG:HD3	2.20	0.42
1:0:912:A:C4	1:0:1294:A:C2	3.06	0.42
1:0:1909:A:N1	1:0:2128:G:H1'	2.35	0.42
1:0:2568:A:H2'	1:0:2569:A:O4'	2.19	0.42
2:9:3005:G:OP1	16:N:17:ARG:NH2	2.52	0.42
4:A:36:ASP:OD2	4:A:85:SER:HB2	2.20	0.42
5:B:84:LEU:HD13	5:B:84:LEU:O	2.19	0.42
6:C:123:LEU:HA	6:C:123:LEU:HD23	1.92	0.42
9:F:20:LEU:O	9:F:23:ALA:HB3	2.20	0.42
11:H:144:GLU:HG2	39:H:9535:HOH:O	2.19	0.42
11:H:66:ARG:HD3	39:H:9546:HOH:O	2.20	0.42
32:I:80:LYS:HD3	32:I:86:GLU:O	2.19	0.42
1:0:1980:U:O2	1:0:2008:U:H4'	2.20	0.42
1:0:2508:C:H2'	39:0:7270:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2635:A:HO2'	1:0:2636:C:H5'	1.84	0.42
1:0:2697:A:H2'	1:0:2698:G:O4'	2.20	0.42
1:0:308:U:H5'	22:T:97:ARG:HH21	1.85	0.42
30:2:10:ARG:HH11	30:2:49:GLU:CD	2.23	0.42
2:9:3003:A:OP2	2:9:3025:G:N2	2.52	0.42
5:B:301:VAL:HG11	5:B:309:VAL:HG11	2.02	0.42
7:D:60:GLU:O	7:D:61:PHE:C	2.57	0.42
9:F:28:ALA:CB	9:F:99:THR:HG23	2.49	0.42
10:G:23:ILE:O	10:G:27:ILE:HG13	2.20	0.42
11:H:28:ILE:HA	11:H:63:GLU:OE1	2.19	0.42
11:H:77:LEU:HD12	11:H:83:TYR:CD2	2.55	0.42
16:N:152:GLU:HA	16:N:152:GLU:OE1	2.20	0.42
25:W:41:TYR:HA	25:W:44:MET:HE3	2.02	0.42
1:0:1149:U:H5''	1:0:1151:G:O4'	2.20	0.41
1:0:1476:A:O2'	1:0:1477:C:H5'	2.20	0.41
1:0:1768:C:H2'	1:0:1769:C:O4'	2.19	0.41
1:0:2015:A:H2'	1:0:2016:U:O4'	2.20	0.41
1:0:462:A:H2'	39:0:5457:HOH:O	2.20	0.41
1:0:87:C:C2	30:2:30:ASP:OD2	2.72	0.41
10:G:64:ASN:N	10:G:64:ASN:ND2	2.67	0.41
11:H:45:VAL:HG13	39:H:9525:HOH:O	2.19	0.41
32:I:138:THR:HG22	32:I:139:ILE:H	1.84	0.41
12:J:71:TYR:CG	12:J:72:PRO:HD2	2.55	0.41
16:N:93:GLN:HE21	16:N:127:LEU:HD12	1.84	0.41
1:0:2388:C:H5'	19:Q:83:THR:O	2.20	0.41
20:R:16:ALA:HB1	20:R:94:ASN:HD22	1.85	0.41
27:Y:155:ARG:HH21	27:Y:157:ILE:HD11	1.85	0.41
1:0:2896:A:H5''	39:X:5399:HOH:O	2.21	0.41
1:0:920:C:OP1	14:L:37:LYS:NZ	2.51	0.41
4:A:94:LEU:HG	4:A:99:ILE:HD11	2.02	0.41
6:C:127:ARG:HD3	6:C:129:HIS:CE1	2.53	0.41
6:C:132:ASP:HB2	6:C:161:ASP:HB3	2.02	0.41
11:H:29:ALA:CB	11:H:66:ARG:HH12	2.20	0.41
24:V:29:ASN:O	24:V:33:VAL:HG23	2.20	0.41
26:X:80:GLU:HG2	26:X:80:GLU:O	2.20	0.41
1:0:1878:G:O2'	1:0:1879:U:C5	2.68	0.41
1:0:2256:G:H2'	1:0:2257:G:C5'	2.51	0.41
1:0:2337:G:O3'	7:D:97:GLN:HA	2.20	0.41
1:0:349:U:O2'	1:0:350:C:H5'	2.21	0.41
2:9:3064:C:C2'	2:9:3065:A:H5'	2.49	0.41
4:A:57:ALA:HA	4:A:67:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:166:ILE:HD11	6:C:207:LEU:HD13	2.02	0.41
8:E:102:VAL:HG13	8:E:116:THR:HG23	2.02	0.41
11:H:63:GLU:HA	39:H:9546:HOH:O	2.19	0.41
16:N:49:THR:HG22	16:N:56:ASP:CB	2.50	0.41
21:S:42:GLU:O	21:S:46:ASP:HA	2.21	0.41
22:T:112:LEU:CD2	22:T:119:ALA:HB3	2.50	0.41
1:O:2866:U:C4	23:U:50:GLU:HB3	2.55	0.41
39:O:5855:HOH:O	25:W:119:HIS:CG	2.73	0.41
1:O:2506:A:O2'	1:O:2507:G:P	2.79	0.41
1:O:314:G:N2	1:O:316:A:H3'	2.35	0.41
1:O:583:G:H2'	1:O:584:U:C6	2.56	0.41
1:O:883:U:C2'	1:O:883:U:O2	2.66	0.41
1:O:932:U:H2'	1:O:933:C:C6	2.56	0.41
5:B:217:ARG:CG	5:B:257:THR:HG22	2.48	0.41
1:O:2101:A:H2'	6:C:63:SER:OG	2.20	0.41
9:F:79:GLN:HB2	9:F:82:ASP:OD2	2.20	0.41
12:J:19:MET:HE2	12:J:79:PHE:HA	2.02	0.41
13:K:109:LEU:CD1	13:K:113:ILE:HD11	2.42	0.41
14:L:92:ASP:HB3	14:L:95:ASP:OD2	2.21	0.41
17:O:45:LEU:HD12	17:O:88:LYS:HD2	2.02	0.41
20:R:39:THR:HG22	20:R:41:GLY:N	2.36	0.41
21:S:38:ALA:O	21:S:42:GLU:HG3	2.20	0.41
22:T:78:THR:HB	22:T:87:VAL:O	2.21	0.41
1:O:2265:U:H2'	1:O:2266:A:H8	1.82	0.41
1:O:2503:A:OP1	11:H:151:ARG:NH2	2.46	0.41
1:O:414:C:H5'	39:O:3274:HOH:O	2.20	0.41
1:O:506:G:H22	1:O:509:A:H5'	1.79	0.41
1:O:936:C:OP1	17:O:35:LYS:NZ	2.46	0.41
32:I:135:LEU:HB2	32:I:137:VAL:HG23	2.02	0.41
12:J:39:VAL:HG11	12:J:107:ASN:CB	2.50	0.41
12:J:75:PRO:HB3	12:J:132:LEU:HB3	2.02	0.41
16:N:66:LEU:HG	16:N:175:LEU:HD21	2.02	0.41
1:O:500:G:O2'	20:R:94:ASN:ND2	2.53	0.41
26:X:43:VAL:CG1	26:X:47:ALA:HB3	2.51	0.41
27:Y:107:PRO:HD3	27:Y:182:PHE:CE1	2.56	0.41
1:O:1279:U:O2	1:O:1279:U:H2'	2.20	0.41
1:O:1304:U:H2'	1:O:1305:C:C6	2.56	0.41
1:O:177:A:H2'	1:O:178:U:O4'	2.20	0.41
1:O:1787:C:H4'	1:O:2883:A:O4'	2.20	0.41
1:O:611:U:H2'	1:O:612:U:C6	2.56	0.41
1:O:1881:A:OP1	4:A:199:HIS:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:16:ARG:NH2	39:B:9556:HOH:O	2.43	0.41
5:B:62:ARG:CB	5:B:65:MET:HE3	2.50	0.41
1:O:1363:G:P	6:C:76:ARG:HH22	2.43	0.41
7:D:139:TYR:CE2	7:D:143:LYS:HE3	2.56	0.41
1:O:2338:G:OP1	7:D:97:GLN:HG2	2.21	0.41
8:E:137:ASP:OD1	8:E:139:GLU:HB2	2.20	0.41
14:L:73:VAL:HG21	14:L:116:HIS:CD2	2.54	0.41
15:M:159:VAL:HG13	15:M:160:PHE:N	2.36	0.41
15:M:167:GLY:O	15:M:171:ARG:HG3	2.20	0.41
22:T:18:GLU:O	22:T:21:LYS:HG2	2.21	0.41
23:U:9:CYS:CA	23:U:52:THR:HG23	2.51	0.41
28:Z:10:ARG:HG3	28:Z:11:SER:N	2.36	0.41
1:O:1162:G:H1'	32:I:117:LEU:HD11	2.02	0.41
1:O:1181:A:H4'	32:I:92:PRO:HG2	2.02	0.41
1:O:2281:C:C2'	1:O:2282:U:H5'	2.50	0.41
1:O:2443:C:H5'	14:L:57:VAL:HG21	2.03	0.41
1:O:2456:A:H5'	39:O:6254:HOH:O	2.20	0.41
1:O:2564:G:OP2	1:O:2565:C:H5''	2.20	0.41
29:1:42:SER:HB2	39:1:9465:HOH:O	2.20	0.41
7:D:22:VAL:HG22	7:D:74:THR:HG22	2.02	0.41
8:E:20:ILE:HD12	8:E:33:LEU:CD1	2.50	0.41
1:O:2784:A:H1'	8:E:60:SER:OG	2.21	0.41
9:F:111:ILE:O	9:F:115:VAL:HG23	2.19	0.41
12:J:63:ILE:HG22	12:J:64:GLY:N	2.35	0.41
1:O:1132:A:N6	1:O:1229:C:H2'	2.36	0.41
1:O:559:U:H2'	1:O:560:C:O4'	2.21	0.41
1:O:960:G:N3	1:O:960:G:C2'	2.84	0.41
2:9:3064:C:H2'	2:9:3065:A:H5'	2.02	0.41
4:A:52:SER:HB2	4:A:164:ARG:HH11	1.86	0.41
4:A:65:ARG:HH11	4:A:65:ARG:HG2	1.86	0.41
5:B:104:GLU:HB2	39:B:9631:HOH:O	2.20	0.41
7:D:135:VAL:HG21	7:D:139:TYR:CG	2.54	0.41
8:E:7:ILE:CD1	8:E:12:ASP:HA	2.48	0.41
1:O:2283:G:C6	11:H:113:MET:HB3	2.56	0.41
1:O:1163:G:H5'	32:I:115:ASP:O	2.21	0.41
14:L:144:ASP:O	14:L:147:GLU:HB2	2.21	0.41
15:M:27:ARG:HH22	15:M:44:THR:HG23	1.85	0.41
16:N:42:HIS:CG	16:N:62:HIS:HE1	2.39	0.41
16:N:77:ASN:OD1	16:N:79:PRO:HD2	2.21	0.41
25:W:119:HIS:HD2	25:W:120:PRO:O	2.04	0.41
25:W:125:HIS:HD2	25:W:127:GLY:N	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1755:A:H2'	1:0:1756:G:O4'	2.21	0.41
1:0:2699:A:H2'	1:0:2700:G:O4'	2.20	0.41
1:0:855:U:H4'	1:0:856:G:O4'	2.20	0.41
31:3:24:LYS:HA	31:3:67:LEU:HD23	2.02	0.41
4:A:103:VAL:O	4:A:105:VAL:HG23	2.21	0.41
4:A:36:ASP:CB	4:A:85:SER:H	2.33	0.41
4:A:68:ILE:HG12	4:A:69:LEU:N	2.35	0.41
4:A:94:LEU:HD12	4:A:98:GLU:CB	2.51	0.41
9:F:60:VAL:O	9:F:60:VAL:CG1	2.68	0.41
1:0:2365:G:H4'	19:Q:45:PRO:O	2.21	0.41
25:W:38:THR:HG22	25:W:40:ALA:H	1.85	0.41
1:0:1754:A:H2'	1:0:1755:A:O4'	2.20	0.41
1:0:185:G:O3'	1:0:186:A:H4'	2.21	0.41
1:0:2094:G:O6	1:0:2649:A:H2	2.03	0.41
1:0:517:U:H1'	39:0:8147:HOH:O	2.20	0.41
1:0:553:G:P	27:Y:204:ARG:NH2	2.86	0.41
4:A:194:MET:HE1	4:A:199:HIS:HB2	2.02	0.41
5:B:277:GLU:N	5:B:278:PRO:CD	2.84	0.41
7:D:56:ARG:N	39:D:6752:HOH:O	2.52	0.41
20:R:33:ARG:NH1	39:R:9452:HOH:O	2.45	0.41
22:T:27:LEU:HD23	22:T:98:VAL:HB	2.02	0.41
22:T:85:GLU:HG2	22:T:86:GLU:N	2.36	0.41
23:U:14:GLU:O	23:U:17:THR:HB	2.21	0.41
24:V:59:ILE:O	24:V:63:GLU:HG2	2.20	0.41
26:X:23:HIS:NE2	26:X:24:LYS:HD2	2.36	0.41
1:0:1352:A:HO2'	1:0:1353:C:P	2.44	0.41
1:0:17:G:H2'	1:0:18:C:C6	2.56	0.41
1:0:2681:A:H4'	1:0:2682:C:H5'	2.03	0.41
1:0:2748:G:H4'	1:0:2749:U:C5'	2.51	0.41
1:0:830:G:O2'	1:0:831:U:H5'	2.21	0.41
1:0:941:G:C5	1:0:942:U:C4	3.09	0.41
4:A:171:LYS:NZ	39:A:9514:HOH:O	2.54	0.41
4:A:173:GLY:O	4:A:176:HIS:HB3	2.20	0.41
12:J:80:LYS:HE2	12:J:98:PHE:CE1	2.56	0.41
13:K:115:ARG:CG	13:K:116:GLU:N	2.84	0.41
13:K:38:SER:O	39:K:4183:HOH:O	2.22	0.41
14:L:93:VAL:HG12	14:L:97:VAL:HG23	2.02	0.41
15:M:68:ARG:NH2	15:M:73:ARG:HD3	2.36	0.41
16:N:176:ARG:HG3	16:N:180:LEU:CD1	2.51	0.41
18:P:131:PHE:CE1	18:P:137:LEU:HD13	2.56	0.41
22:T:14:ALA:HA	22:T:15:PRO:HD3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2523:U:O2'	1:0:2524:G:H5'	2.22	0.40
1:0:2748:G:H4'	1:0:2749:U:H5'	2.02	0.40
1:0:380:A:H2'	39:0:7729:HOH:O	2.21	0.40
1:0:2807:U:OP2	5:B:28:SER:HB2	2.21	0.40
6:C:133:ARG:NH1	39:C:9216:HOH:O	2.54	0.40
2:9:3056:A:HO2'	7:D:155:HIS:CE1	2.39	0.40
8:E:126:ILE:HB	8:E:131:LEU:CD2	2.51	0.40
12:J:54:VAL:HG11	12:J:138:THR:HG21	2.02	0.40
16:N:37:ARG:HD3	36:N:9307:CL:CL	2.58	0.40
17:O:112:ARG:HE	17:O:112:ARG:HB2	1.77	0.40
18:P:37:ARG:O	18:P:41:ARG:HG3	2.20	0.40
20:R:13:THR:CG2	20:R:14:ALA:N	2.84	0.40
25:W:149:LEU:HG	25:W:153:MET:HE1	2.03	0.40
27:Y:177:LYS:HD3	27:Y:181:GLY:O	2.21	0.40
1:0:1044:C:H3'	1:0:1045:G:H5''	2.03	0.40
1:0:1131:G:H4'	2:9:3091:C:O4'	2.21	0.40
1:0:1745:G:H22	1:0:2033:G:H5'	1.86	0.40
1:0:2611:G:H5'	1:0:2613:G:C8	2.56	0.40
1:0:2754:G:H2'	1:0:2755:G:O4'	2.21	0.40
1:0:294:C:H2'	1:0:295:C:O4'	2.21	0.40
1:0:951:A:O2'	1:0:952:G:H5'	2.21	0.40
31:3:55:VAL:HB	31:3:56:PRO:HD2	2.03	0.40
4:A:186:TRP:CG	4:A:187:PRO:HA	2.57	0.40
6:C:133:ARG:HG3	6:C:133:ARG:HH11	1.85	0.40
6:C:162:VAL:CG2	6:C:232:LEU:HD21	2.48	0.40
11:H:39:ASP:HB3	11:H:41:ASP:OD2	2.21	0.40
13:K:78:LYS:HA	13:K:79:PRO:HD3	1.93	0.40
14:L:77:ALA:C	14:L:79:ASP:H	2.25	0.40
16:N:112:GLY:HA2	16:N:137:ALA:N	2.36	0.40
39:9:1361:HOH:O	16:N:41:LYS:HE3	2.21	0.40
21:S:81:ILE:HG22	24:V:29:ASN:OD1	2.21	0.40
22:T:106:GLU:HG3	39:T:4913:HOH:O	2.21	0.40
26:X:9:VAL:HG13	26:X:88:GLU:CD	2.41	0.40
1:0:1099:G:OP1	25:W:129:LYS:HE3	2.22	0.40
1:0:1168:C:H5''	32:I:87:THR:CG2	2.51	0.40
1:0:1657:A:H2'	1:0:1658:A:C8	2.56	0.40
1:0:2428:G:N7	31:3:60:LYS:NZ	2.68	0.40
1:0:629:A:H2'	1:0:630:A:O4'	2.22	0.40
1:0:644:G:H5'	1:0:644:G:N3	2.37	0.40
1:0:921:G:H4'	1:0:924:G:N1	2.36	0.40
39:0:6895:HOH:O	4:A:205:GLY:HA3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:255:GLY:O	5:B:257:THR:HG23	2.20	0.40
5:B:305:ASP:O	5:B:306:LYS:CB	2.67	0.40
32:I:99:ASP:HA	32:I:138:THR:O	2.21	0.40
17:O:97:SER:H	17:O:100:GLN:NE2	2.20	0.40
20:R:39:THR:CG2	20:R:107:GLU:O	2.70	0.40
24:V:60:GLN:O	24:V:65:ASP:N	2.54	0.40
1:O:1477:C:H5'	1:O:1868:G:H5'	2.04	0.40
1:O:1972:U:C2'	1:O:1973:A:H5''	2.51	0.40
1:O:2499:U:H2'	1:O:2500:C:H6	1.86	0.40
1:O:2565:C:H4'	39:O:5409:HOH:O	2.22	0.40
4:A:192:VAL:HG13	4:A:208:HIS:N	2.37	0.40
5:B:41:PHE:CD1	5:B:79:MET:CE	3.04	0.40
20:R:16:ALA:CB	20:R:94:ASN:HD22	2.34	0.40
23:U:35:LYS:HE2	23:U:51:TRP:CZ2	2.57	0.40
27:Y:95:THR:N	27:Y:236:VAL:O	2.54	0.40
1:O:1117:A:C2	1:O:1244:U:C2	3.10	0.40
1:O:2038:A:O2'	1:O:2039:A:H5'	2.21	0.40
1:O:204:A:H2'	1:O:205:U:H5'	2.02	0.40
1:O:226:A:H1'	1:O:393:G:C5	2.56	0.40
1:O:2374:A:H2'	1:O:2375:G:C8	2.57	0.40
1:O:2857:C:H2'	1:O:2858:U:C6	2.57	0.40
1:O:285:A:H2'	1:O:286:U:O4'	2.21	0.40
1:O:370:G:O2'	1:O:371:U:H5'	2.21	0.40
1:O:582:C:O2'	1:O:583:G:H5'	2.22	0.40
1:O:920:C:H5'	1:O:921:G:C4	2.56	0.40
29:1:8:GLN:HE22	29:1:11:LYS:HZ1	1.68	0.40
4:A:166:ASP:HA	39:A:9607:HOH:O	2.20	0.40
6:C:140:VAL:CG1	6:C:141:SER:N	2.85	0.40
7:D:40:ILE:HG13	7:D:41:LEU:N	2.37	0.40
7:D:49:PRO:HB3	39:D:5828:HOH:O	2.21	0.40
7:D:28:GLY:CA	7:D:69:ILE:HG23	2.37	0.40
12:J:64:GLY:HA3	36:J:9321:CL:CL	2.58	0.40
15:M:66:SER:HB3	15:M:128:TRP:CD1	2.56	0.40
1:O:1864:C:C5	15:M:75:ARG:HD2	2.57	0.40
19:Q:62:THR:O	19:Q:64:GLU:HG2	2.22	0.40
25:W:91:ASP:HB2	39:W:5425:HOH:O	2.22	0.40
28:Z:39:CYS:SG	28:Z:41:ASN:HB3	2.60	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	235/240 (98%)	208 (88%)	25 (11%)	2 (1%)	17	16
5	B	335/338 (99%)	315 (94%)	16 (5%)	4 (1%)	13	10
6	C	244/246 (99%)	225 (92%)	19 (8%)	0	100	100
7	D	134/177 (76%)	107 (80%)	16 (12%)	11 (8%)	1	0
8	E	170/178 (96%)	164 (96%)	6 (4%)	0	100	100
9	F	117/120 (98%)	105 (90%)	8 (7%)	4 (3%)	3	1
10	G	25/348 (7%)	25 (100%)	0	0	100	100
11	H	156/171 (91%)	137 (88%)	15 (10%)	4 (3%)	5	3
12	J	140/145 (97%)	132 (94%)	5 (4%)	3 (2%)	7	4
13	K	130/132 (98%)	125 (96%)	5 (4%)	0	100	100
14	L	141/165 (86%)	119 (84%)	20 (14%)	2 (1%)	11	8
15	M	192/195 (98%)	183 (95%)	8 (4%)	1 (0%)	29	31
16	N	184/187 (98%)	165 (90%)	12 (6%)	7 (4%)	3	1
17	O	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
18	P	141/149 (95%)	136 (96%)	5 (4%)	0	100	100
19	Q	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
20	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
21	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
22	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	17	16
23	U	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
24	V	63/71 (89%)	58 (92%)	4 (6%)	1 (2%)	9	7
25	W	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
26	X	80/92 (87%)	72 (90%)	8 (10%)	0	100	100
27	Y	140/241 (58%)	137 (98%)	3 (2%)	0	100	100
28	Z	71/83 (86%)	62 (87%)	6 (8%)	3 (4%)	3	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	86 (96%)	4 (4%)	0	100	100
32	I	68/162 (42%)	56 (82%)	10 (15%)	2 (3%)	4	2
All	All	3705/4431 (84%)	3432 (93%)	228 (6%)	45 (1%)	13	10

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	27	LEU
5	B	139	ASP
11	H	166	SER
11	H	168	ALA
12	J	143	LYS
14	L	80	ASP
16	N	154	LEU
16	N	184	ILE
28	Z	81	ARG
4	A	37	VAL
7	D	27	ILE
7	D	60	GLU
7	D	61	PHE
7	D	97	GLN
7	D	171	ASP
9	F	101	ALA
22	T	53	GLY
24	V	43	PRO
28	Z	20	ARG
28	Z	21	VAL
7	D	28	GLY
7	D	56	ARG
11	H	16	ARG
11	H	81	GLY
12	J	5	GLU
12	J	65	ASN
14	L	102	ASP
16	N	65	ASP
16	N	155	GLU
16	N	164	ASP
16	N	167	ASP
5	B	34	GLY

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Mol	Chain	Res	Type
5	B	185	GLY
7	D	16	PRO
7	D	137	PRO
7	D	173	GLU
9	F	71	GLY
32	I	132	CYS
7	D	164	ALA
15	M	83	SER
16	N	160	SER
32	I	129	VAL
9	F	100	ASP
9	F	27	GLY
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%)	168 (94%)	11 (6%)	18	21
5	B	282/283 (100%)	265 (94%)	17 (6%)	19	22
6	C	193/193 (100%)	176 (91%)	17 (9%)	10	10
7	D	117/148 (79%)	111 (95%)	6 (5%)	24	29
8	E	152/156 (97%)	147 (97%)	5 (3%)	38	49
9	F	93/94 (99%)	92 (99%)	1 (1%)	73	85
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	128 (97%)	4 (3%)	41	53
12	J	118/121 (98%)	111 (94%)	7 (6%)	19	23
13	K	106/106 (100%)	102 (96%)	4 (4%)	33	42
14	L	113/127 (89%)	110 (97%)	3 (3%)	44	57
15	M	158/159 (99%)	153 (97%)	5 (3%)	39	50
16	N	149/150 (99%)	144 (97%)	5 (3%)	37	47
17	O	93/94 (99%)	91 (98%)	2 (2%)	52	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	P	113/117 (97%)	111 (98%)	2 (2%)	59	72
19	Q	79/80 (99%)	76 (96%)	3 (4%)	33	42
20	R	117/122 (96%)	115 (98%)	2 (2%)	60	74
21	S	71/74 (96%)	71 (100%)	0	100	100
22	T	105/106 (99%)	101 (96%)	4 (4%)	33	42
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	50 (98%)	1 (2%)	55	69
25	W	130/130 (100%)	125 (96%)	5 (4%)	33	42
26	X	66/74 (89%)	62 (94%)	4 (6%)	18	21
27	Y	120/196 (61%)	107 (89%)	13 (11%)	6	6
28	Z	60/68 (88%)	60 (100%)	0	100	100
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	41 (98%)	1 (2%)	49	62
31	3	79/79 (100%)	78 (99%)	1 (1%)	69	81
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3612 (86%)	2970 (96%)	123 (4%)	31	40

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

Mol	Chain	Res	Type
4	A	3	ARG
4	A	36	ASP
4	A	78	ASP
4	A	94	LEU
4	A	131	HIS
4	A	151	GLN
4	A	153	ARG
4	A	165	THR
4	A	179	MET
4	A	206	ARG
4	A	217	ARG
5	B	7	ARG
5	B	11	LEU
5	B	27	ASN
5	B	56	ASP
5	B	82	VAL
5	B	149	ASP

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Mol	Chain	Res	Type
5	B	175	LEU
5	B	180	ASP
5	B	190	MET
5	B	234	ARG
5	B	251	VAL
5	B	254	GLN
5	B	264	GLU
5	B	265	LEU
5	B	277	GLU
5	B	307	ARG
5	B	312	ARG
6	C	2	GLN
6	C	67	GLN
6	C	76	ARG
6	C	91	PRO
6	C	94	THR
6	C	101	ASP
6	C	136	VAL
6	C	162	VAL
6	C	187	ARG
6	C	214	THR
6	C	222	ASP
6	C	223	LEU
6	C	234	VAL
6	C	236	THR
6	C	240	LEU
6	C	243	VAL
6	C	246	ARG
7	D	24	HIS
7	D	50	VAL
7	D	61	PHE
7	D	133	ASN
7	D	137	PRO
7	D	170	TYR
8	E	7	ILE
8	E	102	VAL
8	E	108	LEU
8	E	155	ASN
8	E	164	ASP
9	F	12	LEU
11	H	84	LYS
11	H	154	TYR

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Mol	Chain	Res	Type
11	H	159	PRO
11	H	170	ASN
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
13	K	4	LEU
13	K	10	GLN
13	K	49	LEU
13	K	84	ASP
14	L	35	ARG
14	L	43	HIS
14	L	89	PHE
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	26	LEU
16	N	49	THR
16	N	65	ASP
16	N	139	TRP
17	O	3	THR
17	O	111	VAL
18	P	81	LYS
18	P	98	ILE
19	Q	16	ASN
19	Q	57	ASP
19	Q	95	GLU
20	R	82	GLU
20	R	132	ARG
22	T	39	ASN
22	T	73	HIS
22	T	89	ARG
22	T	96	VAL
24	V	65	ASP
25	W	26	ILE
25	W	35	VAL

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Mol	Chain	Res	Type
25	W	52	VAL
25	W	142	ASP
25	W	146	ILE
26	X	8	ARG
26	X	79	GLU
26	X	82	GLU
26	X	85	VAL
27	Y	103	THR
27	Y	108	ASP
27	Y	141	THR
27	Y	144	ARG
27	Y	154	ARG
27	Y	163	THR
27	Y	186	ARG
27	Y	189	ASN
27	Y	200	THR
27	Y	203	VAL
27	Y	204	ARG
27	Y	220	GLU
27	Y	235	GLU
30	2	18	ASN
31	3	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	47	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	332	ASN
6	C	2	GLN
6	C	39	GLN
6	C	129	HIS
7	D	47	GLN
7	D	85	GLN
7	D	103	ASN
7	D	133	ASN

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Mol	Chain	Res	Type
8	E	106	ASN
8	E	143	GLN
10	G	64	ASN
11	H	31	HIS
11	H	56	GLN
11	H	59	HIS
11	H	70	ASN
11	H	170	ASN
12	J	25	GLN
12	J	52	GLN
12	J	107	ASN
12	J	126	ASN
13	K	10	GLN
14	L	18	HIS
14	L	41	HIS
14	L	42	ASN
15	M	24	GLN
15	M	26	GLN
15	M	58	GLN
15	M	77	HIS
15	M	143	ASN
15	M	170	ASN
16	N	93	GLN
16	N	107	ASN
16	N	153	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
22	T	43	ASN

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Mol	Chain	Res	Type
22	T	73	HIS
23	U	39	ASN
23	U	48	ASN
24	V	60	GLN
25	W	12	ASN
25	W	27	HIS
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	22	ASN
27	Y	133	HIS
27	Y	134	HIS
27	Y	149	GLN
27	Y	189	ASN
29	1	8	GLN
29	1	16	HIS
29	1	28	HIS
30	2	16	ASN
30	2	18	ASN
30	2	41	HIS
30	2	45	ASN
31	3	30	GLN
31	3	48	ASN
32	I	104	GLN
32	I	113	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	232 (8%)	35 (1%)
2	9	121/122 (99%)	16 (13%)	2 (1%)
3	4	1/3 (33%)	0	0
All	All	2867/3047 (94%)	248 (8%)	37 (1%)

All (248) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A

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Mol	Chain	Res	Type
1	0	70	A
1	0	71	G
1	0	86	A
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	169	A
1	0	170	U
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	461	C
1	0	487	G
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

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Mol	Chain	Res	Type
1	0	545	G
1	0	553	G
1	0	559	U
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	698	A
1	0	701	U
1	0	702	G
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	846	A
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	875	A
1	0	877	G
1	0	878	G
1	0	885	G
1	0	898	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

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Mol	Chain	Res	Type
1	0	1072	G
1	0	1081	A
1	0	1087	G
1	0	1088	A
1	0	1100	G
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	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	1564	C
1	0	1592	G

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Mol	Chain	Res	Type
1	0	1625	U
1	0	1626	A
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	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

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Mol	Chain	Res	Type
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2110	G
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2465	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	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	2645	U
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2719	A
1	0	2726	U

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Mol	Chain	Res	Type
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	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	2853	U
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3040	C
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3052	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (37) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A
1	0	129	A
1	0	169	A

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Mol	Chain	Res	Type
1	0	338	C
1	0	603	A
1	0	644	G
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1232	A
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1506	U
1	0	1563	G
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1752	G
1	0	1856	C
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2320	U
1	0	2467	A
1	0	2536	C
1	0	2649	A
1	0	2718	C
1	0	2761	A
1	0	2791	U
1	0	2852	A
2	9	3043	G
2	9	3065	A

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PPU	4	76	1,3	32,40,41	1.14	1 (3%)	33,57,60	0.79	1 (3%)
1	OMU	0	2587	1	14,22,23	1.08	1 (7%)	14,31,34	1.20	1 (7%)
1	PSU	0	2621	1	17,21,22	1.61	3 (17%)	20,30,33	5.43	4 (20%)
1	1MA	0	628	1	15,25,26	0.72	0	15,37,40	1.39	2 (13%)
1	UR3	0	2619	1	14,22,23	0.83	1 (7%)	15,32,35	0.61	0
1	OMG	0	2588	1,3	18,26,27	1.08	2 (11%)	20,38,41	2.62	5 (25%)

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
3	PPU	4	76	1,3	-	0/21/43/44	0/4/4/4
1	OMU	0	2587	1	-	0/7/27/28	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3
1	UR3	0	2619	1	-	0/5/25/26	0/2/2/2
1	OMG	0	2588	1,3	-	0/5/27/28	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	76	PPU	OC-CM	-5.38	1.26	1.42
1	0	2621	PSU	C5-C1'	-4.72	1.48	1.52
1	0	2588	OMG	C6-N1	3.29	1.38	1.33
1	0	2587	OMU	C4-N3	3.02	1.38	1.33
1	0	2621	PSU	C4-N3	2.98	1.38	1.33
1	0	2621	PSU	C2-N1	2.90	1.43	1.38
1	0	2619	UR3	C6-C5	-2.21	1.33	1.38
1	0	2588	OMG	C8-N7	-2.11	1.30	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	-17.10	114.84	128.43
1	0	2621	PSU	C4-N3-C2	14.40	127.30	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2588	OMG	C5-C6-N1	-8.65	111.59	123.43
1	0	2621	PSU	C5-C4-N3	-8.36	114.59	125.36
1	0	2588	OMG	C6-N1-C2	5.89	125.29	115.93
1	0	628	1MA	C2-N3-C4	-4.55	110.90	116.58
1	0	2587	OMU	C5-C4-N3	-3.90	114.74	123.31
1	0	2588	OMG	C2-N3-C4	-3.05	111.87	115.36
1	0	2621	PSU	C6-N1-C2	2.56	119.58	115.36
1	0	2588	OMG	N3-C2-N1	-2.36	124.07	127.22
3	4	76	PPU	CM-OC-CZ	2.21	122.31	117.51
1	0	628	1MA	O4'-C1'-C2'	-2.05	103.93	106.93
1	0	2588	OMG	C6-C5-C4	-2.04	118.85	120.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	0	2749/2922 (94%)	-0.23	90 (3%) 46 44	26, 46, 90, 148	0
2	9	122/122 (100%)	0.00	5 (4%) 37 35	39, 62, 87, 147	0
3	4	2/3 (66%)	-0.53	0 100 100	52, 52, 52, 62	0
4	A	237/240 (98%)	0.42	17 (7%) 15 14	30, 52, 82, 104	0
5	B	337/338 (99%)	0.12	6 (1%) 68 66	31, 50, 72, 85	0
6	C	246/246 (100%)	-0.05	4 (1%) 72 70	28, 47, 68, 81	0
7	D	140/177 (79%)	1.76	51 (36%) 0 0	56, 90, 119, 127	0
8	E	172/178 (96%)	0.63	22 (12%) 3 3	42, 60, 78, 83	0
9	F	119/120 (99%)	1.14	31 (26%) 0 0	47, 71, 99, 108	0
10	G	29/348 (8%)	2.58	17 (58%) 0 0	68, 89, 97, 98	0
11	H	160/171 (93%)	0.64	22 (13%) 2 2	44, 60, 92, 99	0
12	J	142/145 (97%)	-0.09	3 (2%) 63 61	36, 47, 66, 86	0
13	K	132/132 (100%)	-0.18	3 (2%) 60 58	34, 45, 66, 69	0
14	L	145/165 (87%)	0.73	25 (17%) 1 1	30, 64, 110, 119	0
15	M	194/195 (99%)	0.41	11 (5%) 23 22	35, 46, 67, 79	0
16	N	186/187 (99%)	0.79	31 (16%) 1 1	44, 62, 104, 112	0
17	O	115/116 (99%)	0.02	2 (1%) 70 68	41, 53, 66, 74	0
18	P	143/149 (95%)	0.12	3 (2%) 63 61	40, 51, 65, 78	0
19	Q	95/96 (98%)	0.01	3 (3%) 47 45	41, 47, 63, 74	0
20	R	150/155 (96%)	-0.11	2 (1%) 77 75	31, 44, 62, 70	0
21	S	81/85 (95%)	0.38	6 (7%) 14 13	43, 62, 82, 95	0
22	T	119/120 (99%)	0.60	9 (7%) 13 12	43, 56, 79, 107	0
23	U	53/66 (80%)	0.30	3 (5%) 23 22	42, 51, 67, 75	0
24	V	65/71 (91%)	2.01	23 (35%) 0 0	54, 78, 111, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	154/154 (100%)	-0.03	2 (1%) 77 75	36, 48, 69, 78	0
26	X	82/92 (89%)	0.54	7 (8%) 10 9	41, 53, 79, 97	0
27	Y	142/241 (58%)	0.13	8 (5%) 24 23	31, 43, 62, 82	0
28	Z	73/83 (87%)	0.94	19 (26%) 0 0	49, 73, 86, 92	0
29	1	56/57 (98%)	-0.45	0 100 100	30, 35, 42, 50	0
30	2	46/50 (92%)	0.63	6 (13%) 3 3	38, 58, 73, 83	0
31	3	92/92 (100%)	0.14	4 (4%) 35 33	37, 55, 68, 79	0
32	I	70/162 (43%)	5.42	64 (91%) 0 0	107, 120, 137, 139	0
All	All	6648/7478 (88%)	0.18	499 (7%) 14 13	26, 51, 95, 148	0

All (499) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	71	GLY	16.2
24	V	1	THR	15.4
7	D	63	ILE	13.9
32	I	133	THR	13.3
32	I	96	PHE	11.8
32	I	137	VAL	11.5
16	N	166	ALA	11.0
32	I	79	ILE	10.9
24	V	39	ALA	10.2
32	I	85	PHE	10.0
32	I	76	ALA	10.0
7	D	57	THR	9.2
24	V	40	PRO	8.8
7	D	10	PHE	8.6
32	I	89	SER	8.3
32	I	88	GLY	8.3
2	9	3001	U	8.1
32	I	111	GLN	8.0
32	I	98	ALA	7.9
32	I	75	THR	7.9
7	D	61	PHE	7.8
15	M	70	GLY	7.8
32	I	132	CYS	7.7
32	I	116	LEU	7.7
32	I	113	HIS	7.6
1	0	1951	G	7.5

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Mol	Chain	Res	Type	RSRZ
32	I	72	VAL	7.4
22	T	119	ALA	7.4
32	I	107	GLN	7.4
30	2	49	GLU	7.2
32	I	93	GLN	7.2
32	I	102	VAL	7.0
32	I	109	ALA	7.0
4	A	37	VAL	7.0
32	I	97	VAL	6.9
22	T	118	SER	6.9
32	I	91	GLU	6.8
32	I	81	ASP	6.8
10	G	24	VAL	6.7
32	I	118	SER	6.5
32	I	87	THR	6.5
24	V	38	GLY	6.4
1	0	282	C	6.4
7	D	170	TYR	6.4
32	I	121	LEU	6.2
10	G	23	ILE	6.1
7	D	69	ILE	6.1
28	Z	22	SER	6.0
26	X	88	GLU	6.0
32	I	108	ILE	6.0
32	I	114	PRO	6.0
17	O	22	GLY	6.0
1	0	2237	G	5.9
22	T	116	ASP	5.8
11	H	111	ASP	5.8
32	I	86	GLU	5.8
32	I	78	LEU	5.8
32	I	74	PRO	5.7
10	G	27	ILE	5.7
2	9	3024	U	5.5
7	D	64	ARG	5.5
14	L	80	ASP	5.4
32	I	104	GLN	5.4
32	I	77	GLU	5.4
28	Z	20	ARG	5.3
32	I	105	VAL	5.3
28	Z	11	SER	5.3
12	J	70	PHE	5.3

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Mol	Chain	Res	Type	RSRZ
1	0	280	C	5.3
1	0	1199	A	5.2
22	T	115	GLU	5.1
24	V	37	GLY	5.1
24	V	36	ALA	5.0
1	0	2004	U	5.0
2	9	3002	U	4.9
14	L	130	ARG	4.9
32	I	129	VAL	4.9
1	0	1173	A	4.9
1	0	1202	A	4.8
8	E	45	ASP	4.8
1	0	2508	C	4.8
9	F	119	ARG	4.7
26	X	80	GLU	4.7
4	A	35	GLY	4.7
32	I	117	LEU	4.6
1	0	2637	A	4.6
1	0	1172	G	4.6
7	D	90	LEU	4.6
1	0	10	U	4.6
7	D	66	GLY	4.6
7	D	11	HIS	4.6
1	0	285	A	4.6
9	F	117	GLU	4.5
10	G	26	MET	4.5
14	L	81	VAL	4.5
16	N	161	GLY	4.5
32	I	126	LYS	4.5
32	I	103	ASP	4.5
4	A	237	GLY	4.4
17	O	23	GLY	4.4
1	0	1177	A	4.4
14	L	91	VAL	4.4
2	9	3023	U	4.4
14	L	82	ALA	4.4
7	D	62	ASP	4.4
32	I	138	THR	4.4
7	D	53	LYS	4.3
32	I	106	LYS	4.3
1	0	1950	G	4.3
32	I	110	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	0	2238	A	4.2
4	A	31	LYS	4.2
9	F	108	VAL	4.2
11	H	171	ALA	4.2
4	A	133	ARG	4.2
21	S	81	ILE	4.1
7	D	56	ARG	4.1
4	A	36	ASP	4.1
16	N	183	ASP	4.1
32	I	119	TYR	4.1
14	L	75	LEU	4.1
1	0	514	G	4.1
1	0	272	A	4.1
7	D	44	ILE	4.1
28	Z	45	ASP	4.1
9	F	110	ASP	4.1
24	V	10	ASP	4.0
1	0	288	A	4.0
1	0	497	A	4.0
15	M	74	LYS	4.0
32	I	125	ALA	4.0
16	N	184	ILE	4.0
1	0	1965	C	4.0
24	V	59	ILE	3.9
8	E	10	ASP	3.9
10	G	69	ARG	3.9
1	0	1163	G	3.9
9	F	16	ALA	3.9
1	0	970	U	3.9
11	H	37	GLN	3.9
1	0	1948	G	3.9
28	Z	19	GLY	3.9
28	Z	24	ARG	3.9
26	X	85	VAL	3.9
23	U	47	ARG	3.9
14	L	99	GLU	3.9
7	D	26	GLY	3.8
32	I	84	GLY	3.8
28	Z	25	ARG	3.8
2	9	3122	C	3.8
16	N	163	PHE	3.8
4	A	97	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
5	B	57	GLU	3.8
32	I	115	ASP	3.8
7	D	65	GLU	3.8
28	Z	12	GLY	3.7
32	I	123	ASN	3.7
1	0	2748	G	3.7
24	V	3	LEU	3.7
32	I	99	ASP	3.7
22	T	117	ASP	3.7
1	0	1200	A	3.7
16	N	175	LEU	3.7
9	F	22	VAL	3.7
25	W	86	GLU	3.6
16	N	155	GLU	3.6
9	F	99	THR	3.6
7	D	134	LEU	3.6
16	N	68	GLU	3.6
32	I	135	LEU	3.6
4	A	82	VAL	3.6
8	E	87	PHE	3.6
32	I	134	SER	3.5
30	2	35	ARG	3.5
24	V	43	PRO	3.5
1	0	1171	A	3.5
19	Q	17	LYS	3.5
7	D	88	LEU	3.5
24	V	2	VAL	3.5
7	D	107	GLY	3.5
1	0	2344	G	3.5
4	A	32	VAL	3.4
9	F	28	ALA	3.4
19	Q	95	GLU	3.4
9	F	100	ASP	3.4
1	0	279	C	3.4
30	2	39	ARG	3.4
16	N	156	GLU	3.4
1	0	1947	G	3.4
28	Z	31	SER	3.4
1	0	358	G	3.4
16	N	152	GLU	3.3
1	0	1169	U	3.3
1	0	960	G	3.3

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Mol	Chain	Res	Type	RSRZ
21	S	45	TYR	3.3
1	0	1164	U	3.3
9	F	103	GLU	3.3
1	0	1198	U	3.3
6	C	61	PHE	3.3
9	F	25	ASP	3.3
16	N	154	LEU	3.2
8	E	100	ASP	3.2
32	I	120	ASP	3.2
9	F	118	LEU	3.2
7	D	27	ILE	3.2
32	I	140	GLU	3.2
16	N	162	ASP	3.2
10	G	66	LEU	3.2
27	Y	95	THR	3.2
26	X	77	PHE	3.1
7	D	58	VAL	3.1
10	G	22	ALA	3.1
16	N	165	ALA	3.1
32	I	95	ASP	3.1
1	0	999	C	3.1
1	0	281	U	3.1
8	E	154	ILE	3.1
27	Y	236	VAL	3.1
14	L	79	ASP	3.1
16	N	164	ASP	3.1
9	F	26	THR	3.1
9	F	90	GLU	3.1
11	H	149	ALA	3.1
26	X	7	GLU	3.1
9	F	49	PHE	3.1
32	I	80	LYS	3.1
10	G	63	ARG	3.1
21	S	2	TRP	3.1
1	0	2511	A	3.1
1	0	138	U	3.1
16	N	180	LEU	3.1
9	F	106	ALA	3.1
11	H	35	ARG	3.1
1	0	1966	U	3.0
32	I	83	ALA	3.0
7	D	55	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
11	H	143	ALA	3.0
21	S	20	PHE	3.0
7	D	135	VAL	3.0
7	D	171	ASP	3.0
7	D	154	LYS	3.0
11	H	146	VAL	3.0
14	L	150	GLN	3.0
28	Z	23	ARG	3.0
7	D	25	MET	2.9
8	E	99	GLY	2.9
1	0	1525	G	2.9
9	F	107	ASP	2.9
24	V	41	GLU	2.9
7	D	166	ILE	2.9
24	V	8	ILE	2.9
32	I	112	LYS	2.9
9	F	79	GLN	2.9
1	0	1168	C	2.9
1	0	2747	C	2.9
7	D	35	ALA	2.9
5	B	1	PRO	2.9
1	0	1192	A	2.9
32	I	92	PRO	2.9
1	0	291	C	2.8
14	L	102	ASP	2.8
7	D	51	ARG	2.8
1	0	362	G	2.8
28	Z	33	MET	2.8
14	L	147	GLU	2.8
10	G	15	TRP	2.8
9	F	115	VAL	2.8
12	J	4	ALA	2.8
15	M	49	ALA	2.8
31	3	41	GLU	2.8
9	F	98	VAL	2.8
26	X	10	VAL	2.8
32	I	73	PRO	2.8
16	N	134	ASP	2.8
32	I	100	LEU	2.8
1	0	289	G	2.8
31	3	62	THR	2.8
32	I	122	THR	2.8

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Mol	Chain	Res	Type	RSRZ
7	D	18	ILE	2.8
11	H	138	CYS	2.8
24	V	63	GLU	2.8
27	Y	216	ARG	2.8
13	K	132	VAL	2.7
1	0	1279	U	2.7
1	0	284	C	2.7
15	M	132	ILE	2.7
14	L	100	ALA	2.7
28	Z	14	PHE	2.7
14	L	76	LEU	2.7
14	L	148	GLU	2.7
31	3	92	GLU	2.7
7	D	92	GLU	2.7
1	0	370	G	2.7
1	0	969	G	2.7
16	N	145	ALA	2.7
1	0	2345	A	2.7
27	Y	108	ASP	2.7
7	D	172	VAL	2.7
9	F	12	LEU	2.7
1	0	2507	G	2.7
4	A	85	SER	2.6
16	N	174	GLU	2.6
25	W	76	ASP	2.6
7	D	40	ILE	2.6
8	E	126	ILE	2.6
1	0	293	A	2.6
24	V	5	VAL	2.6
32	I	136	GLY	2.6
1	0	1201	C	2.6
27	Y	235	GLU	2.6
28	Z	34	ASN	2.6
4	A	38	ILE	2.6
32	I	139	ILE	2.6
11	H	83	TYR	2.6
11	H	137	TYR	2.6
14	L	105	TYR	2.6
22	T	112	LEU	2.6
28	Z	21	VAL	2.6
11	H	74	ILE	2.6
7	D	70	GLY	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
7	D	67	ASP	2.6
8	E	11	VAL	2.6
11	H	73	LEU	2.6
11	H	140	VAL	2.6
1	0	716	G	2.6
1	0	735	C	2.6
7	D	68	PRO	2.6
4	A	33	GLU	2.6
10	G	21	ASP	2.6
9	F	29	VAL	2.6
18	P	141	ILE	2.6
1	0	1174	A	2.6
9	F	19	ALA	2.6
24	V	14	ALA	2.6
15	M	75	ARG	2.5
15	M	88	VAL	2.5
9	F	15	ASP	2.5
1	0	1175	G	2.5
16	N	178	THR	2.5
14	L	145	LEU	2.5
9	F	27	GLY	2.5
28	Z	59	TYR	2.5
1	0	1967	U	2.5
9	F	101	ALA	2.5
10	G	25	GLU	2.5
11	H	141	GLU	2.5
16	N	177	GLU	2.5
1	0	1203	G	2.5
15	M	164	THR	2.5
24	V	12	THR	2.5
19	Q	18	PRO	2.5
24	V	45	ARG	2.5
15	M	71	SER	2.5
6	C	132	ASP	2.5
1	0	278	A	2.5
1	0	363	A	2.5
24	V	46	ILE	2.5
8	E	128	GLY	2.5
10	G	67	LEU	2.5
7	D	23	VAL	2.5
1	0	2769	C	2.5
7	D	167	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	0	1929	G	2.5
1	0	295	C	2.4
1	0	1000	C	2.4
10	G	64	ASN	2.4
11	H	154	TYR	2.4
1	0	1190	G	2.4
8	E	6	GLU	2.4
7	D	165	PHE	2.4
7	D	52	THR	2.4
16	N	149	GLU	2.4
27	Y	102	LEU	2.4
16	N	95	ALA	2.4
14	L	97	VAL	2.4
16	N	70	GLY	2.4
5	B	104	GLU	2.4
14	L	60	GLU	2.4
4	A	60	PHE	2.4
14	L	89	PHE	2.4
22	T	82	THR	2.4
11	H	39	ASP	2.4
14	L	90	ARG	2.4
8	E	124	VAL	2.4
1	0	1180	U	2.4
15	M	87	GLY	2.4
9	F	17	LEU	2.4
28	Z	16	ALA	2.4
30	2	26	MET	2.4
7	D	104	PHE	2.4
24	V	33	VAL	2.4
30	2	44	ARG	2.3
6	C	143	ASP	2.3
10	G	12	ILE	2.3
18	P	135	ALA	2.3
24	V	6	GLN	2.3
27	Y	234	VAL	2.3
4	A	86	ALA	2.3
11	H	32	LYS	2.3
8	E	43	ASP	2.3
10	G	65	THR	2.3
1	0	128	A	2.3
1	0	372	A	2.3
1	0	290	C	2.3

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Mol	Chain	Res	Type	RSRZ
8	E	127	ASP	2.3
1	0	2250	G	2.3
7	D	54	ALA	2.3
8	E	4	GLU	2.3
1	0	1904	A	2.3
16	N	139	TRP	2.3
16	N	172	PHE	2.3
30	2	27	LEU	2.2
16	N	185	GLU	2.2
8	E	86	VAL	2.2
7	D	85	GLN	2.2
7	D	38	GLU	2.2
16	N	67	ALA	2.2
7	D	93	LEU	2.2
21	S	19	ASP	2.2
8	E	15	GLN	2.2
31	3	56	PRO	2.2
1	0	1181	A	2.2
32	I	124	ALA	2.2
8	E	123	ASP	2.2
14	L	142	LEU	2.2
14	L	141	GLU	2.2
1	0	1170	U	2.2
9	F	6	PHE	2.2
4	A	236	GLY	2.2
4	A	64	ASP	2.2
12	J	5	GLU	2.2
7	D	157	LEU	2.2
1	0	1165	G	2.2
11	H	33	MET	2.2
13	K	126	SER	2.2
7	D	173	GLU	2.2
16	N	170	GLU	2.2
14	L	119	THR	2.2
1	0	1964	U	2.2
1	0	2645	U	2.2
6	C	1	MET	2.2
16	N	72	GLU	2.2
9	F	102	GLY	2.2
5	B	2	GLN	2.2
15	M	159	VAL	2.2
11	H	47	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
8	E	129	GLU	2.2
1	0	1665	G	2.1
28	Z	10	ARG	2.1
1	0	2850	C	2.1
7	D	84	LEU	2.1
11	H	82	ASP	2.1
24	V	49	LEU	2.1
9	F	24	ARG	2.1
7	D	43	GLU	2.1
32	I	82	GLU	2.1
1	0	283	U	2.1
1	0	1625	U	2.1
5	B	183	GLU	2.1
8	E	98	GLU	2.1
10	G	18	GLU	2.1
20	R	13	THR	2.1
16	N	167	ASP	2.1
1	0	2103	A	2.1
1	0	2506	A	2.1
5	B	133	GLU	2.1
7	D	81	GLU	2.1
21	S	78	ALA	2.1
28	Z	18	TYR	2.1
1	0	1949	G	2.1
28	Z	37	HIS	2.1
27	Y	96	GLU	2.1
16	N	160	SER	2.1
18	P	67	LYS	2.1
20	R	150	PRO	2.1
10	G	71	LEU	2.1
1	0	1189	A	2.1
22	T	106	GLU	2.1
32	I	94	GLU	2.1
24	V	9	ARG	2.1
7	D	106	PHE	2.1
9	F	21	GLU	2.0
26	X	71	ARG	2.0
1	0	368	C	2.0
1	0	1919	A	2.0
8	E	125	GLU	2.0
8	E	16	ASP	2.0
11	H	45	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
23	U	53	ASP	2.0
22	T	57	GLY	2.0
14	L	77	ALA	2.0
4	A	209	PRO	2.0
14	L	144	ASP	2.0
11	H	144	GLU	2.0
1	0	292	G	2.0
23	U	10	GLY	2.0
8	E	89	SER	2.0
13	K	118	ALA	2.0
15	M	79	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	PPU	4	76	37/38	0.94	0.14	48,54,66,71	0
1	PSU	0	2621	20/21	0.97	0.11	37,40,50,51	0
1	1MA	0	628	23/24	0.97	0.14	29,33,36,37	0
1	UR3	0	2619	21/22	0.97	0.14	45,45,49,50	0
1	OMG	0	2588	24/25	0.97	0.12	30,35,40,41	0
1	OMU	0	2587	21/22	0.99	0.10	33,36,38,39	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
37	SR	0	9601	1/1	-0.13	0.75	200,200,200,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8047	1/1	0.20	0.48	91,91,91,91	0
35	NA	0	9122	1/1	0.24	0.30	96,96,96,96	0
37	SR	0	9501	1/1	0.43	0.37	200,200,200,200	0
33	MG	0	8082	1/1	0.45	0.32	107,107,107,107	0
35	NA	0	9184	1/1	0.51	0.51	102,102,102,102	0
37	SR	0	9547	1/1	0.54	1.06	200,200,200,200	0
35	NA	0	9129	1/1	0.57	0.22	85,85,85,85	0
35	NA	0	9171	1/1	0.61	0.28	61,61,61,61	0
33	MG	0	8072	1/1	0.61	0.33	96,96,96,96	0
33	MG	0	8014	1/1	0.66	0.35	73,73,73,73	0
35	NA	0	9182	1/1	0.67	0.21	78,78,78,78	0
35	NA	0	9179	1/1	0.68	1.02	100,100,100,100	0
33	MG	0	8065	1/1	0.69	0.41	93,93,93,93	0
37	SR	B	9521	1/1	0.70	0.49	199,199,199,199	0
33	MG	0	8093	1/1	0.71	0.12	42,42,42,42	0
35	NA	0	9173	1/1	0.74	0.38	70,70,70,70	0
37	SR	0	9590	1/1	0.75	0.13	178,178,178,178	0
33	MG	0	8092	1/1	0.76	0.72	81,81,81,81	0
37	SR	0	9452	1/1	0.76	0.19	114,114,114,114	0
33	MG	0	8045	1/1	0.78	0.33	84,84,84,84	0
33	MG	0	8061	1/1	0.78	0.12	95,95,95,95	0
37	SR	0	9529	1/1	0.78	0.14	138,138,138,138	0
37	SR	0	9537	1/1	0.79	0.14	154,154,154,154	0
35	NA	0	9168	1/1	0.79	0.11	57,57,57,57	0
34	K	0	9001	1/1	0.79	0.45	116,116,116,116	0
35	NA	0	9164	1/1	0.79	0.35	59,59,59,59	0
33	MG	B	8055	1/1	0.80	0.21	108,108,108,108	0
37	SR	0	9500	1/1	0.80	1.52	200,200,200,200	0
33	MG	0	8103	1/1	0.81	0.19	62,62,62,62	0
35	NA	D	9151	1/1	0.81	0.10	63,63,63,63	0
33	MG	0	8024	1/1	0.81	1.41	77,77,77,77	0
33	MG	0	8052	1/1	0.82	0.38	68,68,68,68	0
35	NA	S	9112	1/1	0.82	0.13	59,59,59,59	0
36	CL	A	9309	1/1	0.83	0.14	68,68,68,68	0
33	MG	0	8054	1/1	0.83	0.09	58,58,58,58	0
33	MG	0	8076	1/1	0.83	0.12	61,61,61,61	0
35	NA	0	9185	1/1	0.83	0.32	46,46,46,46	0
35	NA	J	9146	1/1	0.83	0.09	55,55,55,55	0
35	NA	0	9169	1/1	0.84	0.47	104,104,104,104	0
33	MG	0	8040	1/1	0.84	0.37	100,100,100,100	0
35	NA	B	9161	1/1	0.84	0.53	62,62,62,62	0
35	NA	0	9163	1/1	0.84	0.20	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8118	1/1	0.85	0.18	76,76,76,76	0
33	MG	0	8050	1/1	0.85	0.16	93,93,93,93	0
33	MG	0	8108	1/1	0.86	0.18	74,74,74,74	0
35	NA	0	9127	1/1	0.86	0.12	57,57,57,57	0
37	SR	0	9484	1/1	0.86	0.11	147,147,147,147	0
35	NA	0	9170	1/1	0.86	0.45	94,94,94,94	0
35	NA	0	9118	1/1	0.87	0.23	60,60,60,60	0
33	MG	0	8085	1/1	0.87	0.33	91,91,91,91	0
33	MG	0	8059	1/1	0.87	0.38	78,78,78,78	0
35	NA	0	9141	1/1	0.87	0.10	62,62,62,62	0
35	NA	0	9126	1/1	0.87	0.11	59,59,59,59	0
33	MG	0	8113	1/1	0.88	0.08	50,50,50,50	0
37	SR	0	9490	1/1	0.88	0.08	109,109,109,109	0
37	SR	0	9539	1/1	0.88	0.21	162,162,162,162	0
35	NA	0	9157	1/1	0.88	0.15	47,47,47,47	0
35	NA	0	9113	1/1	0.88	0.14	65,65,65,65	0
33	MG	0	8057	1/1	0.88	0.22	85,85,85,85	0
35	NA	0	9166	1/1	0.88	0.10	67,67,67,67	0
33	MG	0	8042	1/1	0.88	0.09	60,60,60,60	0
37	SR	0	9465	1/1	0.88	0.07	100,100,100,100	0
33	MG	9	8095	1/1	0.89	0.20	46,46,46,46	0
37	SR	0	9626	1/1	0.89	0.30	128,128,128,128	0
35	NA	0	9102	1/1	0.89	0.28	57,57,57,57	0
33	MG	0	8094	1/1	0.89	0.23	67,67,67,67	0
33	MG	0	8039	1/1	0.89	0.07	65,65,65,65	0
33	MG	0	8104	1/1	0.89	0.23	76,76,76,76	0
35	NA	0	9108	1/1	0.90	0.10	35,35,35,35	0
36	CL	0	9315	1/1	0.90	0.12	58,58,58,58	0
33	MG	0	8090	1/1	0.90	0.47	80,80,80,80	0
33	MG	0	8058	1/1	0.90	0.26	45,45,45,45	0
37	SR	0	9459	1/1	0.91	0.07	101,101,101,101	0
35	NA	0	9172	1/1	0.91	0.40	70,70,70,70	0
37	SR	0	9475	1/1	0.91	0.08	77,77,77,77	0
35	NA	0	9152	1/1	0.91	0.74	78,78,78,78	0
33	MG	0	8089	1/1	0.91	0.09	54,54,54,54	0
35	NA	0	9149	1/1	0.91	0.18	42,42,42,42	0
35	NA	0	9134	1/1	0.91	0.07	51,51,51,51	0
33	MG	0	8063	1/1	0.91	0.07	70,70,70,70	0
35	NA	0	9165	1/1	0.91	0.21	47,47,47,47	0
35	NA	0	9139	1/1	0.92	0.12	52,52,52,52	0
37	SR	0	9534	1/1	0.92	0.10	100,100,100,100	0
33	MG	0	8097	1/1	0.92	0.16	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8096	1/1	0.92	0.14	46,46,46,46	0
33	MG	0	8030	1/1	0.92	0.10	39,39,39,39	0
37	SR	0	9468	1/1	0.92	0.05	113,113,113,113	0
37	SR	0	9530	1/1	0.92	0.10	84,84,84,84	0
35	NA	0	9167	1/1	0.92	0.09	56,56,56,56	0
33	MG	0	8107	1/1	0.92	0.23	67,67,67,67	0
35	NA	0	9150	1/1	0.92	0.11	38,38,38,38	0
33	MG	0	8021	1/1	0.92	0.20	55,55,55,55	0
33	MG	0	8101	1/1	0.92	0.16	59,59,59,59	0
35	NA	C	9104	1/1	0.92	0.20	34,34,34,34	0
35	NA	R	9186	1/1	0.92	0.47	69,69,69,69	0
35	NA	0	9177	1/1	0.93	0.23	63,63,63,63	0
33	MG	0	8043	1/1	0.93	0.05	49,49,49,49	0
35	NA	R	9138	1/1	0.93	0.07	56,56,56,56	0
35	NA	0	9125	1/1	0.93	0.73	115,115,115,115	0
35	NA	0	9174	1/1	0.93	0.17	65,65,65,65	0
35	NA	0	9110	1/1	0.93	0.14	46,46,46,46	0
35	NA	0	9162	1/1	0.93	0.15	58,58,58,58	0
37	SR	9	9503	1/1	0.93	0.04	114,114,114,114	0
33	MG	0	8056	1/1	0.93	0.20	46,46,46,46	0
35	NA	0	9140	1/1	0.93	0.25	60,60,60,60	0
33	MG	0	8060	1/1	0.93	0.28	71,71,71,71	0
34	K	0	9002	1/1	0.94	0.14	89,89,89,89	0
37	SR	0	9581	1/1	0.94	0.08	121,121,121,121	0
33	MG	0	8114	1/1	0.94	0.19	63,63,63,63	0
35	NA	9	9183	1/1	0.94	0.15	66,66,66,66	0
35	NA	0	9120	1/1	0.94	0.18	64,64,64,64	0
33	MG	0	8028	1/1	0.94	0.16	37,37,37,37	0
33	MG	0	8022	1/1	0.94	0.69	74,74,74,74	0
37	SR	9	9588	1/1	0.94	0.08	114,114,114,114	0
35	NA	0	9178	1/1	0.94	0.22	51,51,51,51	0
33	MG	0	8041	1/1	0.94	0.18	50,50,50,50	0
33	MG	0	8088	1/1	0.94	0.08	45,45,45,45	0
35	NA	R	9137	1/1	0.94	0.10	36,36,36,36	0
33	MG	0	8091	1/1	0.94	0.08	45,45,45,45	0
37	SR	0	9474	1/1	0.94	0.09	112,112,112,112	0
35	NA	0	9101	1/1	0.94	0.15	47,47,47,47	0
35	NA	0	9154	1/1	0.94	0.16	59,59,59,59	0
35	NA	0	9175	1/1	0.94	0.16	52,52,52,52	0
33	MG	0	8046	1/1	0.94	0.09	40,40,40,40	0
33	MG	Y	8109	1/1	0.94	0.08	41,41,41,41	0
35	NA	0	9158	1/1	0.94	0.23	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8015	1/1	0.94	0.12	34,34,34,34	0
33	MG	0	8037	1/1	0.94	0.08	39,39,39,39	0
35	NA	Q	9148	1/1	0.94	0.08	44,44,44,44	0
36	CL	N	9307	1/1	0.95	0.14	52,52,52,52	0
35	NA	0	9132	1/1	0.95	0.21	51,51,51,51	0
33	MG	0	8027	1/1	0.95	0.19	39,39,39,39	0
37	SR	0	9505	1/1	0.95	0.09	85,85,85,85	0
33	MG	0	8036	1/1	0.95	0.09	60,60,60,60	0
35	NA	M	9147	1/1	0.95	0.18	43,43,43,43	0
35	NA	0	9181	1/1	0.95	0.12	50,50,50,50	0
33	MG	0	8067	1/1	0.95	0.09	42,42,42,42	0
37	SR	0	9447	1/1	0.95	0.09	67,67,67,67	0
33	MG	0	8116	1/1	0.95	0.07	62,62,62,62	0
37	SR	0	9480	1/1	0.95	0.06	87,87,87,87	0
33	MG	0	8001	1/1	0.95	0.26	20,20,20,20	0
35	NA	0	9111	1/1	0.95	0.10	57,57,57,57	0
37	SR	0	9504	1/1	0.95	0.08	105,105,105,105	0
35	NA	0	9124	1/1	0.95	0.09	47,47,47,47	0
33	MG	0	8115	1/1	0.95	0.11	56,56,56,56	0
35	NA	0	9116	1/1	0.95	0.20	58,58,58,58	0
37	SR	0	9405	1/1	0.95	0.15	60,60,60,60	0
33	MG	0	8012	1/1	0.96	0.26	41,41,41,41	0
33	MG	0	8013	1/1	0.96	0.38	22,22,22,22	0
37	SR	F	9595	1/1	0.96	0.14	105,105,105,105	0
36	CL	L	9310	1/1	0.96	0.09	54,54,54,54	0
37	SR	0	9469	1/1	0.96	0.05	79,79,79,79	0
37	SR	0	9506	1/1	0.96	0.03	66,66,66,66	0
35	NA	0	9123	1/1	0.96	0.10	41,41,41,41	0
33	MG	0	8084	1/1	0.96	0.74	74,74,74,74	0
33	MG	0	8102	1/1	0.96	0.08	56,56,56,56	0
37	SR	0	9467	1/1	0.96	0.09	67,67,67,67	0
37	SR	0	9515	1/1	0.96	0.15	87,87,87,87	0
36	CL	0	9316	1/1	0.96	0.17	69,69,69,69	0
33	MG	0	8099	1/1	0.96	0.10	59,59,59,59	0
37	SR	0	9532	1/1	0.96	0.07	103,103,103,103	0
37	SR	0	9488	1/1	0.96	0.09	76,76,76,76	0
37	SR	0	9566	1/1	0.96	0.04	77,77,77,77	0
37	SR	0	9483	1/1	0.96	0.08	68,68,68,68	0
33	MG	0	8051	1/1	0.96	0.20	26,26,26,26	0
33	MG	0	8032	1/1	0.96	0.08	43,43,43,43	0
35	NA	0	9128	1/1	0.96	0.11	45,45,45,45	0
33	MG	A	8066	1/1	0.96	0.18	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8019	1/1	0.96	0.07	58,58,58,58	0
37	SR	0	9489	1/1	0.97	0.07	85,85,85,85	0
37	SR	0	9509	1/1	0.97	0.12	81,81,81,81	0
33	MG	0	8117	1/1	0.97	0.09	43,43,43,43	0
37	SR	0	9568	1/1	0.97	0.08	75,75,75,75	0
33	MG	T	8073	1/1	0.97	0.12	46,46,46,46	0
37	SR	0	9560	1/1	0.97	0.07	97,97,97,97	0
37	SR	H	9486	1/1	0.97	0.15	109,109,109,109	0
35	NA	0	9130	1/1	0.97	0.08	49,49,49,49	0
35	NA	0	9160	1/1	0.97	0.09	39,39,39,39	0
33	MG	0	8044	1/1	0.97	0.08	39,39,39,39	0
35	NA	0	9159	1/1	0.97	0.11	46,46,46,46	0
37	SR	0	9570	1/1	0.97	0.03	98,98,98,98	0
33	MG	0	8110	1/1	0.97	0.07	36,36,36,36	0
36	CL	J	9321	1/1	0.97	0.06	53,53,53,53	0
37	SR	0	9522	1/1	0.97	0.04	104,104,104,104	0
33	MG	0	8080	1/1	0.97	0.18	47,47,47,47	0
37	SR	0	9429	1/1	0.97	0.09	60,60,60,60	0
36	CL	M	9318	1/1	0.97	0.17	41,41,41,41	0
33	MG	0	8075	1/1	0.97	0.09	36,36,36,36	0
35	NA	0	9143	1/1	0.97	0.10	43,43,43,43	0
35	NA	0	9107	1/1	0.97	0.23	61,61,61,61	0
36	CL	0	9313	1/1	0.97	0.09	51,51,51,51	0
37	SR	0	9435	1/1	0.97	0.08	65,65,65,65	0
35	NA	0	9131	1/1	0.97	0.06	48,48,48,48	0
35	NA	0	9156	1/1	0.98	0.14	53,53,53,53	0
37	SR	0	9414	1/1	0.98	0.12	52,52,52,52	0
37	SR	0	9445	1/1	0.98	0.07	56,56,56,56	0
36	CL	J	9302	1/1	0.98	0.07	48,48,48,48	0
37	SR	0	9454	1/1	0.98	0.05	74,74,74,74	0
37	SR	0	9438	1/1	0.98	0.06	63,63,63,63	0
37	SR	0	9425	1/1	0.98	0.10	55,55,55,55	0
37	SR	0	9421	1/1	0.98	0.08	64,64,64,64	0
37	SR	0	9427	1/1	0.98	0.11	52,52,52,52	0
37	SR	0	9477	1/1	0.98	0.10	84,84,84,84	0
36	CL	0	9322	1/1	0.98	0.15	53,53,53,53	0
37	SR	0	9434	1/1	0.98	0.09	55,55,55,55	0
33	MG	0	8083	1/1	0.98	0.10	54,54,54,54	0
36	CL	0	9311	1/1	0.98	0.08	57,57,57,57	0
35	NA	0	9115	1/1	0.98	0.08	39,39,39,39	0
33	MG	0	8079	1/1	0.98	0.12	34,34,34,34	0
36	CL	B	9319	1/1	0.98	0.11	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
37	SR	A	9437	1/1	0.98	0.14	67,67,67,67	0
37	SR	0	9495	1/1	0.98	0.08	88,88,88,88	0
37	SR	0	9517	1/1	0.98	0.06	91,91,91,91	0
37	SR	0	9585	1/1	0.98	0.06	83,83,83,83	0
33	MG	0	8074	1/1	0.98	0.19	23,23,23,23	0
33	MG	0	8112	1/1	0.98	0.04	43,43,43,43	0
37	SR	0	9422	1/1	0.98	0.10	54,54,54,54	0
37	SR	R	9418	1/1	0.98	0.13	54,54,54,54	0
33	MG	0	8009	1/1	0.98	0.10	28,28,28,28	0
37	SR	0	9464	1/1	0.98	0.04	74,74,74,74	0
38	CD	Z	9203	1/1	0.98	0.07	78,78,78,78	0
37	SR	0	9446	1/1	0.98	0.07	83,83,83,83	0
33	MG	0	8026	1/1	0.98	0.15	27,27,27,27	0
37	SR	0	9461	1/1	0.98	0.04	76,76,76,76	0
38	CD	3	9204	1/1	0.98	0.04	60,60,60,60	0
37	SR	0	9455	1/1	0.98	0.07	67,67,67,67	0
35	NA	0	9114	1/1	0.98	0.10	46,46,46,46	0
33	MG	0	8029	1/1	0.98	0.23	33,33,33,33	0
37	SR	0	9441	1/1	0.98	0.06	60,60,60,60	0
37	SR	0	9431	1/1	0.98	0.12	55,55,55,55	0
35	NA	0	9117	1/1	0.98	0.19	39,39,39,39	0
37	SR	0	9466	1/1	0.98	0.03	84,84,84,84	0
37	SR	S	9470	1/1	0.98	0.13	100,100,100,100	0
37	SR	0	9545	1/1	0.98	0.04	79,79,79,79	0
33	MG	0	8106	1/1	0.98	0.04	43,43,43,43	0
35	NA	0	9105	1/1	0.98	0.14	43,43,43,43	0
33	MG	K	8069	1/1	0.98	0.22	29,29,29,29	0
33	MG	0	8003	1/1	0.98	0.17	32,32,32,32	0
37	SR	0	9417	1/1	0.98	0.09	59,59,59,59	0
33	MG	0	8098	1/1	0.98	0.07	39,39,39,39	0
37	SR	0	9453	1/1	0.98	0.04	69,69,69,69	0
37	SR	0	9498	1/1	0.98	0.06	59,59,59,59	0
37	SR	0	9442	1/1	0.99	0.09	59,59,59,59	0
37	SR	0	9440	1/1	0.99	0.03	61,61,61,61	0
37	SR	9	9481	1/1	0.99	0.05	80,80,80,80	0
37	SR	0	9482	1/1	0.99	0.23	102,102,102,102	0
37	SR	A	9497	1/1	0.99	0.07	91,91,91,91	0
37	SR	0	9432	1/1	0.99	0.13	62,62,62,62	0
37	SR	0	9444	1/1	0.99	0.04	50,50,50,50	0
35	NA	0	9155	1/1	0.99	0.30	55,55,55,55	0
33	MG	0	8031	1/1	0.99	0.07	50,50,50,50	0
37	SR	0	9473	1/1	0.99	0.04	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	CL	0	9303	1/1	0.99	0.12	46,46,46,46	0
37	SR	A	9436	1/1	0.99	0.04	61,61,61,61	0
37	SR	0	9508	1/1	0.99	0.05	80,80,80,80	0
36	CL	0	9317	1/1	0.99	0.05	50,50,50,50	0
38	CD	O	9205	1/1	0.99	0.08	75,75,75,75	0
37	SR	0	9412	1/1	0.99	0.12	42,42,42,42	0
36	CL	R	9306	1/1	0.99	0.14	44,44,44,44	0
33	MG	0	8005	1/1	0.99	0.07	35,35,35,35	0
37	SR	B	9458	1/1	0.99	0.06	68,68,68,68	0
33	MG	0	8020	1/1	0.99	0.15	37,37,37,37	0
36	CL	Y	9320	1/1	0.99	0.06	43,43,43,43	0
37	SR	0	9462	1/1	0.99	0.09	64,64,64,64	0
37	SR	0	9457	1/1	0.99	0.07	47,47,47,47	0
33	MG	0	8017	1/1	0.99	0.15	28,28,28,28	0
37	SR	3	9439	1/1	0.99	0.05	63,63,63,63	0
37	SR	0	9428	1/1	0.99	0.04	49,49,49,49	0
37	SR	0	9423	1/1	0.99	0.08	54,54,54,54	0
33	MG	0	8002	1/1	0.99	0.16	28,28,28,28	0
37	SR	0	9408	1/1	0.99	0.14	39,39,39,39	0
35	NA	0	9106	1/1	0.99	0.19	37,37,37,37	0
37	SR	0	9433	1/1	0.99	0.10	76,76,76,76	0
37	SR	1	9460	1/1	0.99	0.08	52,52,52,52	0
37	SR	0	9407	1/1	0.99	0.12	43,43,43,43	0
36	CL	J	9301	1/1	0.99	0.08	53,53,53,53	0
35	NA	0	9136	1/1	0.99	0.11	34,34,34,34	0
37	SR	0	9629	1/1	0.99	0.07	65,65,65,65	0
33	MG	0	8025	1/1	0.99	0.37	25,25,25,25	0
36	CL	K	9312	1/1	0.99	0.06	46,46,46,46	0
37	SR	0	9420	1/1	0.99	0.12	56,56,56,56	0
33	MG	0	8008	1/1	0.99	0.21	17,17,17,17	0
37	SR	0	9426	1/1	0.99	0.07	67,67,67,67	0
33	MG	0	8004	1/1	0.99	0.11	30,30,30,30	0
33	MG	0	8068	1/1	0.99	0.10	46,46,46,46	0
37	SR	0	9410	1/1	0.99	0.12	37,37,37,37	0
37	SR	0	9415	1/1	0.99	0.10	50,50,50,50	0
33	MG	0	8038	1/1	0.99	0.25	20,20,20,20	0
37	SR	0	9450	1/1	0.99	0.09	62,62,62,62	0
38	CD	U	9201	1/1	0.99	0.10	48,48,48,48	0
36	CL	3	9304	1/1	0.99	0.08	55,55,55,55	0
36	CL	0	9305	1/1	0.99	0.08	54,54,54,54	0
37	SR	0	9416	1/1	0.99	0.11	43,43,43,43	0
37	SR	0	9451	1/1	0.99	0.10	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
37	SR	1	9419	1/1	0.99	0.11	40,40,40,40	0
37	SR	0	9456	1/1	0.99	0.07	69,69,69,69	0
37	SR	0	9406	1/1	0.99	0.18	38,38,38,38	0
35	NA	0	9135	1/1	0.99	0.15	50,50,50,50	0
33	MG	0	8070	1/1	0.99	0.16	26,26,26,26	0
37	SR	0	9478	1/1	0.99	0.07	70,70,70,70	0
37	SR	0	9411	1/1	0.99	0.12	40,40,40,40	0
38	CD	1	9202	1/1	0.99	0.05	51,51,51,51	0
36	CL	0	9314	1/1	0.99	0.06	45,45,45,45	0
36	CL	O	9308	1/1	0.99	0.06	60,60,60,60	0
37	SR	0	9449	1/1	0.99	0.08	59,59,59,59	0
37	SR	L	9409	1/1	1.00	0.11	40,40,40,40	0
37	SR	0	9424	1/1	1.00	0.13	45,45,45,45	0
37	SR	0	9413	1/1	1.00	0.10	44,44,44,44	0
37	SR	0	9448	1/1	1.00	0.05	60,60,60,60	0
37	SR	0	9430	1/1	1.00	0.13	44,44,44,44	0
37	SR	0	9443	1/1	1.00	0.09	57,57,57,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.