



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:26 PM GMT

PDB ID : 1VT2  
Title : Crystal structure of the E. coli ribosome bound to CEM-101. This file contains the 50S subunit of the second 70S ribosome.  
Authors : Dunkle, J.A.; Zhang, W.; Cate, J.H.D.; Mankin, A.S.  
Deposited on : 2010-09-06  
Resolution : 3.30 Å(reported)

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

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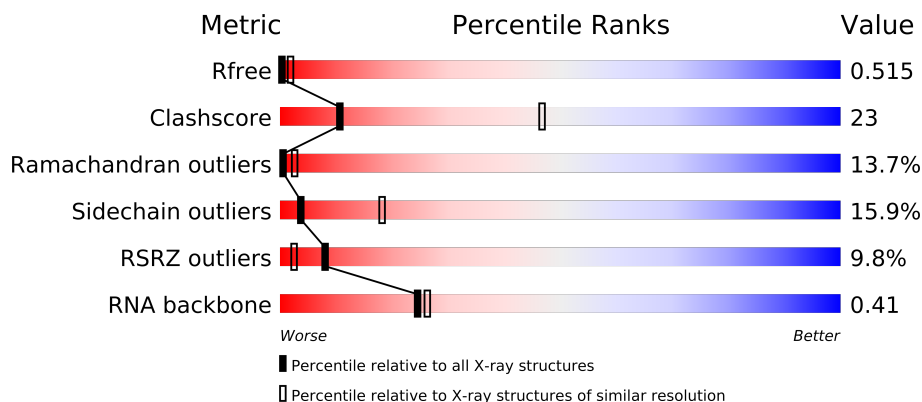
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)
RNA backbone	1838	1042 (3.90-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	2904	
2	B	120	
3	C	273	
4	D	209	
5	E	201	
6	F	179	
7	G	177	
8	H	149	
9	I	142	
10	J	142	
11	K	123	
12	L	144	

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Mol	Chain	Length	Quality of chain
13	M	136	
14	N	127	
15	O	117	
16	P	115	
17	Q	118	
18	R	103	
19	S	110	
20	T	100	
21	U	104	
22	V	94	
23	W	85	
24	X	78	
25	Y	63	
26	Z	59	
27	0	57	
28	1	55	
29	2	46	
30	3	65	
31	4	38	

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

Mol	Type	Chain	Res	Geometry	Electron density
32	MG	A	2906	-	X
32	MG	A	2909	-	X
32	MG	A	2913	-	X
32	MG	A	2915	-	X
32	MG	A	2917	-	X
32	MG	A	2919	-	X
32	MG	A	2923	-	X
32	MG	A	2925	-	X
32	MG	A	2930	-	X
32	MG	A	2933	-	X
32	MG	A	2936	-	X
32	MG	A	2937	-	X
32	MG	A	2938	-	X
32	MG	A	2942	-	X
32	MG	A	2960	-	X
32	MG	A	2961	-	X
32	MG	A	2962	-	X
32	MG	A	2964	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
32	MG	A	2966	-	X
32	MG	A	2967	-	X
32	MG	A	2979	-	X
32	MG	A	2982	-	X
32	MG	A	2983	-	X
32	MG	A	2992	-	X
32	MG	A	2995	-	X
32	MG	A	2996	-	X
32	MG	A	3001	-	X
32	MG	A	3002	-	X
32	MG	A	3012	-	X
32	MG	A	3013	-	X
32	MG	A	3019	-	X
32	MG	A	3027	-	X
32	MG	A	3031	-	X
32	MG	A	3034	-	X
32	MG	A	3036	-	X
32	MG	C	722	-	X
32	MG	J	747	-	X

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 90428 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	116	Total	C	N	O		0	0	0
			892	552	178	162				

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	117	Total	C	N	O		0	0	0
			947	604	192	151				

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	102	Total	C	N	O			
			779	492	146	141	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	94	Total	C	N	O	S			
			753	479	137	134	3	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	79	Total	C	N	O	S			
			596	367	120	108	1	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	77	Total	C	N	O	S			
			625	388	129	106	2	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	63	Total	C	N	O	S			
			509	313	99	95	2	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	58	Total	C	N	O	S			
			449	281	87	79	2	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	0	56	Total	C	N	O	S			
			444	269	94	80	1	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L33.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	B	1	Total	Mg	0	0
			1	1		
32	A	133	Total	Mg	0	0
			133	133		
32	C	1	Total	Mg	0	0
			1	1		
32	J	1	Total	Mg	0	0
			1	1		
32	E	1	Total	Mg	0	0
			1	1		

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	4	1	Total	Zn	0	0
			1	1		

- Molecule 34 is water.

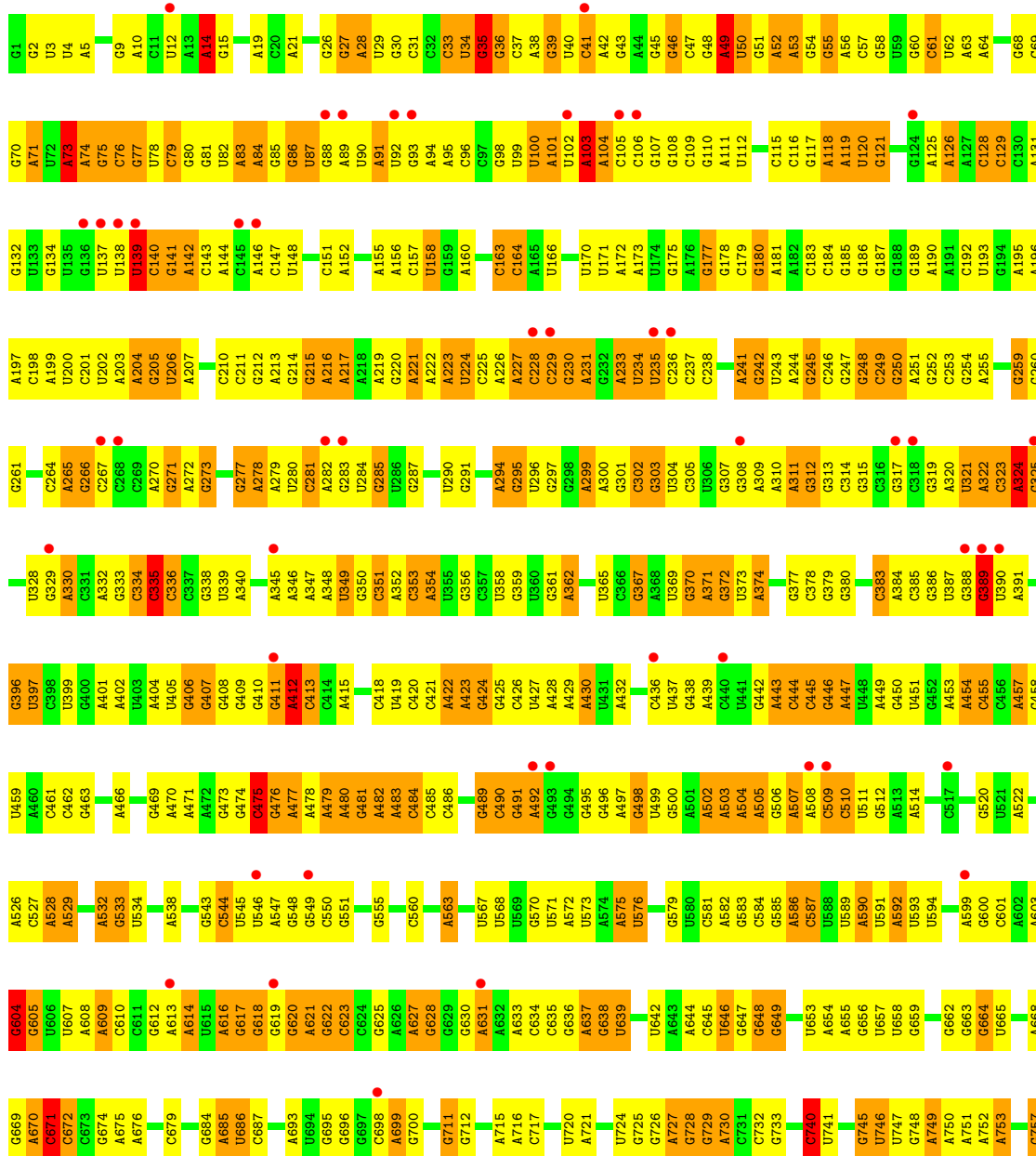
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	612	Total O 612 612	0	0
34	B	4	Total O 4 4	0	0
34	C	4	Total O 4 4	0	0
34	D	1	Total O 1 1	0	0
34	E	3	Total O 3 3	0	0
34	J	6	Total O 6 6	0	0
34	L	2	Total O 2 2	0	0
34	N	1	Total O 1 1	0	0
34	T	2	Total O 2 2	0	0
34	U	2	Total O 2 2	0	0
34	V	1	Total O 1 1	0	0
34	2	1	Total O 1 1	0	0
34	3	2	Total O 2 2	0	0
34	4	2	Total O 2 2	0	0

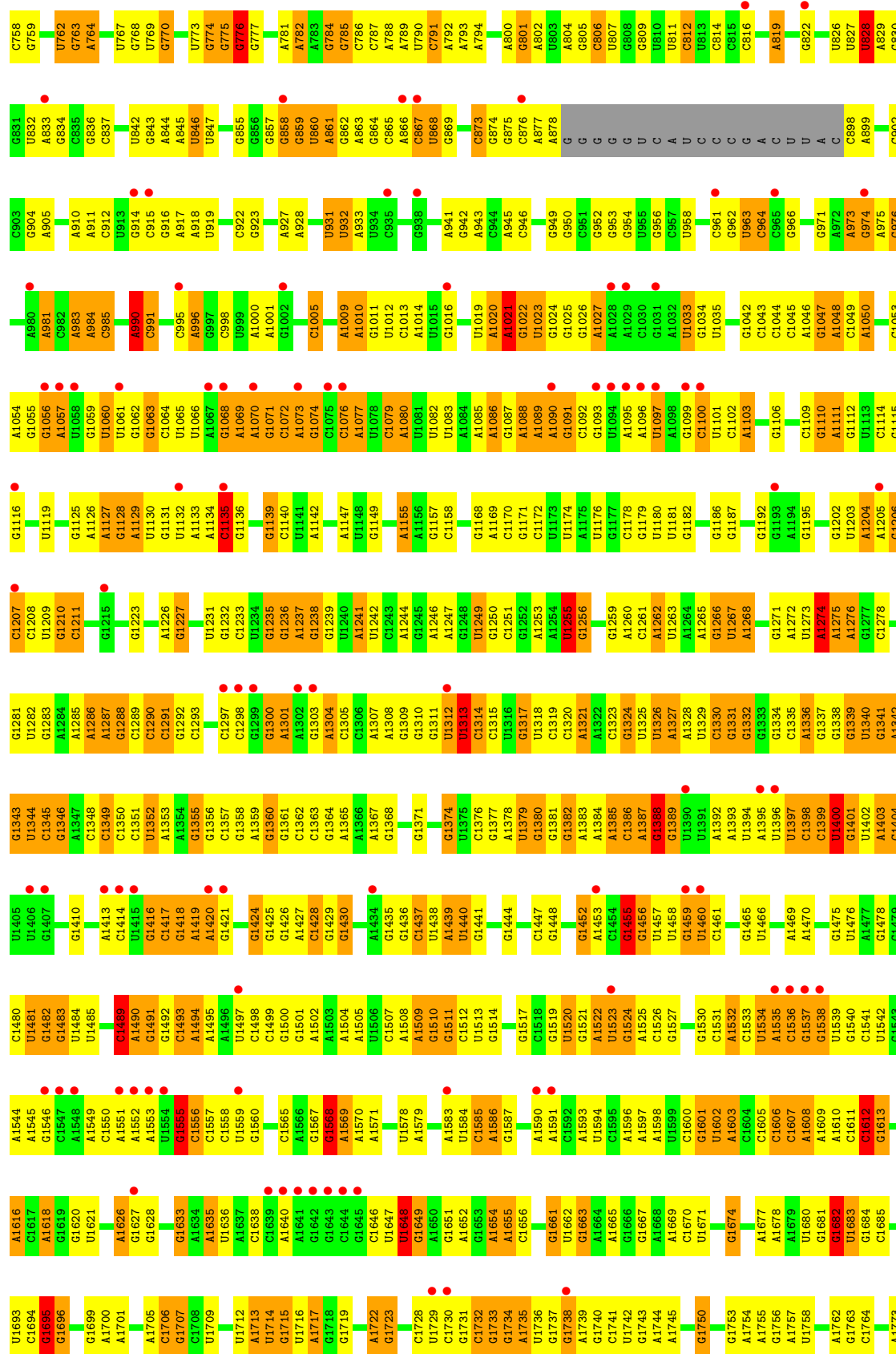
### 3 Residue-property plots

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

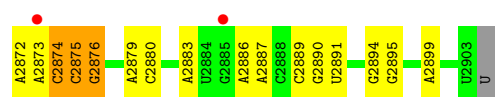
#### • Molecule 1: 23S rRNA

Chain A: 



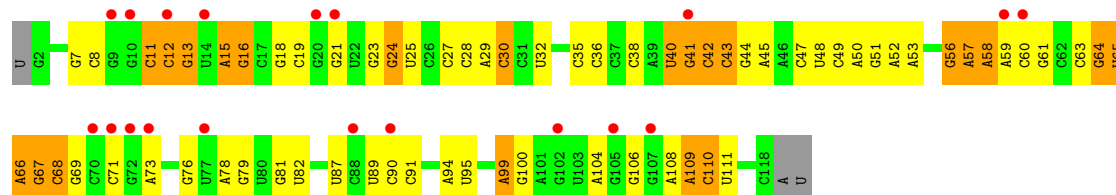


A2778	U2707	C2619	G2445	U2384	G2307	U2333	C	C2104	U2028	G1846	C1774
A2781	G2708	C2620	G2446	C2385	G2308	G2234	C	U2105	G2029	A1847	U1775
U2784	A2711	U2621	A2447	A2386	U2309	G2235	U	A2030	A1848	G1776	
C2785	C2712	G2623	A2448	A2387	C2310	U2236	U	G2107	A2031		
	U2713	G2624	G2454	A2388	A2311	G2237	G	A2108	U1856	U1779	
C2788	G2714	G2627	G2455	A2389	U2312	G2238	A	U2109	G1857	A1780	
		C2628	G2456	U2390	C2313	G2239	A	G2110	U1858	U1781	
G2718	G2718	U2629	G2458	G2391	A2314	G2243	A	U	U1859	U1782	
U2719	U2719	G2630	A2459	G2392	A2315	U2244	U	G	U1865	A1783	
U2720	G2631	U2632	U2460	U2393	G2316	G2245	A	U2037	U1866	A1784	
A2721	A2461	G2633	A2462	C2394	A2317	G2250	C	U2038	G1867		
	C2463	G2634	C2463	G2397	G2318	G2251	C	U1963	A1868	A1787	
A2725	U2552	U2553	C2466	U2398	U2320	G2252	A	G1964	G1869	C1788	
A2726	G2553	U2554	C2467	G2399	U2321	G2253	C	C2043	U1870	A1789	
A2727	U2555	U2556	C2468	G2400	A2322	G2254	C	C2044	G1871	C1790	
U2728	G2559	U2560	U2469	U2401	G2323	G2255	A	U2039	C1872	A1791	
U2729	U2563	U2564	A2469	U2402	U2324	G2256	C	G2040	G1873		
A2800	U2565	U2566	U2474	C2403	G2325	G2257	C	C2045	A1874		
U2807	G2566	A2566	C2475	U2404	G2330	G2258		G2048	C1875	C1795	
U2808	U2567	U2568	A2476	G2405	G2331	G2259		U2181	U1796	U1796	
A2809	G2569	U2569	U2477	A2406	G2332	G2260		U2182	G1876	G1797	
	A2478	G2570	A2478	A2407	U2333	G2261		U2183	A1877	U1798	
G2812	G2571	U2571	G2488	G2409	A2334	G2262		U2184	G1884	C1800	
C2815	U2572	U2572	U2489	G2410	A2335	G2263		U2185	A1889	A1801	
G2816	G2573	G2573	A2490	A2411	A2336	G2264		U2186	A1890	A1802	
A2820	U2574	U2574	U2491	A2412	G2337	G2265		U2187	A1891	A1803	
A2821	G2575	U2575	G2494	G2413	C2338	G2266		U2188	A1892		
C2824	U2576	U2576	G2495	G2414	C2339	G2267		U2189	A1893		
G2825	G2577	U2577	G2496	A2415	U2194	G2268		U2190	A1894		
	U2578	U2578	U2497	C2416	U2197	G2269		U2191	A1895		
U2831	U2579	U2579	A2498	G2417	A2198	G2270		U2192	A1896		
U2832	G2580	U2580	C2498	U2418	C2200	G2271		U2193	A1897		
U2833	U2581	U2581	G2502	U2419	G2201	G2272		U2194	A1898		
U2836	U2582	U2582	U2503	C2420	U2202	G2273		U2195	A1899		
U2837	U2583	U2583	A2504	G2421	U2203	G2274		U2196	A1900		
G2838	U2584	U2584	G2505	C2422	U2204	G2275		U2197	A1901		
	A2585	U2585	U2506	U2423	G2205	G2276		U2198	A1902		
U2844	A2586	U2586	A2513	A2424	U2206	G2277		U2199	A1903		
G2846	U2587	U2587	C2514	A2425	U2207	G2278		U2200	A1904		
U2847	A2588	U2588	C2515	A2426	U2208	G2279		U2201	A1905		
A2850	A2589	U2589	A2518	G2427	U2209	G2280		U2202	A1906		
A2851	C2601	U2601	U2519	C2428	U2210	G2281		U2203	A1907		
	G2602	U2602	C2520	G2429	U2211	G2282		U2204	A1908		
G2857	G2603	U2603	A2518	U2430	A2358	G2283		U2205	A1909		
	C2606	U2606	U2519	U2431	G2361	G2284		U2206	A1910		
A2860	G2607	U2607	C2520	A2432	G2362	U2291		U2207	A1911		
U2861	G2608	U2608	G2526	A2433	G2363	G2296		U2208	A1912		
G2862	U2609	U2609	U2527	A2434	G2371	U2297		U2209	A1913		
	C2610	U2610	C2528	A2435	U2372	A2297		U2210	A1914		
U2866	G2611	U2611	U2529	G2436	G2373	A2298		U2211	U1915		
G2867	C2612	U2612	G2529	U2437	G2374	U2299		U2212	U1916		
A2868	U2613	U2613	A2530	U2438	C2375	G2300		U2213	A1917		
G2869	A2531	U2614	C2532	A2439	G2376	C2301		U2214	A1918		
U2700	U2615	U2615	U2533	U2441	G2377	U2302		U2215	A1919		
A2776	U2616	U2616	A2534	C2442	G2378	U2303		U2216	A1920		
G2777	U2617	U2617	U2535	C2443	G2379	U2304		U2217	A1921		
	G2618	U2618	G2535	G2444	G2380	U2305		U2218	A1922		
					A2381	U2306		U2219	A1923		
					G2382			U2220	A1924		
					G2383			U2221	U1931		
								G2222	G1935		
								C2223	A1936		
								A2094	A1937		
								U2022	A1938		
								C2023	U1939		
								G2024	U1940		
								U2098	G1941		



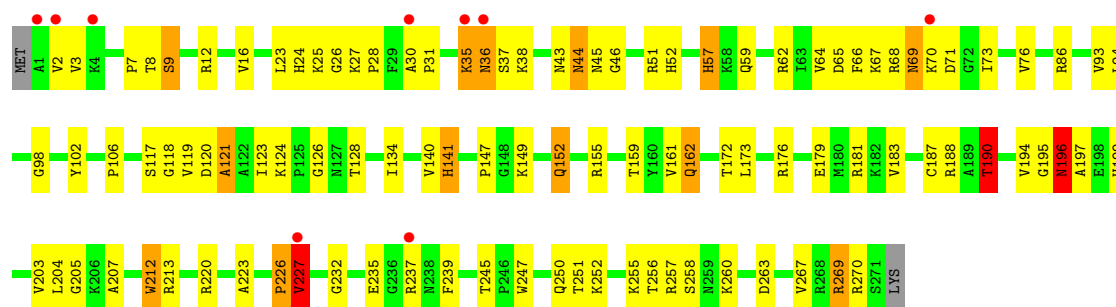
• Molecule 2: 5S rRNA

Chain B:



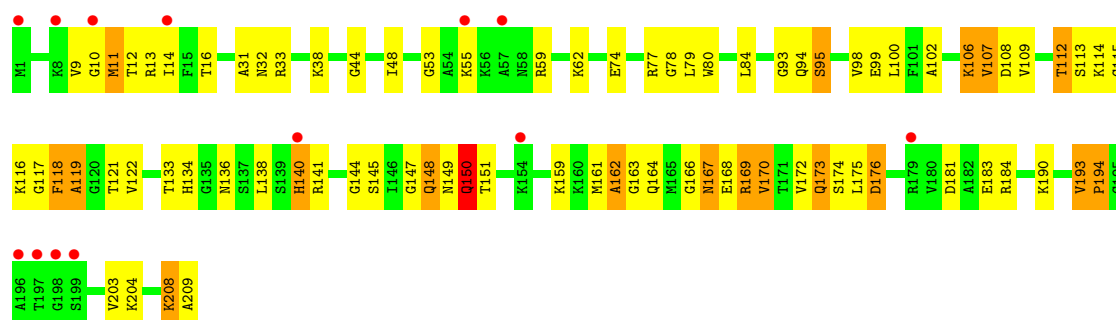
• Molecule 3: 50S ribosomal protein L2

Chain C:



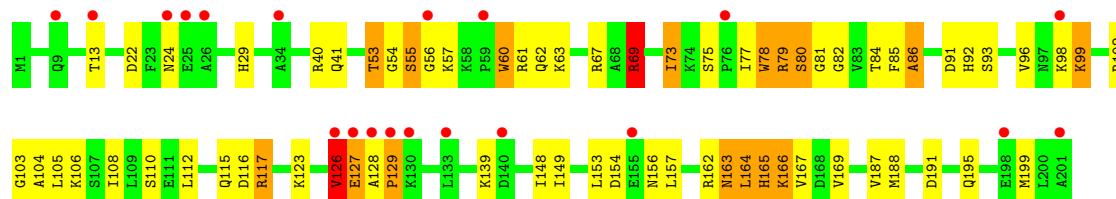
• Molecule 4: 50S ribosomal protein L3

Chain D:

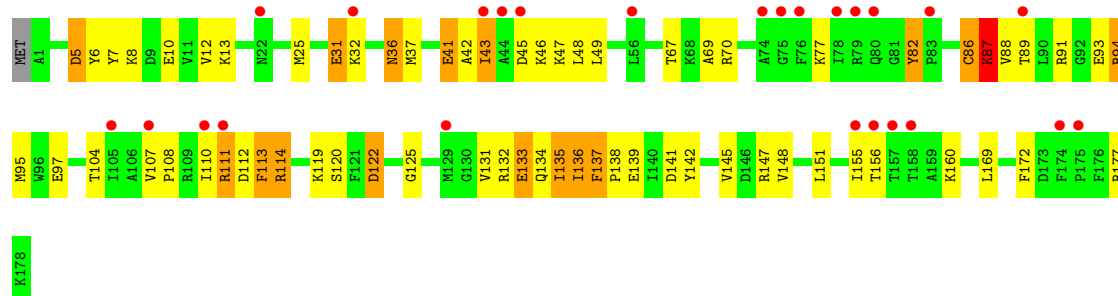


• Molecule 5: 50S ribosomal protein L4

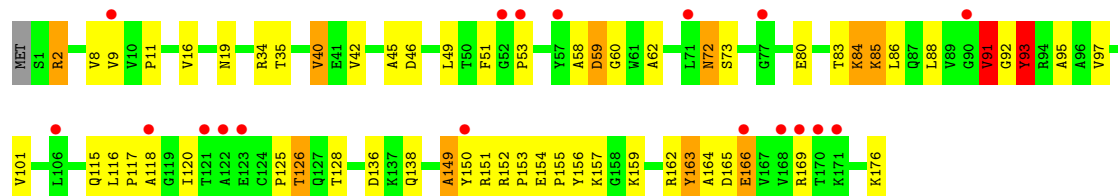
Chain E:



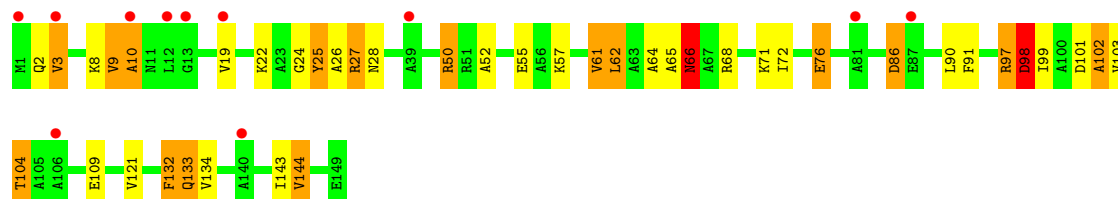
• Molecule 6: 50S ribosomal protein L5

Chain F: 

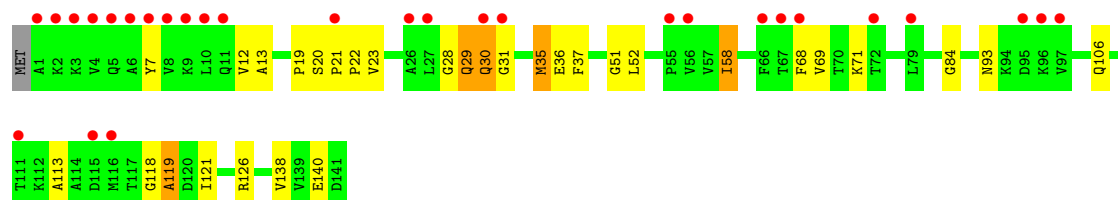
- Molecule 7: 50S ribosomal protein L6

Chain G: 

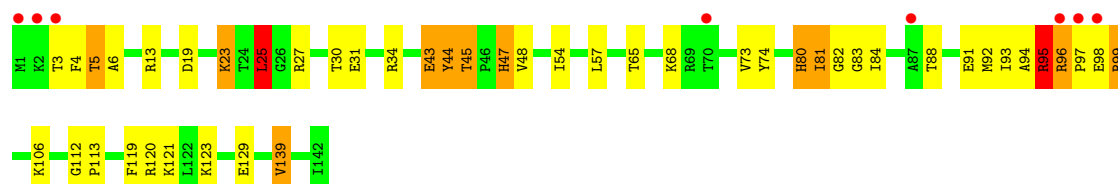
- Molecule 8: 50S ribosomal protein L9

Chain H: 

- Molecule 9: 50S ribosomal protein L11

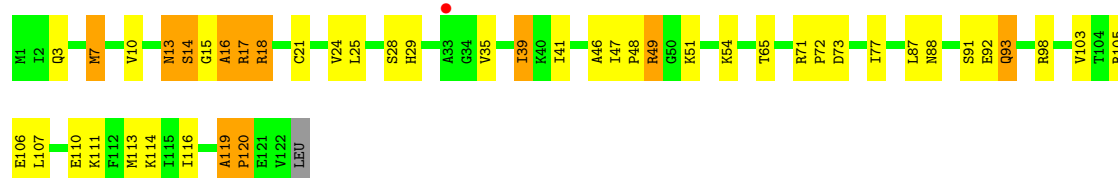
Chain I: 

- Molecule 10: 50S ribosomal protein L13

Chain J: 

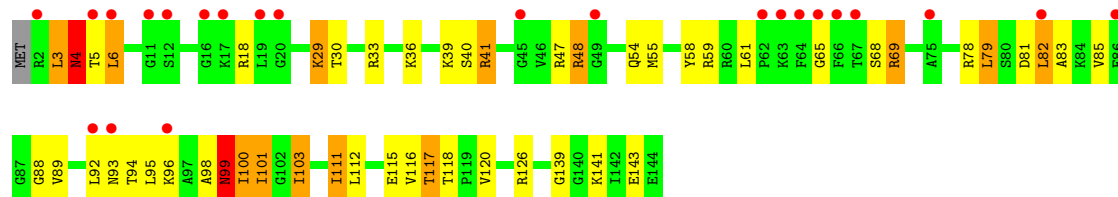
- Molecule 11: 50S ribosomal protein L14

Chain K: 



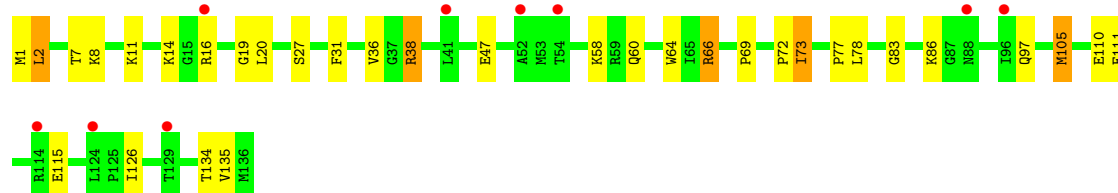
- Molecule 12: 50S ribosomal protein L15

Chain L: 



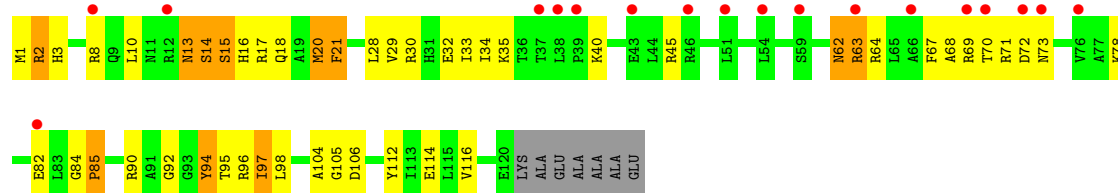
- Molecule 13: 50S ribosomal protein L16

Chain M: 



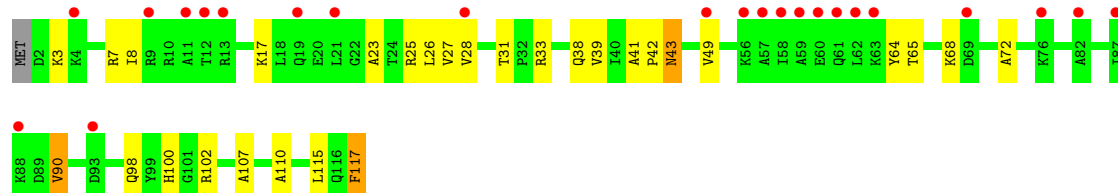
- Molecule 14: 50S ribosomal protein L17

Chain N: 



- Molecule 15: 50S ribosomal protein L18

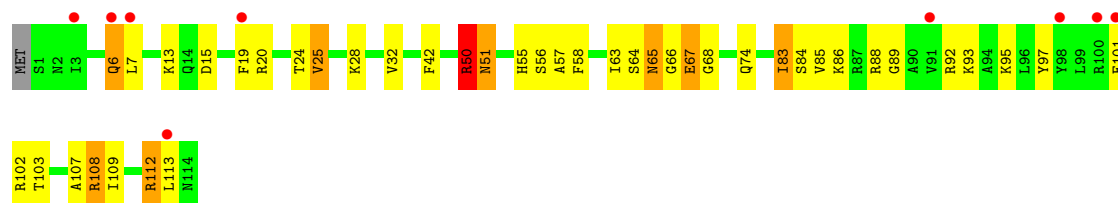
Chain O: 



- Molecule 16: 50S ribosomal protein L19

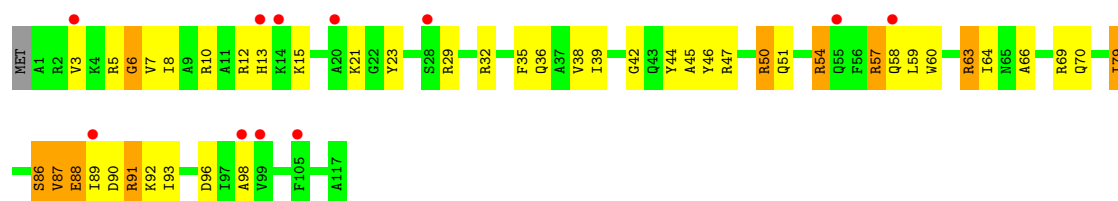


Chain P: 



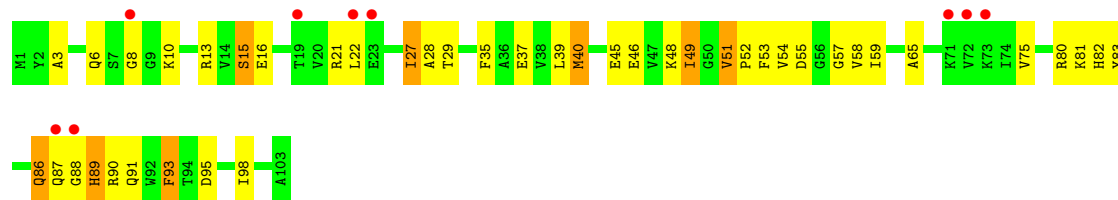
- Molecule 17: 50S ribosomal protein L20

Chain Q: 



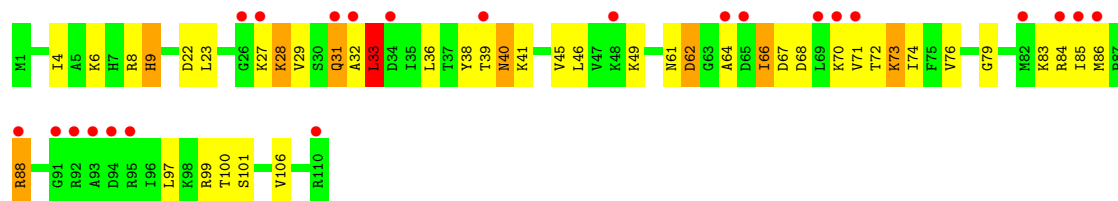
- Molecule 18: 50S ribosomal protein L21

Chain R: 



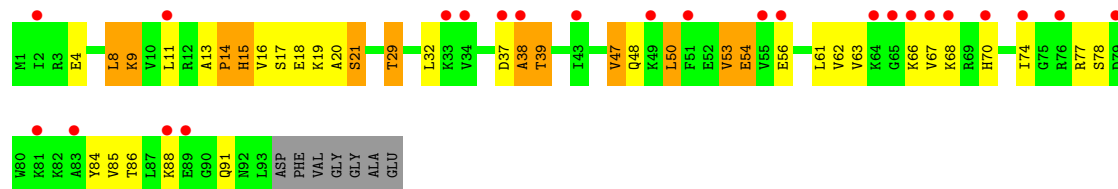
- Molecule 19: 50S ribosomal protein L22

Chain S: 



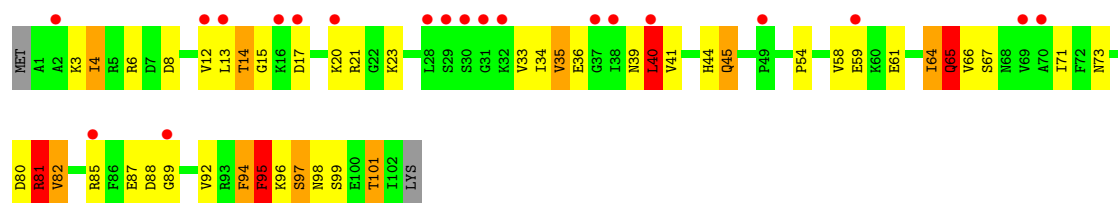
- Molecule 20: 50S ribosomal protein L23

Chain T: 



- Molecule 21: 50S ribosomal protein L24

Chain U: 



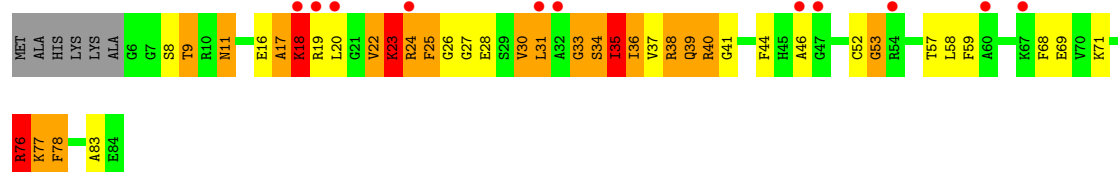
- Molecule 22: 50S ribosomal protein L25

Chain V:



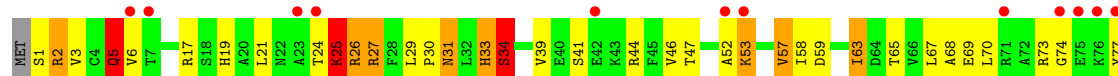
- Molecule 23: 50S ribosomal protein L27

Chain W:



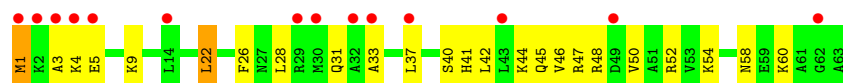
- Molecule 24: 50S ribosomal protein L28

Chain X:



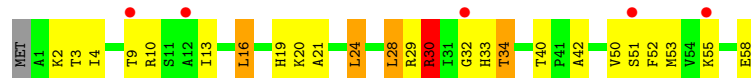
- Molecule 25: 50S ribosomal protein L29

Chain Y:



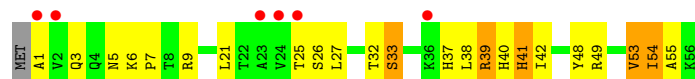
- Molecule 26: 50S ribosomal protein L30

Chain Z:



- Molecule 27: 50S ribosomal protein L32

Chain 0:



- Molecule 28: 50S ribosomal protein L33

Chain 1: 



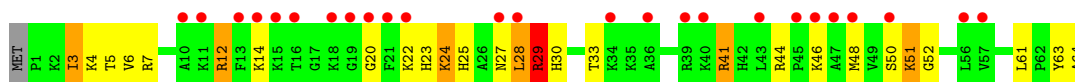
- Molecule 29: 50S ribosomal protein L34

Chain 2: 



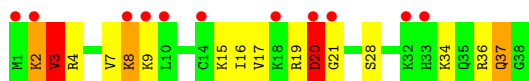
- Molecule 30: 50S ribosomal protein L35

Chain 3: 



- Molecule 31: 50S ribosomal protein L36

Chain 4: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.76Å 433.27Å 618.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.78 – 3.30 69.78 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.8 (69.78-3.30) 95.9 (69.78-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 3.13Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_501)	Depositor
R, $R_{free}$	0.187 , 0.244 0.515 , 0.515	Depositor DCC
$R_{free}$ test set	19610 reflections (2.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.1	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 72.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 971020 reflections	Xtriage
$F_o, F_c$ correlation	0.53	EDS
Total number of atoms	90428	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.38	0/68314	0.83	60/106569 (0.1%)
2	B	0.30	0/2803	0.76	1/4371 (0.0%)
3	C	0.32	0/2121	0.55	0/2852
4	D	0.31	0/1586	0.57	0/2134
5	E	0.27	0/1571	0.51	0/2113
6	F	0.24	0/1444	0.50	0/1937
7	G	0.24	0/1343	0.50	0/1816
8	H	0.29	0/1122	0.52	0/1515
9	I	0.22	0/1046	0.47	0/1410
10	J	0.29	0/1152	0.60	1/1551 (0.1%)
11	K	0.34	0/947	0.58	0/1268
12	L	0.28	0/1054	0.56	0/1403
13	M	0.29	0/1093	0.50	0/1460
14	N	0.30	0/973	0.53	0/1301
15	O	0.24	0/902	0.45	0/1209
16	P	0.32	0/929	0.52	0/1242
17	Q	0.30	0/960	0.47	0/1278
18	R	0.30	0/829	0.52	0/1107
19	S	0.29	0/864	0.54	1/1156 (0.1%)
20	T	0.26	0/744	0.54	0/994
21	U	0.26	0/787	0.51	0/1051
22	V	0.24	0/766	0.44	0/1025
23	W	0.29	0/603	0.54	0/797
24	X	0.28	0/635	0.58	0/848
25	Y	0.23	0/510	0.50	0/677
26	Z	0.28	0/453	0.53	0/605
27	0	0.30	0/450	0.52	0/599
28	1	0.27	0/416	0.49	0/554
29	2	0.30	0/380	0.54	0/498
30	3	0.29	0/513	0.56	0/676
31	4	0.33	0/303	0.53	0/397
All	All	0.35	0/97613	0.76	63/146413 (0.0%)

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	C	C2-N1-C1'	6.54	125.99	118.80
1	A	1428	C	C2-N1-C1'	-6.53	111.62	118.80
10	J	25	LEU	CA-CB-CG	6.38	129.97	115.30
1	A	740	C	C6-N1-C2	6.25	122.80	120.30
1	A	2405	G	C4-N9-C1'	6.17	134.53	126.50
1	A	776	G	C4-N9-C1'	6.14	134.48	126.50
1	A	828	U	C2-N1-C1'	5.99	124.89	117.70
1	A	1799	G	N3-C4-C5	-5.89	125.66	128.60
1	A	2620	C	C6-N1-C2	5.84	122.64	120.30
1	A	1255	U	C2-N1-C1'	5.73	124.58	117.70
1	A	774	G	C4-N9-C1'	-5.70	119.09	126.50
1	A	757	G	N3-C4-C5	5.68	131.44	128.60
1	A	246	C	C6-N1-C2	5.62	122.55	120.30
1	A	1428	C	C6-N1-C1'	5.61	127.53	120.80
1	A	2405	G	C8-N9-C1'	-5.61	119.70	127.00
1	A	475	C	C2-N1-C1'	5.57	124.92	118.80
1	A	1021	A	C3'-C2'-C1'	5.54	105.93	101.50
1	A	139	U	C2-N1-C1'	5.50	124.30	117.70
1	A	1568	G	C8-N9-C1'	-5.48	119.87	127.00
1	A	2310	C	C3'-C2'-C1'	5.43	105.84	101.50
19	S	97	LEU	CA-CB-CG	5.41	127.75	115.30
1	A	49	A	C3'-C2'-C1'	5.37	105.80	101.50
1	A	476	G	C4-N9-C1'	5.36	133.47	126.50
1	A	671	C	C2-N1-C1'	5.36	124.69	118.80
1	A	1455	G	C3'-C2'-C1'	5.36	105.78	101.50
1	A	335	C	C6-N1-C1'	-5.34	114.39	120.80
1	A	2061	G	N1-C6-O6	5.28	123.07	119.90
1	A	2347	C	C3'-C2'-C1'	5.28	105.72	101.50
1	A	2682	A	C3'-C2'-C1'	5.26	105.71	101.50
1	A	389	G	C3'-C2'-C1'	5.25	105.70	101.50
1	A	412	A	C3'-C2'-C1'	5.24	105.69	101.50
1	A	1314	C	C2-N1-C1'	5.23	124.56	118.80
1	A	1274	A	C3'-C2'-C1'	5.23	105.68	101.50
1	A	73	A	C3'-C2'-C1'	5.22	105.68	101.50
1	A	2615	U	C3'-C2'-C1'	5.22	105.67	101.50
1	A	1648	U	C3'-C2'-C1'	5.21	105.67	101.50
1	A	1555	G	C3'-C2'-C1'	5.21	105.67	101.50
1	A	35	G	C3'-C2'-C1'	5.21	105.66	101.50
1	A	1568	G	C4-N9-C1'	5.20	133.26	126.50
1	A	2458	G	C4-N9-C1'	5.20	133.25	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1400	U	C3'-C2'-C1'	5.19	105.65	101.50
1	A	1682	G	C3'-C2'-C1'	5.16	105.63	101.50
1	A	1612	C	C3'-C2'-C1'	5.15	105.62	101.50
1	A	990	A	C3'-C2'-C1'	5.14	105.61	101.50
1	A	1915	U	C3'-C2'-C1'	5.12	105.60	101.50
1	A	475	C	C6-N1-C1'	-5.12	114.65	120.80
1	A	1695	G	C3'-C2'-C1'	5.12	105.60	101.50
1	A	1388	G	C3'-C2'-C1'	5.12	105.59	101.50
1	A	1439	A	C4-C5-C6	5.11	119.56	117.00
1	A	103	A	C3'-C2'-C1'	5.11	105.58	101.50
1	A	2656	U	C3'-C2'-C1'	5.09	105.57	101.50
1	A	2777	G	C3'-C2'-C1'	5.08	105.56	101.50
1	A	1489	C	C3'-C2'-C1'	5.07	105.56	101.50
1	A	1799	G	C4-N9-C1'	5.07	133.09	126.50
1	A	604	G	C3'-C2'-C1'	5.06	105.55	101.50
2	B	41	G	C4-N9-C1'	5.06	133.08	126.50
1	A	1789	A	C8-N9-C4	5.06	107.82	105.80
1	A	324	A	C3'-C2'-C1'	5.04	105.53	101.50
1	A	2752	C	C3'-C2'-C1'	5.04	105.53	101.50
1	A	2727	A	C3'-C2'-C1'	5.03	105.53	101.50
1	A	1135	C	C3'-C2'-C1'	5.03	105.52	101.50
1	A	14	A	C3'-C2'-C1'	5.02	105.52	101.50
1	A	1313	U	N3-C2-O2	-5.02	118.69	122.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	60995	0	0	1547	0
2	B	2507	0	0	67	0
3	C	2082	0	0	41	0
4	D	1565	0	0	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1552	0	0	26	0
6	F	1420	0	12	17	0
7	G	1323	0	0	19	0
8	H	1111	0	0	15	0
9	I	1032	0	0	7	0
10	J	1129	0	0	26	0
11	K	938	0	0	12	0
12	L	1045	0	0	26	0
13	M	1074	0	0	9	0
14	N	960	0	0	24	0
15	O	892	0	0	11	0
16	P	917	0	0	21	0
17	Q	947	0	0	28	0
18	R	816	0	0	15	0
19	S	857	0	0	16	0
20	T	738	0	0	13	0
21	U	779	0	0	16	0
22	V	753	0	0	10	0
23	W	596	0	0	31	0
24	X	625	0	0	21	0
25	Y	509	0	0	12	0
26	Z	449	0	0	8	0
27	0	444	0	0	9	0
28	1	409	0	0	6	0
29	2	377	0	0	16	0
30	3	504	0	0	13	0
31	4	302	0	0	7	0
32	A	133	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	E	1	0	0	0	0
32	J	1	0	0	0	0
33	4	1	0	0	0	0
34	2	1	0	0	1	0
34	3	2	0	0	0	0
34	4	2	0	0	0	0
34	A	612	0	0	23	0
34	B	4	0	0	1	0
34	C	4	0	0	0	0
34	D	1	0	0	0	0
34	E	3	0	0	0	0
34	J	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	L	2	0	0	0	0
34	N	1	0	0	0	0
34	T	2	0	0	0	0
34	U	2	0	0	0	0
34	V	1	0	0	0	0
All	All	90428	0	12	1981	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

All (1981) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:216:A:O2'	1:A:217:A:C8	2.20	0.94
2:B:57:A:O2'	2:B:58:A:C8	2.24	0.91
1:A:1809:A:O2'	1:A:1810:A:C8	2.26	0.88
1:A:1135:C:N4	1:A:1139:G:C6	2.45	0.84
1:A:975:A:O2'	1:A:976:G:C8	2.30	0.83
1:A:1489:C:C4'	1:A:1490:A:OP1	2.26	0.83
2:B:12:C:C4'	2:B:13:G:OP1	2.25	0.83
1:A:1847:A:O2'	1:A:1848:A:C8	2.31	0.82
1:A:2197:U:O2'	1:A:2198:A:C8	2.32	0.82
1:A:2336:A:N7	23:W:40:ARG:CZ	2.42	0.81
1:A:1913:A:C4'	1:A:1914:C:OP1	2.29	0.80
1:A:310:A:O2'	1:A:311:A:C8	2.35	0.80
1:A:867:C:O2'	1:A:868:U:C6	2.35	0.79
1:A:2297:A:O2'	1:A:2298:A:C8	2.36	0.78
1:A:412:A:N6	1:A:2412:A:O4'	2.17	0.77
1:A:1071:G:N7	1:A:1089:A:C6	2.53	0.77
1:A:482:A:N6	1:A:506:G:C4	2.52	0.76
1:A:226:A:C2	1:A:230:G:O6	2.38	0.76
1:A:762:U:C4'	1:A:763:G:O5'	2.33	0.76
1:A:2093:G:O6	1:A:2225:A:C8	2.38	0.76
1:A:1780:A:OP1	34:A:3521:HOH:O	2.04	0.75
1:A:84:A:C5	1:A:103:A:N6	2.55	0.75
1:A:1857:G:O2'	1:A:1884:G:N2	2.19	0.75
1:A:1606:C:O2'	1:A:1607:C:OP2	2.04	0.75
1:A:2056:G:C2	1:A:2057:G:C8	2.74	0.74
1:A:1387:A:N6	1:A:1401:G:C6	2.54	0.74
1:A:2261:C:C2	1:A:2280:G:N2	2.56	0.74
1:A:163:C:O2'	1:A:164:C:O4'	2.05	0.74
1:A:118:A:C8	1:A:119:A:C8	2.76	0.74
1:A:2333:A:C2	1:A:2335:A:N6	2.55	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1210:G:C6	1:A:1237:A:N7	2.56	0.74
1:A:335:C:O2'	1:A:336:C:C6	2.40	0.74
1:A:532:A:N1	1:A:2020:A:O2'	2.21	0.73
1:A:223:A:N6	1:A:422:A:N6	2.37	0.73
1:A:2875:C:O2'	1:A:2876:G:C8	2.41	0.73
1:A:984:A:O2'	1:A:985:C:OP1	2.06	0.73
1:A:2056:G:N2	27:0:1:ALA:N	2.36	0.73
1:A:128:C:O2'	1:A:129:C:C6	2.42	0.73
1:A:1343:G:O2'	1:A:1344:U:C6	2.41	0.73
1:A:616:A:O2'	1:A:617:G:C8	2.42	0.73
1:A:454:A:C4'	1:A:455:C:OP2	2.36	0.72
1:A:379:G:C6	1:A:396:G:O6	2.42	0.72
1:A:1521:G:C6	1:A:1522:A:N6	2.57	0.72
4:D:118:PHE:CD1	4:D:119:ALA:N	2.58	0.72
2:B:18:G:C2	2:B:67:G:O6	2.43	0.72
1:A:2571:U:C4	1:A:2574:G:C8	2.78	0.71
1:A:422:A:O2'	1:A:423:A:C8	2.43	0.71
1:A:1343:G:C5	1:A:1597:A:N6	2.58	0.71
7:G:93:TYR:N	7:G:93:TYR:CD2	2.55	0.71
1:A:1648:U:O2'	1:A:1649:G:O4'	2.08	0.71
1:A:1416:G:C6	1:A:1417:C:N4	2.57	0.71
1:A:410:G:C6	1:A:2407:A:N6	2.58	0.71
1:A:396:G:O2'	1:A:397:U:C6	2.43	0.71
1:A:1324:G:O2'	1:A:1616:A:C6	2.44	0.71
1:A:1056:G:N2	1:A:1102:C:C5	2.58	0.71
1:A:302:C:O2'	1:A:303:G:C8	2.42	0.71
1:A:1281:G:C6	1:A:1290:C:N4	2.58	0.71
1:A:132:G:N2	1:A:148:U:C2	2.58	0.71
1:A:397:U:OP1	24:X:30:PRO:CA	2.39	0.71
12:L:81:ASP:O	12:L:83:ALA:N	2.23	0.71
1:A:68:G:N2	1:A:74:A:OP2	2.24	0.71
1:A:2298:A:O2'	1:A:2299:U:C6	2.44	0.70
1:A:502:A:C5	1:A:505:A:N7	2.59	0.70
1:A:301:G:C6	1:A:302:C:N4	2.59	0.70
1:A:1352:U:C5	1:A:1377:G:C6	2.79	0.70
1:A:1682:G:O2'	1:A:1683:U:C6	2.43	0.70
1:A:1797:G:O3'	3:C:255:LYS:O	2.09	0.70
1:A:5:A:C2	1:A:2899:A:C2	2.79	0.70
1:A:1809:A:C2	1:A:1810:A:C4	2.80	0.69
1:A:675:A:OP1	5:E:60:TRP:CZ2	2.45	0.69
1:A:2212:A:C8	1:A:2214:C:N4	2.61	0.69
1:A:1938:A:OP2	34:A:3559:HOH:O	2.11	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2788:C:O2'	1:A:2809:A:N3	2.25	0.69
1:A:332:A:C4	1:A:335:C:N4	2.61	0.69
1:A:226:A:C4	1:A:227:A:N7	2.61	0.69
1:A:1722:A:N6	1:A:1739:A:C8	2.61	0.69
1:A:2850:A:N7	1:A:2868:A:O2'	2.25	0.69
1:A:2336:A:N7	23:W:40:ARG:NH2	2.40	0.69
29:2:15:SER:O	29:2:16:HIS:CD2	2.45	0.69
23:W:40:ARG:NH1	23:W:40:ARG:CG	2.55	0.68
21:U:95:PHE:O	21:U:97:SER:N	2.26	0.68
1:A:1388:G:N1	1:A:1400:U:N3	2.40	0.68
2:B:56:G:C4'	2:B:57:A:O5'	2.41	0.68
1:A:142:A:O2'	1:A:143:C:C6	2.46	0.68
1:A:229:C:O2'	1:A:230:G:O4'	2.10	0.68
1:A:1303:G:O2'	1:A:1304:A:C8	2.47	0.68
24:X:31:ASN:ND2	24:X:31:ASN:N	2.41	0.68
1:A:1315:C:OP2	34:A:3587:HOH:O	2.12	0.68
1:A:1439:A:N7	1:A:1440:U:C1'	2.57	0.68
1:A:956:G:C2	1:A:962:G:O6	2.47	0.67
1:A:227:A:C4'	1:A:228:C:OP1	2.42	0.67
1:A:21:A:C2	1:A:520:G:C2	2.82	0.67
1:A:1716:U:O2'	1:A:1717:A:C8	2.47	0.67
1:A:2331:G:N1	1:A:2385:C:N4	2.43	0.67
1:A:1357:C:C5	34:A:3256:HOH:O	2.47	0.67
1:A:2667:C:O2'	1:A:2668:G:C8	2.48	0.67
6:F:136:ILE:O	6:F:137:PHE:O	2.13	0.67
1:A:1063:G:C6	1:A:1064:C:N4	2.63	0.67
1:A:822:G:O6	1:A:943:A:C2	2.48	0.67
1:A:187:G:C2	1:A:210:C:C2	2.84	0.66
1:A:1973:G:C6	1:A:1974:C:C4	2.83	0.66
1:A:2540:C:C2	1:A:2541:A:C8	2.83	0.66
1:A:1400:U:O2'	1:A:1401:G:O4'	2.13	0.66
2:B:13:G:N2	2:B:16:G:C4	2.64	0.66
1:A:617:G:O2'	1:A:618:G:C8	2.48	0.66
1:A:1510:G:N2	1:A:1511:G:C4	2.63	0.66
1:A:2264:C:C2	1:A:2277:G:N2	2.64	0.66
1:A:241:A:C8	1:A:243:U:C4	2.84	0.66
1:A:1385:A:C4'	1:A:1386:C:OP1	2.43	0.65
1:A:1568:G:N2	3:C:57:HIS:CE1	2.64	0.65
1:A:1109:C:C5	1:A:1110:G:C6	2.84	0.65
14:N:28:LEU:O	14:N:32:GLU:N	2.30	0.65
1:A:223:A:C5	1:A:422:A:N7	2.65	0.65
1:A:63:A:N6	1:A:91:A:N6	2.44	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2836:U:O2'	1:A:2837:A:C8	2.49	0.65
1:A:2147:A:OP1	1:A:2147:A:C4'	2.45	0.65
1:A:2468:A:O2'	1:A:2469:A:C8	2.50	0.65
1:A:1654:A:O2'	1:A:1655:A:O4'	2.15	0.65
1:A:845:A:N6	1:A:932:U:N3	2.45	0.65
1:A:752:A:O2'	1:A:753:A:OP2	2.15	0.65
1:A:2332:C:O2'	23:W:40:ARG:NH2	2.30	0.64
1:A:249:C:C5'	1:A:2394:C:O2'	2.45	0.64
1:A:769:U:C4	1:A:770:G:N7	2.65	0.64
1:A:1358:G:N2	1:A:1374:G:C6	2.65	0.64
1:A:1973:G:C6	1:A:1974:C:N4	2.66	0.64
1:A:2627:G:O2'	1:A:2781:A:N1	2.31	0.64
2:B:52:A:O2'	2:B:53:A:C8	2.51	0.64
1:A:2093:G:N2	1:A:2094:A:C4	2.66	0.64
1:A:1416:G:C4	1:A:1417:C:C5	2.86	0.64
2:B:109:A:C2	2:B:110:C:C2	2.86	0.64
1:A:1281:G:C2	1:A:1290:C:N3	2.65	0.64
1:A:764:A:C2	1:A:781:A:C2	2.85	0.64
1:A:303:G:C2	1:A:304:U:C2	2.86	0.64
11:K:15:GLY:O	11:K:16:ALA:O	2.16	0.64
1:A:324:A:O2'	1:A:325:G:O4'	2.16	0.64
1:A:319:G:C6	1:A:333:G:N1	2.66	0.64
21:U:95:PHE:CD1	21:U:95:PHE:N	2.64	0.63
1:A:279:A:N6	1:A:361:G:O2'	2.31	0.63
1:A:2135:A:C2'	1:A:2136:G:O4'	2.46	0.63
1:A:2666:C:O2'	1:A:2667:C:C5'	2.46	0.63
7:G:154:GLU:O	7:G:156:TYR:N	2.30	0.63
1:A:630:G:N2	1:A:633:A:OP2	2.31	0.63
1:A:2550:G:C2	1:A:2559:C:O2	2.51	0.63
1:A:223:A:N6	1:A:422:A:C6	2.67	0.63
1:A:1817:G:O2'	1:A:1818:U:C5'	2.46	0.63
1:A:230:G:N2	1:A:231:A:C5	2.67	0.63
1:A:857:G:N7	1:A:858:G:C8	2.66	0.63
1:A:137:U:C4	1:A:138:U:C2	2.86	0.63
1:A:2622:U:O2'	1:A:2825:G:N7	2.32	0.63
1:A:1313:U:C2'	1:A:1313:U:O2	2.46	0.63
1:A:2815:C:O2	27:O:40:HIS:CE1	2.52	0.63
1:A:152:A:C2	1:A:175:G:C2	2.87	0.63
1:A:200:U:C5	1:A:201:C:C4	2.87	0.63
1:A:1608:A:N7	1:A:1611:C:N4	2.46	0.62
4:D:117:GLY:O	4:D:119:ALA:N	2.32	0.62
2:B:42:C:O2'	2:B:43:C:C5'	2.46	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1059:G:N1	1:A:1088:A:C2	2.67	0.62
1:A:1398:C:O2'	1:A:1399:C:O4'	2.18	0.62
1:A:2345:G:C8	1:A:2347:C:C5	2.87	0.62
1:A:2345:G:C6	1:A:2347:C:N4	2.67	0.62
1:A:2812:G:N2	1:A:2889:C:C2	2.67	0.62
1:A:185:G:C6	1:A:212:G:C2	2.87	0.62
1:A:311:A:O2'	1:A:312:G:OP1	2.17	0.62
1:A:503:A:C4	1:A:506:G:N7	2.67	0.62
2:B:109:A:O2'	2:B:110:C:C6	2.53	0.62
1:A:1417:C:C2'	1:A:1418:G:C8	2.82	0.62
1:A:529:A:C8	1:A:2023:C:N4	2.68	0.62
1:A:503:A:C4'	1:A:504:A:O5'	2.47	0.62
1:A:479:A:C4'	1:A:480:A:OP1	2.47	0.62
1:A:2344:U:C4'	1:A:2345:G:OP1	2.48	0.62
10:J:43:GLU:O	10:J:45:THR:N	2.33	0.62
2:B:49:C:OP1	15:O:102:ARG:N	2.33	0.62
1:A:1345:C:C5'	1:A:1396:U:O4	2.48	0.61
1:A:1358:G:C5	34:A:3256:HOH:O	2.53	0.61
1:A:192:C:OP1	34:A:3566:HOH:O	2.16	0.61
1:A:975:A:O2'	1:A:976:G:O5'	2.17	0.61
1:A:1439:A:C2	1:A:1553:A:N7	2.68	0.61
1:A:1552:A:O2'	1:A:1553:A:C5'	2.49	0.61
1:A:201:C:C4	1:A:202:U:C5	2.88	0.61
1:A:311:A:C2	1:A:328:U:O4	2.53	0.61
1:A:1255:U:O2'	1:A:1256:G:OP1	2.18	0.61
1:A:749:A:C5	1:A:750:A:N7	2.68	0.61
2:B:16:G:O6	2:B:69:G:C5	2.53	0.61
1:A:686:U:OP2	34:A:3550:HOH:O	2.16	0.61
1:A:1019:U:O2'	1:A:1021:A:N1	2.34	0.61
13:M:27:SER:N	13:M:66:ARG:NH2	2.49	0.61
1:A:2406:A:OP2	1:A:2411:A:N6	2.34	0.61
1:A:2406:A:C2	12:L:69:ARG:NH2	2.68	0.61
10:J:4:PHE:O	10:J:44:TYR:CZ	2.53	0.61
1:A:508:A:N6	19:S:9:HIS:CE1	2.68	0.61
1:A:379:G:C6	1:A:396:G:C6	2.89	0.61
1:A:1071:G:N7	1:A:1089:A:C5	2.69	0.60
1:A:538:A:N6	1:A:555:G:O2'	2.34	0.60
1:A:151:C:OP1	1:A:1359:A:O2'	2.19	0.60
1:A:2022:U:O2'	1:A:2616:C:O2'	2.18	0.60
1:A:867:C:O2'	1:A:868:U:O5'	2.18	0.60
1:A:1551:A:C4	1:A:1552:A:C8	2.89	0.60
1:A:379:G:C6	1:A:380:G:C5	2.90	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:48:ARG:NH1	12:L:48:ARG:CG	2.64	0.60
1:A:2638:G:O2'	1:A:2639:A:C8	2.55	0.60
1:A:2:G:C6	1:A:3:U:C4	2.90	0.60
1:A:226:A:N6	1:A:227:A:N6	2.50	0.60
1:A:1521:G:C6	1:A:1522:A:C6	2.89	0.60
1:A:1844:C:O3'	3:C:255:LYS:NZ	2.34	0.60
1:A:2850:A:OP2	1:A:2866:U:N3	2.35	0.60
1:A:2234:G:C5	1:A:2235:G:C8	2.89	0.60
1:A:1286:A:O2'	1:A:1288:G:N2	2.35	0.60
1:A:478:A:N1	1:A:480:A:C4	2.70	0.60
1:A:1249:U:O2'	1:A:1250:G:OP2	2.19	0.60
17:Q:46:TYR:CZ	17:Q:50:ARG:NH1	2.70	0.60
1:A:1608:A:C8	1:A:1611:C:N4	2.70	0.59
1:A:247:G:N7	1:A:249:C:C2	2.70	0.59
1:A:2313:C:O2'	1:A:2314:A:C8	2.54	0.59
4:D:140:HIS:CD2	4:D:140:HIS:N	2.69	0.59
1:A:532:A:C4	1:A:2021:C:O2	2.55	0.59
1:A:242:G:C8	30:3:3:ILE:O	2.55	0.59
1:A:481:G:O2'	1:A:507:A:N6	2.35	0.59
1:A:80:G:O2'	1:A:346:A:C2	2.55	0.59
1:A:311:A:O2'	1:A:332:A:O4'	2.21	0.59
1:A:370:G:N1	1:A:424:G:C5	2.70	0.59
1:A:410:G:N1	1:A:2407:A:N6	2.49	0.59
1:A:647:G:C5	1:A:648:G:N7	2.70	0.59
1:A:1475:G:O2'	1:A:1476:U:C6	2.55	0.59
4:D:149:ASN:O	4:D:151:THR:N	2.35	0.59
1:A:2478:A:N7	1:A:2529:G:C6	2.69	0.59
1:A:560:C:O2	17:Q:47:ARG:NH1	2.35	0.59
1:A:33:C:C4'	1:A:34:U:OP1	2.51	0.59
1:A:301:G:C5	1:A:302:C:N4	2.71	0.59
1:A:2776:A:C4'	1:A:2777:G:O5'	2.50	0.59
1:A:1413:A:C6	1:A:1414:C:N4	2.71	0.59
1:A:483:A:C8	21:U:44:HIS:CG	2.90	0.59
1:A:1079:C:O2'	1:A:1080:A:O4'	2.20	0.59
1:A:1062:G:O4'	1:A:1088:A:N7	2.35	0.59
1:A:84:A:C4	1:A:103:A:N6	2.71	0.59
4:D:108:ASP:N	4:D:204:LYS:O	2.35	0.59
1:A:1553:A:N7	1:A:1555:G:C6	2.71	0.59
1:A:2725:A:C4	1:A:2727:A:N7	2.71	0.59
1:A:353:C:N4	1:A:354:A:N6	2.51	0.59
1:A:2310:C:O2'	1:A:2311:A:C4'	2.50	0.59
1:A:226:A:C5	1:A:227:A:N7	2.71	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:746:U:O2'	1:A:2611:C:O2'	2.21	0.59
1:A:1593:A:C6	1:A:1594:U:C4	2.91	0.59
1:A:1808:A:N7	24:X:27:ARG:NH1	2.51	0.59
1:A:1062:G:OP1	1:A:1070:A:OP2	2.20	0.59
1:A:2808:G:O2'	1:A:2809:A:C8	2.55	0.59
1:A:711:G:C2	1:A:721:A:C2	2.90	0.59
1:A:621:A:O2'	1:A:622:G:O4'	2.21	0.59
1:A:459:U:C5	1:A:469:G:N2	2.71	0.59
1:A:2857:G:N2	1:A:2860:A:OP2	2.36	0.58
1:A:1303:G:O2'	1:A:1304:A:O5'	2.21	0.58
1:A:2415:G:C6	1:A:2416:C:C4	2.90	0.58
1:A:230:G:O2'	1:A:231:A:C8	2.57	0.58
1:A:1612:C:O2'	1:A:1613:G:O5'	2.21	0.58
1:A:1048:A:N6	1:A:1111:A:C4	2.71	0.58
1:A:1358:G:C6	34:A:3256:HOH:O	2.52	0.58
1:A:2386:A:O2'	1:A:2387:U:C6	2.56	0.58
29:2:11:LYS:NZ	34:2:647:HOH:O	2.37	0.58
1:A:1048:A:C6	1:A:1111:A:C2	2.90	0.58
1:A:860:U:O4	1:A:2268:A:C5	2.57	0.58
1:A:478:A:C6	1:A:480:A:C5	2.92	0.58
8:H:2:GLN:O	8:H:3:VAL:O	2.22	0.58
1:A:684:G:C2	1:A:794:A:C2	2.92	0.58
1:A:845:A:N1	1:A:932:U:O2	2.37	0.58
23:W:25:PHE:O	23:W:27:GLY:N	2.37	0.58
1:A:1826:G:C6	1:A:1827:U:C4	2.92	0.58
1:A:1062:G:O2'	1:A:1063:G:C8	2.56	0.58
1:A:858:G:C4	1:A:2268:A:C2	2.92	0.58
1:A:2310:C:O2'	1:A:2311:A:C5'	2.52	0.58
2:B:81:G:C6	2:B:82:U:C4	2.92	0.58
1:A:811:U:C5'	1:A:812:C:OP2	2.51	0.58
1:A:46:G:C2	1:A:47:C:C5	2.91	0.58
1:A:1669:A:OP2	34:A:3553:HOH:O	2.17	0.58
1:A:1494:A:C2	1:A:1495:A:C4	2.92	0.58
1:A:307:G:N2	1:A:310:A:C8	2.72	0.58
1:A:1739:A:C6	1:A:1740:G:C5	2.92	0.58
1:A:1510:G:N2	1:A:1511:G:N3	2.50	0.58
1:A:647:G:C8	1:A:648:G:N7	2.72	0.58
1:A:259:G:C6	1:A:260:G:N7	2.72	0.58
1:A:1266:G:O2'	1:A:2012:G:O6	2.21	0.58
7:G:163:TYR:N	7:G:163:TYR:CD2	2.71	0.58
1:A:2298:A:C6	1:A:2321:U:C5	2.92	0.58
18:R:82:HIS:O	18:R:82:HIS:CG	2.57	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:616:A:C2'	1:A:617:G:C8	2.86	0.57
1:A:1510:G:O2'	1:A:1511:G:O4'	2.22	0.57
1:A:1073:A:O2'	1:A:1074:G:C8	2.57	0.57
1:A:215:G:C4'	1:A:216:A:OP1	2.51	0.57
1:A:1071:G:O2'	1:A:1072:C:O5'	2.21	0.57
1:A:2267:A:N6	1:A:2272:U:N3	2.53	0.57
4:D:13:ARG:NH1	16:P:74:GLN:NE2	2.53	0.57
1:A:1342:A:C5	1:A:1345:C:N4	2.73	0.57
1:A:1609:A:N6	1:A:1616:A:C2	2.72	0.57
1:A:1131:G:O6	1:A:2024:G:O2'	2.22	0.57
1:A:489:G:C4	1:A:491:G:C8	2.92	0.57
12:L:94:THR:O	12:L:98:ALA:N	2.38	0.57
1:A:82:U:N3	1:A:83:A:C8	2.72	0.57
1:A:2023:C:O2'	1:A:2024:G:C8	2.57	0.57
1:A:1237:A:C2	1:A:1238:G:C1'	2.87	0.57
1:A:100:U:OP1	1:A:100:U:C6	2.57	0.57
1:A:1914:C:O2'	1:A:1915:U:O4'	2.21	0.57
1:A:1782:U:O2	1:A:2608:G:O2'	2.22	0.57
1:A:729:G:O6	3:C:207:ALA:N	2.37	0.57
1:A:1259:G:C4	1:A:1260:A:C8	2.93	0.57
6:F:107:VAL:N	6:F:108:PRO:CD	2.68	0.57
1:A:1287:A:O2'	1:A:1288:G:N3	2.38	0.57
1:A:265:A:N7	1:A:427:U:O2'	2.37	0.57
19:S:66:ILE:O	19:S:68:ASP:N	2.38	0.57
1:A:612:G:N2	1:A:614:A:O2'	2.38	0.57
1:A:617:G:O2'	1:A:618:G:O4'	2.23	0.57
1:A:1458:U:O3'	1:A:1459:G:C4'	2.53	0.57
2:B:23:G:N2	2:B:61:G:C2	2.73	0.57
1:A:1555:G:N2	1:A:1556:C:C2	2.73	0.57
10:J:65:THR:O	10:J:68:LYS:NZ	2.38	0.57
1:A:28:A:C6	1:A:29:U:O2	2.58	0.57
1:A:864:G:C6	1:A:865:C:N4	2.72	0.57
1:A:308:G:C6	1:A:309:A:C6	2.93	0.56
1:A:819:A:OP2	1:A:1187:G:N2	2.38	0.56
1:A:1401:G:C5	1:A:1402:U:C4	2.93	0.56
1:A:1553:A:C8	1:A:1555:G:C6	2.92	0.56
1:A:1809:A:N3	1:A:1810:A:C8	2.73	0.56
1:A:370:G:O2'	1:A:423:A:O2'	2.23	0.56
1:A:111:A:C2	1:A:112:U:C2	2.93	0.56
1:A:1301:A:C4	1:A:1303:G:N7	2.73	0.56
1:A:648:G:O2'	1:A:649:G:C8	2.58	0.56
1:A:2725:A:C4	1:A:2727:A:C8	2.93	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:120:U:O4	1:A:177:G:C8	2.58	0.56
2:B:78:A:C2	2:B:99:A:C4	2.93	0.56
1:A:1992:G:N2	1:A:1996:C:O2'	2.39	0.56
1:A:1651:G:N2	1:A:2007:U:C2	2.72	0.56
6:F:5:ASP:C	6:F:7:TYR:N	2.59	0.56
1:A:1734:G:O2'	1:A:1735:A:C8	2.59	0.56
1:A:504:A:O2'	1:A:505:A:P	2.63	0.56
1:A:620:G:C8	1:A:622:G:O6	2.59	0.56
1:A:1831:G:N2	1:A:1975:G:C4	2.73	0.56
26:Z:16:LEU:N	26:Z:16:LEU:CD2	2.69	0.56
1:A:2336:A:C8	23:W:40:ARG:NH2	2.73	0.56
1:A:2135:A:O2'	1:A:2136:G:O4'	2.23	0.56
1:A:1019:U:OP1	1:A:1035:U:O2'	2.24	0.56
1:A:1651:G:C2	1:A:2007:U:C2	2.94	0.56
1:A:2232:C:P	24:X:26:ARG:NH1	2.79	0.56
1:A:2200:C:N4	1:A:2224:G:N2	2.52	0.56
1:A:2345:G:C6	1:A:2381:A:C6	2.94	0.56
1:A:1275:A:O3'	1:A:1276:A:O4'	2.24	0.56
1:A:2212:A:N7	1:A:2214:C:N4	2.54	0.56
1:A:2314:A:C2	1:A:2315:G:C5	2.93	0.56
1:A:241:A:C4'	1:A:242:G:OP1	2.54	0.56
4:D:149:ASN:OD1	4:D:150:GLN:N	2.39	0.56
1:A:221:A:C2	1:A:233:A:C5	2.94	0.56
1:A:453:A:N3	1:A:457:A:O2'	2.39	0.56
1:A:1071:G:O2'	1:A:1072:C:C5'	2.54	0.56
1:A:2415:G:C5	1:A:2416:C:C4	2.94	0.56
1:A:83:A:N6	1:A:101:A:C5'	2.69	0.56
14:N:62:ASN:O	14:N:63:ARG:CB	2.54	0.56
1:A:571:U:C4	1:A:2030:A:C6	2.93	0.56
1:A:1087:G:C5	1:A:1089:A:C2	2.94	0.55
1:A:49:A:C4'	1:A:50:U:O5'	2.54	0.55
1:A:1324:G:C2	1:A:1328:A:N6	2.74	0.55
1:A:1555:G:C2	1:A:1556:C:C2	2.94	0.55
1:A:294:A:N1	1:A:346:A:N1	2.54	0.55
1:A:352:A:C6	1:A:353:C:C2	2.94	0.55
1:A:1663:G:C6	1:A:1998:A:N6	2.74	0.55
1:A:1275:A:C8	14:N:16:HIS:CD2	2.94	0.55
24:X:70:LEU:O	24:X:74:GLY:N	2.39	0.55
1:A:1856:U:O4	1:A:1857:G:C2	2.59	0.55
10:J:44:TYR:CB	17:Q:63:ARG:CZ	2.84	0.55
1:A:1320:C:O2'	1:A:1321:A:C8	2.60	0.55
1:A:1009:A:O2'	1:A:1010:A:C8	2.59	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1016:G:C2	1:A:1147:A:C2	2.94	0.55
2:B:58:A:C8	2:B:59:A:N7	2.75	0.55
1:A:1553:A:N7	1:A:1555:G:C5	2.74	0.55
1:A:571:U:C5	1:A:575:A:C6	2.94	0.55
1:A:2657:A:O3'	7:G:159:LYS:NZ	2.40	0.55
1:A:2287:A:N7	1:A:2289:G:C8	2.74	0.55
20:T:14:PRO:O	20:T:15:HIS:CB	2.53	0.55
1:A:1208:C:N3	1:A:1209:U:C5	2.75	0.55
1:A:1139:G:N2	1:A:1140:C:C2	2.74	0.55
1:A:1520:U:O4	1:A:1521:G:C6	2.59	0.55
1:A:2746:U:C2	1:A:2759:G:N2	2.75	0.55
1:A:299:A:C2	1:A:319:G:N3	2.75	0.55
1:A:2093:G:O2'	1:A:2094:A:P	2.64	0.55
1:A:1552:A:N3	1:A:1552:A:C2'	2.69	0.55
1:A:2285:C:C5	28:1:5:ARG:NH2	2.75	0.55
1:A:2721:A:C2	1:A:2873:A:C5	2.94	0.55
23:W:23:LYS:NZ	23:W:24:ARG:O	2.40	0.55
1:A:1178:C:C2	1:A:1179:G:C8	2.94	0.55
2:B:32:U:C2	2:B:51:G:N2	2.74	0.55
1:A:2407:A:C2	1:A:2408:U:N3	2.75	0.55
1:A:1551:A:C6	1:A:1552:A:N7	2.74	0.55
1:A:1392:A:N6	1:A:1393:A:N6	2.54	0.55
1:A:1019:U:O4	1:A:1020:A:N6	2.39	0.55
1:A:784:G:C2	3:C:227:VAL:CG2	2.90	0.55
1:A:1537:G:C2'	1:A:1538:G:C4'	2.84	0.55
1:A:303:G:C6	1:A:315:G:O6	2.60	0.55
1:A:1340:U:C4	1:A:1603:A:C8	2.95	0.55
1:A:1021:A:O2'	1:A:1022:G:C4'	2.55	0.55
1:A:1593:A:C5	1:A:1594:U:C4	2.95	0.55
1:A:61:C:N3	1:A:94:A:C2	2.75	0.55
1:A:224:U:C4	1:A:225:C:C5	2.94	0.55
1:A:479:A:C2	1:A:480:A:C6	2.94	0.55
1:A:663:G:O6	1:A:664:G:C6	2.59	0.55
1:A:1223:G:N2	1:A:1226:A:OP2	2.40	0.55
1:A:1286:A:C6	1:A:1289:C:N3	2.75	0.55
1:A:1335:C:N4	34:A:3248:HOH:O	2.40	0.55
1:A:1737:G:C5	1:A:1738:G:C6	2.95	0.55
14:N:35:LYS:NZ	14:N:112:TYR:CE1	2.75	0.55
1:A:1358:G:N7	1:A:1371:G:C6	2.75	0.54
24:X:1:SER:O	24:X:3:VAL:N	2.40	0.54
1:A:1519:G:C6	1:A:1520:U:N3	2.76	0.54
7:G:91:VAL:N	7:G:93:TYR:CE2	2.75	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:Y:47:ARG:O	25:Y:50:VAL:N	2.39	0.54
1:A:1493:C:O2	1:A:1493:C:C2'	2.54	0.54
1:A:532:A:O2'	1:A:532:A:N3	2.40	0.54
1:A:1429:G:O2'	1:A:1430:G:C8	2.60	0.54
1:A:1626:A:C2'	1:A:1627:G:OP2	2.55	0.54
1:A:2148:G:N2	1:A:2149:U:O4	2.40	0.54
1:A:1057:A:N6	1:A:1087:G:OP1	2.40	0.54
1:A:445:C:O2'	1:A:449:A:N3	2.41	0.54
2:B:18:G:C2	2:B:19:C:C2	2.96	0.54
1:A:1817:G:OP1	3:C:86:ARG:NH2	2.41	0.54
16:P:50:ARG:CB	16:P:57:ALA:N	2.71	0.54
1:A:38:A:C2	1:A:442:G:C6	2.94	0.54
1:A:482:A:N6	1:A:506:G:N9	2.54	0.54
1:A:45:G:C5'	1:A:46:G:OP1	2.55	0.54
1:A:657:U:C2	1:A:658:U:C5	2.95	0.54
1:A:1608:A:C5	1:A:1611:C:N4	2.75	0.54
1:A:954:G:C2	1:A:964:C:O2	2.61	0.54
1:A:699:A:C8	1:A:700:G:C8	2.95	0.54
1:A:201:C:C5	1:A:202:U:C5	2.95	0.54
14:N:94:TYR:N	14:N:94:TYR:CD1	2.72	0.54
22:V:80:HIS:CD2	22:V:83:LYS:N	2.76	0.54
1:A:563:A:C4	1:A:2018:G:C2	2.96	0.54
1:A:776:G:N1	1:A:2072:C:OP1	2.41	0.54
1:A:104:A:N7	1:A:105:C:C4	2.75	0.54
4:D:112:THR:CG2	4:D:113:SER:N	2.70	0.54
1:A:1905:C:O4'	1:A:1928:A:C2	2.61	0.54
1:A:214:G:O2'	1:A:216:A:O3'	2.26	0.54
1:A:1857:G:N3	1:A:1884:G:N1	2.55	0.54
1:A:1286:A:C4	1:A:1289:C:N4	2.76	0.54
1:A:1439:A:C8	1:A:1440:U:O4'	2.61	0.54
1:A:249:C:O2'	1:A:250:G:OP2	2.26	0.54
29:2:28:ARG:O	29:2:30:VAL:N	2.41	0.54
1:A:30:G:C5	1:A:31:C:C4	2.95	0.54
10:J:94:ALA:O	10:J:95:ARG:CB	2.56	0.54
1:A:1206:G:C2	1:A:1207:C:C2	2.96	0.54
1:A:301:G:C6	1:A:317:G:C6	2.95	0.54
1:A:95:A:O2'	25:Y:41:HIS:CD2	2.60	0.54
3:C:68:ARG:NH2	3:C:126:GLY:O	2.41	0.54
1:A:2519:U:C6	1:A:2542:A:N6	2.76	0.54
1:A:1317:G:C6	1:A:1318:U:N3	2.75	0.54
1:A:438:G:C6	1:A:439:A:C6	2.96	0.54
1:A:1168:G:C2	1:A:1182:G:C2	2.96	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1536:C:OP2	1:A:1536:C:C2	2.61	0.54
1:A:628:G:C6	1:A:636:G:C2	2.96	0.54
1:A:1285:A:N6	1:A:1329:U:C5	2.76	0.54
15:O:117:PHE:C	15:O:117:PHE:CD2	2.81	0.54
12:L:55:MET:SD	12:L:59:ARG:NE	2.81	0.54
1:A:2221:G:C5	1:A:2222:C:C5	2.96	0.54
1:A:2577:A:C2	27:O:1:ALA:N	2.75	0.53
1:A:1341:G:O2'	1:A:1397:U:O2'	2.26	0.53
1:A:1050:A:C2	1:A:2751:G:N3	2.76	0.53
1:A:917:A:C2	2:B:79:G:N2	2.76	0.53
1:A:749:A:C6	1:A:750:A:N7	2.76	0.53
1:A:729:G:C2'	1:A:729:G:N3	2.70	0.53
1:A:1317:G:C2	1:A:1336:A:C2	2.96	0.53
1:A:1424:G:O6	1:A:1425:G:C2	2.61	0.53
1:A:995:C:O2'	17:Q:60:TRP:CZ2	2.61	0.53
31:4:7:VAL:CG1	31:4:8:LYS:N	2.71	0.53
23:W:11:ASN:ND2	23:W:11:ASN:O	2.41	0.53
1:A:2571:U:O4	1:A:2574:G:C8	2.61	0.53
1:A:764:A:N3	1:A:781:A:C6	2.77	0.53
1:A:345:A:O2'	1:A:346:A:C2	2.61	0.53
1:A:2330:G:N1	1:A:2386:A:C6	2.76	0.53
1:A:2266:A:C4'	1:A:2267:A:O5'	2.57	0.53
14:N:90:ARG:NH2	14:N:116:VAL:CG1	2.70	0.53
14:N:1:MET:O	14:N:2:ARG:CB	2.57	0.53
1:A:30:G:C6	1:A:31:C:N3	2.77	0.53
1:A:2741:A:C8	1:A:2742:G:C8	2.96	0.53
1:A:2034:U:O2'	1:A:2035:G:O5'	2.25	0.53
6:F:113:PHE:O	6:F:114:ARG:CB	2.56	0.53
1:A:56:A:C2	1:A:115:C:C2	2.97	0.53
1:A:502:A:N6	1:A:505:A:C6	2.76	0.53
1:A:1551:A:C5	1:A:1552:A:N7	2.76	0.53
2:B:15:A:C8	2:B:109:A:N6	2.76	0.53
7:G:149:ALA:O	7:G:151:ARG:N	2.41	0.53
24:X:39:VAL:O	24:X:41:SER:N	2.41	0.53
4:D:148:GLN:N	4:D:148:GLN:CD	2.62	0.53
1:A:319:G:O6	1:A:333:G:C6	2.61	0.53
1:A:2235:G:C6	1:A:2236:U:C4	2.97	0.53
1:A:2093:G:N7	1:A:2225:A:C4	2.77	0.53
4:D:118:PHE:CG	4:D:119:ALA:N	2.76	0.53
1:A:1327:A:C6	1:A:1328:A:C4	2.97	0.53
1:A:1378:A:C8	1:A:1380:G:C6	2.96	0.53
1:A:2391:G:O2'	1:A:2392:A:O5'	2.27	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:W:8:SER:O	23:W:9:THR:CB	2.57	0.53
1:A:40:U:C4	1:A:41:C:N4	2.77	0.53
1:A:1936:A:C2	1:A:1945:G:C4	2.96	0.53
1:A:1935:G:C1'	1:A:1964:G:N2	2.71	0.53
1:A:836:G:C6	1:A:837:C:N3	2.76	0.53
1:A:1809:A:C2	1:A:1810:A:C5	2.96	0.53
1:A:1072:C:O2'	1:A:1093:G:O6	2.26	0.53
1:A:1387:A:N3	1:A:1388:G:C8	2.77	0.53
1:A:1596:A:N6	1:A:1597:A:N6	2.57	0.53
1:A:1326:U:O2'	1:A:1327:A:C8	2.61	0.53
1:A:96:C:C4'	25:Y:41:HIS:CD2	2.92	0.53
1:A:1544:A:N1	1:A:1545:A:C2	2.77	0.53
1:A:1684:G:C6	1:A:1685:C:C4	2.96	0.53
1:A:1351:C:C2	1:A:1381:G:C2	2.96	0.53
1:A:1324:G:O2'	1:A:1616:A:N6	2.42	0.53
1:A:279:A:C2	1:A:362:A:C4'	2.92	0.53
1:A:2282:G:C4	1:A:2425:A:N6	2.77	0.53
1:A:2106:U:C4	1:A:2107:G:N7	2.77	0.53
5:E:126:VAL:CG1	5:E:127:GLU:N	2.72	0.53
1:A:2688:G:N1	1:A:2720:U:OP2	2.41	0.53
1:A:1739:A:N6	1:A:1740:G:C6	2.77	0.53
23:W:18:LYS:CD	23:W:19:ARG:N	2.71	0.53
1:A:265:A:C5	1:A:428:A:C8	2.96	0.53
1:A:2191:A:C5'	1:A:2192:U:OP2	2.56	0.53
1:A:2428:G:C2	12:L:54:GLN:NE2	2.77	0.53
2:B:16:G:C6	2:B:69:G:C4	2.97	0.52
1:A:422:A:C2	1:A:423:A:C5	2.96	0.52
1:A:2889:C:N4	1:A:2890:G:C6	2.76	0.52
1:A:3:U:C4	1:A:4:U:C5	2.97	0.52
8:H:2:GLN:O	8:H:19:VAL:O	2.27	0.52
1:A:567:U:O4	1:A:568:U:C4	2.62	0.52
22:V:55:GLU:O	22:V:57:TYR:N	2.42	0.52
1:A:604:G:C6	1:A:625:G:C6	2.97	0.52
31:4:19:ARG:O	31:4:20:ASP:CB	2.56	0.52
1:A:2576:G:C8	1:A:2580:U:O4	2.63	0.52
1:A:1665:A:N7	34:A:3278:HOH:O	2.33	0.52
14:N:21:PHE:CD1	14:N:21:PHE:N	2.77	0.52
1:A:1062:G:C8	1:A:1070:A:OP2	2.63	0.52
1:A:1210:G:C4'	1:A:1211:C:O5'	2.57	0.52
1:A:2214:C:O2'	1:A:2215:C:C5'	2.57	0.52
1:A:469:G:OP2	5:E:54:GLY:O	2.26	0.52
1:A:589:U:O2'	1:A:590:A:OP2	2.27	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2287:A:O2'	1:A:2288:A:O5'	2.26	0.52
1:A:2107:G:C2	1:A:2183:A:C2	2.98	0.52
1:A:2458:G:C8	1:A:2459:A:N6	2.78	0.52
1:A:1319:C:O2	1:A:1334:G:C2	2.63	0.52
24:X:57:VAL:CG1	24:X:58:ILE:N	2.71	0.52
1:A:832:U:OP1	12:L:39:LYS:N	2.43	0.52
30:3:41:ARG:CG	30:3:41:ARG:NH2	2.72	0.52
1:A:1069:A:O2'	1:A:1072:C:OP2	2.26	0.52
1:A:1087:G:C6	1:A:1089:A:C2	2.98	0.52
1:A:860:U:O2'	1:A:861:A:O5'	2.27	0.52
1:A:749:A:C4	1:A:750:A:C8	2.97	0.52
1:A:2727:A:O2'	1:A:2728:U:C5'	2.58	0.52
24:X:53:LYS:O	24:X:57:VAL:N	2.43	0.52
1:A:1868:C:N4	1:A:1869:G:O6	2.42	0.52
1:A:2543:G:C6	1:A:2765:A:C5	2.97	0.52
1:A:768:G:N2	1:A:1379:U:O2'	2.41	0.52
7:G:84:LYS:O	7:G:85:LYS:CB	2.57	0.52
1:A:2093:G:C2	1:A:2094:A:C5	2.97	0.52
1:A:1208:C:C2	1:A:1209:U:C5	2.98	0.52
1:A:2563:U:C1'	1:A:2566:A:N6	2.72	0.52
1:A:528:A:N1	1:A:2043:C:O5'	2.42	0.52
3:C:212:TRP:CD1	3:C:212:TRP:C	2.82	0.52
1:A:1857:G:C4	1:A:1884:G:N1	2.77	0.52
1:A:1596:A:C6	1:A:1597:A:C6	2.98	0.52
1:A:450:G:N1	1:A:454:A:OP2	2.42	0.52
1:A:1722:A:O2'	1:A:1723:G:C8	2.62	0.52
1:A:1789:A:OP2	3:C:220:ARG:NH1	2.43	0.52
1:A:696:G:C2	1:A:767:U:O2	2.63	0.52
1:A:1071:G:O6	1:A:1089:A:C2	2.63	0.52
1:A:1314:C:OP1	1:A:1332:G:OP1	2.26	0.52
2:B:40:U:O2	2:B:43:C:C2'	2.58	0.52
1:A:106:C:O2'	1:A:294:A:O2'	2.27	0.52
1:A:571:U:C4	1:A:575:A:C5	2.97	0.52
1:A:836:G:C5	1:A:837:C:C4	2.97	0.52
8:H:132:PHE:CD1	8:H:133:GLN:N	2.77	0.52
1:A:204:A:C4'	1:A:205:G:OP1	2.58	0.52
1:A:12:U:O2	1:A:12:U:C2'	2.57	0.52
1:A:1063:G:N2	1:A:1076:C:C2	2.78	0.52
1:A:1076:C:O2'	1:A:1077:A:C8	2.63	0.52
30:3:23:HIS:ND1	30:3:24:LYS:O	2.43	0.52
1:A:186:G:N2	1:A:211:C:O2	2.43	0.52
1:A:1447:C:C2'	1:A:1448:G:C8	2.93	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:79:ARG:O	5:E:80:SER:C	2.47	0.52
1:A:372:G:N2	1:A:401:A:OP2	2.42	0.52
1:A:1833:C:C4	1:A:1834:U:C5	2.98	0.52
1:A:1607:C:C4'	1:A:1608:A:C8	2.92	0.52
1:A:406:G:O2'	1:A:407:G:O4'	2.27	0.52
1:A:192:C:N4	1:A:193:U:C2	2.78	0.52
1:A:777:G:N7	1:A:793:A:C2	2.77	0.52
1:A:1931:U:OP2	1:A:1968:G:N2	2.43	0.52
1:A:35:G:C8	1:A:454:A:C2	2.98	0.52
1:A:1049:C:O2'	1:A:1050:A:C8	2.64	0.52
1:A:1338:G:O2'	1:A:1393:A:N1	2.43	0.52
1:A:2345:G:C5	1:A:2347:C:N4	2.78	0.52
1:A:1330:C:O2'	1:A:1331:G:O5'	2.27	0.52
1:A:1532:A:C5	1:A:1533:C:C4	2.98	0.52
1:A:1809:A:C2'	1:A:1810:A:C8	2.93	0.51
1:A:299:A:N3	1:A:319:G:O2'	2.43	0.51
1:A:68:G:C2	1:A:69:C:C2	2.98	0.51
1:A:727:A:O2'	1:A:728:G:C8	2.63	0.51
1:A:2420:C:N4	30:3:29:ARG:O	2.43	0.51
16:P:107:ALA:O	16:P:108:ARG:C	2.48	0.51
1:A:2013:A:N6	1:A:2014:A:C2	2.79	0.51
1:A:334:C:O2'	1:A:335:C:OP1	2.28	0.51
1:A:1612:C:O2'	1:A:1613:G:O4'	2.28	0.51
1:A:379:G:C5	1:A:396:G:C6	2.97	0.51
2:B:108:A:O2'	2:B:109:A:OP1	2.28	0.51
1:A:484:C:N4	1:A:497:A:C2	2.78	0.51
1:A:727:A:C2'	1:A:728:G:C8	2.94	0.51
1:A:1545:A:N6	1:A:1546:G:N2	2.58	0.51
1:A:693:A:O2'	1:A:1353:A:N3	2.44	0.51
1:A:498:G:C2	1:A:499:U:C6	2.99	0.51
1:A:2347:C:O2'	1:A:2348:U:O5'	2.29	0.51
1:A:686:U:C6	1:A:788:A:N1	2.77	0.51
1:A:2282:G:N3	1:A:2425:A:N6	2.58	0.51
1:A:874:G:C2	1:A:904:G:C2	2.99	0.51
19:S:27:LYS:O	19:S:28:LYS:O	2.28	0.51
1:A:1678:A:C8	34:A:3292:HOH:O	2.54	0.51
1:A:305:C:C2	1:A:313:G:C2	2.97	0.51
1:A:118:A:N7	1:A:119:A:C8	2.78	0.51
1:A:301:G:C4	1:A:302:C:C4	2.98	0.51
1:A:860:U:C4	1:A:2268:A:C5	2.99	0.51
5:E:53:THR:OG1	5:E:54:GLY:N	2.43	0.51
1:A:590:A:C5	1:A:591:U:C5	2.97	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:120:ARG:O	10:J:123:LYS:NZ	2.43	0.51
8:H:9:VAL:CG1	8:H:10:ALA:N	2.73	0.51
1:A:1127:A:O2'	1:A:1128:G:C5'	2.58	0.51
1:A:195:A:C6	1:A:198:C:C5	2.98	0.51
1:A:669:G:C2	1:A:801:G:C6	2.98	0.51
1:A:2298:A:O2'	1:A:2299:U:O5'	2.28	0.51
1:A:2093:G:N3	1:A:2094:A:C8	2.78	0.51
1:A:612:G:C2	1:A:617:G:O6	2.64	0.51
1:A:396:G:O2'	1:A:397:U:O5'	2.28	0.51
1:A:1282:U:O4	1:A:1283:G:C6	2.64	0.51
10:J:95:ARG:O	10:J:96:ARG:C	2.49	0.51
1:A:56:A:C2	1:A:57:C:C2	2.97	0.51
1:A:836:G:C6	1:A:837:C:C4	2.99	0.51
1:A:2021:C:C2'	1:A:2021:C:O2	2.58	0.51
1:A:2744:G:C6	1:A:2761:A:C6	2.99	0.51
18:R:27:ILE:CG2	18:R:28:ALA:N	2.73	0.51
18:R:49:ILE:CG2	18:R:54:VAL:N	2.74	0.51
1:A:2216:G:C2'	1:A:2217:G:C8	2.94	0.51
1:A:1202:G:N7	1:A:1203:U:C5	2.78	0.51
1:A:2333:A:OP2	23:W:76:ARG:NH1	2.44	0.51
1:A:1079:C:N4	1:A:1088:A:N3	2.59	0.51
8:H:24:GLY:O	8:H:25:TYR:C	2.48	0.51
1:A:927:A:C6	1:A:928:A:C6	2.99	0.51
13:M:31:PHE:O	13:M:105:MET:N	2.43	0.51
4:D:133:THR:O	4:D:134:HIS:C	2.49	0.51
1:A:1606:C:O2	1:A:1606:C:C5'	2.58	0.51
1:A:617:G:N3	1:A:618:G:C8	2.79	0.51
1:A:491:G:C2'	1:A:492:A:C8	2.94	0.51
11:K:21:CYS:SG	11:K:39:ILE:CG2	2.99	0.51
1:A:1497:U:C5	1:A:1578:U:O5'	2.64	0.51
1:A:1403:A:C2	1:A:1404:C:C2	2.99	0.51
1:A:1417:C:O2'	1:A:1418:G:O4'	2.29	0.51
10:J:44:TYR:O	10:J:45:THR:CB	2.59	0.51
1:A:608:A:C6	1:A:621:A:C8	2.99	0.51
1:A:260:G:C6	1:A:261:G:C5	2.99	0.51
1:A:203:A:OP2	1:A:204:A:O2'	2.29	0.51
1:A:1027:A:N7	1:A:1126:A:C2	2.79	0.51
4:D:161:MET:O	4:D:162:ALA:O	2.29	0.51
1:A:445:C:C2'	1:A:446:G:C8	2.93	0.51
1:A:674:G:O3'	5:E:60:TRP:CH2	2.64	0.51
1:A:1417:C:O2'	1:A:1418:G:C8	2.64	0.51
1:A:2751:G:N3	7:G:2:ARG:NH2	2.59	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:W:33:GLY:O	23:W:34:SER:CB	2.59	0.51
23:W:36:ILE:O	23:W:39:GLN:CB	2.60	0.51
4:D:208:LYS:O	4:D:209:ALA:CB	2.59	0.51
3:C:16:VAL:N	3:C:203:VAL:CG1	2.73	0.51
1:A:295:G:C2	1:A:296:U:C6	2.99	0.51
1:A:842:U:C4	1:A:843:G:N7	2.79	0.51
1:A:668:A:C5	1:A:670:A:C8	2.99	0.51
1:A:1062:G:C8	1:A:1088:A:C8	2.99	0.50
1:A:223:A:C6	1:A:422:A:N7	2.79	0.50
1:A:684:G:OP1	29:2:16:HIS:CE1	2.64	0.50
1:A:2308:G:C2'	1:A:2309:A:OP1	2.58	0.50
12:L:93:ASN:O	12:L:95:LEU:N	2.44	0.50
1:A:2232:C:OP1	24:X:26:ARG:NH1	2.44	0.50
1:A:2044:C:N3	1:A:2045:C:C5	2.79	0.50
1:A:1244:A:O2'	5:E:29:HIS:CE1	2.65	0.50
1:A:319:G:C6	1:A:333:G:C6	2.99	0.50
1:A:84:A:C2	1:A:98:G:N2	2.79	0.50
1:A:1605:C:C3'	1:A:1606:C:C5'	2.89	0.50
1:A:1387:A:O2'	1:A:1388:G:OP2	2.29	0.50
1:A:55:G:N2	1:A:116:C:C2	2.80	0.50
1:A:2408:U:O2'	1:A:2409:G:C8	2.64	0.50
1:A:1300:G:C4'	1:A:1301:A:O5'	2.59	0.50
6:F:135:ILE:O	6:F:137:PHE:N	2.45	0.50
1:A:2392:A:C2	12:L:55:MET:SD	3.04	0.50
1:A:2530:A:C8	7:G:156:TYR:OH	2.64	0.50
12:L:93:ASN:CG	12:L:94:THR:N	2.64	0.50
1:A:371:A:N6	1:A:402:A:OP2	2.44	0.50
1:A:1491:G:O6	1:A:1500:G:C2	2.64	0.50
1:A:2831:G:OP2	4:D:59:ARG:NE	2.44	0.50
1:A:466:A:P	29:2:34:ARG:NH2	2.84	0.50
1:A:976:G:N2	1:A:1155:A:C2	2.80	0.50
1:A:1936:A:C2	1:A:1943:U:C5	2.98	0.50
1:A:1525:A:C6	1:A:1526:C:C2	2.99	0.50
23:W:37:VAL:CG2	23:W:38:ARG:NH1	2.74	0.50
1:A:758:C:C2'	1:A:758:C:O2	2.57	0.50
1:A:2048:G:C6	1:A:2049:G:C5	2.99	0.50
1:A:584:C:N4	1:A:585:G:C6	2.79	0.50
1:A:1973:G:O6	1:A:1974:C:N4	2.44	0.50
1:A:1378:A:N6	1:A:1569:A:N1	2.59	0.50
12:L:61:LEU:O	30:3:12:ARG:NH2	2.43	0.50
1:A:945:A:C8	1:A:2448:A:C2	2.99	0.50
1:A:581:C:OP2	17:Q:32:ARG:NE	2.44	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:998:C:OP2	17:Q:57:ARG:NH2	2.43	0.50
1:A:1348:C:OP2	1:A:1349:C:N4	2.45	0.50
1:A:2201:G:C4	1:A:2202:U:C6	3.00	0.50
1:A:2431:U:O2'	1:A:2433:A:N7	2.45	0.50
1:A:2435:A:C2'	1:A:2436:G:O5'	2.59	0.50
1:A:1973:G:C5	1:A:1974:C:C4	2.99	0.50
1:A:1655:A:C6	1:A:1656:C:C2	2.99	0.50
1:A:858:G:C6	1:A:2268:A:C6	3.00	0.50
1:A:2051:A:C2	1:A:2052:A:N6	2.79	0.50
1:A:604:G:O6	1:A:625:G:C6	2.64	0.50
16:P:64:SER:O	16:P:66:GLY:N	2.43	0.50
1:A:2373:G:C6	1:A:2374:C:C4	3.00	0.50
1:A:1918:A:O2'	1:A:1920:C:N4	2.44	0.50
1:A:1667:G:O2'	1:A:1991:U:O4	2.28	0.50
1:A:2297:A:N3	1:A:2298:A:C8	2.79	0.50
1:A:1342:A:C4	1:A:1345:C:N4	2.79	0.50
1:A:2315:G:C2	1:A:2316:G:C4	2.99	0.50
1:A:2311:A:C5'	1:A:2312:U:C6	2.94	0.50
1:A:2144:G:C2	1:A:2148:G:O6	2.64	0.50
1:A:1525:A:C6	1:A:1526:C:N3	2.79	0.50
1:A:1053:C:N4	1:A:1054:A:N6	2.58	0.50
15:O:41:ALA:O	15:O:43:ASN:N	2.44	0.50
1:A:859:G:C8	1:A:859:G:OP2	2.65	0.50
1:A:2337:G:OP1	1:A:2385:C:OP2	2.29	0.50
1:A:2094:A:C4	1:A:2095:A:C8	3.00	0.50
1:A:1385:A:N6	1:A:1403:A:C5	2.80	0.50
1:A:243:U:O2'	1:A:244:A:C8	2.64	0.50
2:B:110:C:O2'	2:B:111:U:C5'	2.60	0.50
2:B:65:U:C4	2:B:108:A:C4	3.00	0.50
1:A:2623:G:C4'	1:A:2825:G:C8	2.94	0.50
2:B:23:G:C2	2:B:61:G:C2	3.00	0.50
1:A:1783:A:C2	1:A:2588:G:O4'	2.64	0.50
2:B:7:G:O2'	15:O:38:GLN:NE2	2.45	0.50
1:A:1846:G:C5'	1:A:1847:A:OP2	2.60	0.50
1:A:377:G:C6	1:A:378:C:C4	2.99	0.50
1:A:608:A:C5	1:A:621:A:N7	2.80	0.50
1:A:570:G:C5	1:A:2030:A:N7	2.80	0.50
1:A:1500:G:N1	1:A:1501:G:C5	2.80	0.50
1:A:1802:A:O2'	1:A:1803:A:C8	2.65	0.50
1:A:1620:G:C6	1:A:1621:U:C4	3.00	0.50
11:K:92:GLU:O	11:K:93:GLN:O	2.30	0.50
1:A:412:A:O2'	1:A:413:C:C5'	2.60	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:117:G:C2	1:A:119:A:N6	2.80	0.50
1:A:1416:G:C2	1:A:1417:C:C4	3.00	0.50
1:A:142:A:O2'	1:A:143:C:O4'	2.29	0.50
1:A:1714:U:C3'	1:A:1715:G:C5'	2.90	0.50
1:A:1378:A:C8	1:A:1380:G:C5	3.00	0.50
1:A:1049:C:O2'	1:A:1050:A:O5'	2.30	0.50
1:A:918:A:N6	1:A:2268:A:OP2	2.45	0.50
1:A:1019:U:O2'	1:A:1021:A:C2	2.65	0.50
1:A:2415:G:C5	1:A:2416:C:C5	3.00	0.50
1:A:2415:G:C2	1:A:2416:C:C2	3.00	0.50
1:A:1180:U:C4	1:A:1181:U:C4	3.00	0.50
1:A:1671:U:N3	1:A:1674:G:OP2	2.44	0.50
1:A:514:A:N3	1:A:581:C:O2'	2.45	0.50
1:A:1042:G:C6	1:A:1043:C:C4	3.00	0.50
11:K:28:SER:O	11:K:29:HIS:CB	2.60	0.50
1:A:146:A:C6	1:A:147:C:C4	3.00	0.50
2:B:94:A:OP1	22:V:19:ARG:CD	2.60	0.50
24:X:67:LEU:O	24:X:77:TYR:OH	2.28	0.50
1:A:280:U:C5	1:A:281:C:C4	3.00	0.50
1:A:1460:U:C6	1:A:1460:U:OP2	2.64	0.50
1:A:1314:C:OP1	1:A:1332:G:C5'	2.60	0.49
1:A:373:U:O2	1:A:374:A:C8	2.65	0.49
1:A:1719:G:C2	1:A:1742:U:O2	2.65	0.49
1:A:533:G:N2	17:Q:44:TYR:CD1	2.80	0.49
5:E:165:HIS:O	5:E:167:VAL:N	2.45	0.49
1:A:2371:G:O3'	28:1:44:GLN:NE2	2.46	0.49
1:A:1667:G:OP1	11:K:7:MET:N	2.45	0.49
1:A:2823:A:C5	1:A:2824:C:C5	2.99	0.49
1:A:1129:A:N1	1:A:2569:G:O2'	2.45	0.49
12:L:40:SER:OG	12:L:41:ARG:N	2.45	0.49
1:A:2140:G:C6	1:A:2152:G:C6	3.00	0.49
1:A:1274:A:O2'	1:A:1275:A:C5'	2.61	0.49
16:P:50:ARG:CA	16:P:57:ALA:O	2.60	0.49
4:D:114:LYS:CD	4:D:116:LYS:NZ	2.75	0.49
3:C:68:ARG:NE	3:C:128:THR:OG1	2.46	0.49
1:A:1251:C:C5	17:Q:5:ARG:NH1	2.81	0.49
1:A:2290:G:C6	1:A:2291:U:C4	3.00	0.49
1:A:88:G:C2	1:A:89:A:C8	3.00	0.49
1:A:2331:G:N1	1:A:2385:C:C4	2.80	0.49
1:A:309:A:N7	1:A:330:A:N6	2.60	0.49
1:A:2056:G:N2	1:A:2057:G:N9	2.60	0.49
1:A:2667:C:O2'	1:A:2668:G:O4'	2.30	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1313:U:OP1	34:A:3246:HOH:O	2.18	0.49
1:A:1312:U:N3	1:A:1603:A:C6	2.81	0.49
1:A:785:G:O2'	1:A:1779:U:C5'	2.61	0.49
3:C:226:PRO:O	3:C:227:VAL:C	2.51	0.49
1:A:584:C:C4	1:A:585:G:C5	3.00	0.49
1:A:1705:A:C5	1:A:1706:C:C4	3.00	0.49
1:A:2656:U:OP2	1:A:2664:G:N2	2.45	0.49
1:A:1292:G:C6	1:A:1293:C:N4	2.80	0.49
14:N:67:PHE:CE2	14:N:73:ASN:OD1	2.65	0.49
1:A:1069:A:C2	1:A:1072:C:O2'	2.66	0.49
1:A:49:A:C8	1:A:51:G:C2	3.00	0.49
1:A:1056:G:O5'	1:A:1085:A:C2	2.64	0.49
1:A:1553:A:C8	1:A:1555:G:C5	3.00	0.49
1:A:860:U:C4	1:A:2268:A:C4	3.01	0.49
1:A:192:C:OP1	1:A:2243:U:OP1	2.31	0.49
1:A:2620:C:O2'	4:D:162:ALA:O	2.30	0.49
1:A:1491:G:N2	1:A:1492:G:C4	2.80	0.49
1:A:1054:A:C2	1:A:1106:G:C2	3.00	0.49
1:A:19:A:C2	1:A:522:A:C2	2.99	0.49
1:A:1455:G:N7	14:N:64:ARG:NH1	2.60	0.49
1:A:2197:U:C5	1:A:2224:G:C6	3.00	0.49
1:A:2335:A:C4	1:A:2337:G:N7	2.81	0.49
1:A:2054:A:C2	1:A:2616:C:C2	3.00	0.49
1:A:189:G:O6	1:A:205:G:O2'	2.30	0.49
1:A:277:G:O2'	1:A:278:A:C4	2.66	0.49
1:A:470:A:C2	1:A:471:A:C4	3.00	0.49
1:A:646:U:C6	1:A:646:U:OP2	2.65	0.49
1:A:2875:C:O2'	1:A:2876:G:O5'	2.30	0.49
1:A:1816:C:O2'	1:A:1817:G:P	2.70	0.49
1:A:1359:A:C2	1:A:1360:G:C1'	2.95	0.49
1:A:463:G:N2	1:A:466:A:OP2	2.46	0.49
1:A:2634:A:C2	1:A:2635:A:C4	3.01	0.49
1:A:712:G:C2	1:A:720:U:O2	2.65	0.49
4:D:78:GLY:C	4:D:80:TRP:CZ3	2.86	0.49
1:A:873:C:C4'	13:M:64:TRP:NE1	2.75	0.49
1:A:229:C:O2'	1:A:230:G:O5'	2.31	0.49
1:A:983:A:N6	1:A:984:A:C2	2.81	0.49
1:A:2392:A:C8	1:A:2429:G:C2	3.00	0.49
1:A:784:G:O2'	1:A:785:G:C8	2.66	0.49
1:A:949:G:C6	1:A:950:G:N7	2.80	0.49
1:A:2773:C:C2	1:A:2774:C:C5	3.01	0.49
1:A:1808:A:C3'	1:A:1809:A:C8	2.96	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:54:G:C4	1:A:55:G:C8	3.01	0.49
1:A:674:G:O2'	5:E:69:ARG:CG	2.60	0.49
1:A:410:G:N2	1:A:418:C:C2	2.81	0.49
1:A:142:A:C2'	1:A:143:C:C6	2.96	0.49
1:A:1361:G:C6	1:A:1371:G:N2	2.81	0.49
1:A:2345:G:C5	1:A:2381:A:C2	3.01	0.49
1:A:2023:C:O2'	1:A:2024:G:O5'	2.31	0.49
1:A:1364:G:N2	1:A:1367:A:OP2	2.45	0.49
1:A:1869:G:N1	1:A:1873:G:C6	2.81	0.49
4:D:133:THR:CG2	4:D:134:HIS:N	2.76	0.49
1:A:270:A:N1	1:A:369:U:O2'	2.46	0.49
26:Z:30:ARG:NH2	26:Z:33:HIS:CB	2.76	0.49
1:A:635:C:O2'	1:A:639:U:OP1	2.31	0.49
1:A:931:U:O2	1:A:931:U:C2'	2.60	0.49
1:A:117:G:N1	1:A:119:A:N6	2.60	0.49
1:A:2600:A:C6	1:A:2601:C:N4	2.81	0.49
1:A:1517:G:N2	1:A:1732:C:C6	2.81	0.49
1:A:2402:U:O2'	1:A:2403:C:OP1	2.31	0.49
1:A:108:G:C6	1:A:109:C:C4	3.01	0.49
1:A:485:C:C4	1:A:496:G:N1	2.81	0.49
1:A:312:G:C2	1:A:313:G:C8	3.00	0.48
1:A:2868:A:C6	1:A:2869:G:C6	3.01	0.48
1:A:1361:G:C2	1:A:1362:C:C6	3.00	0.48
1:A:2474:U:O4'	1:A:2474:U:O2	2.30	0.48
1:A:593:U:C2	1:A:594:U:C5	3.01	0.48
1:A:1324:G:C2	1:A:1328:A:C6	3.01	0.48
1:A:788:A:OP1	1:A:791:C:N4	2.46	0.48
1:A:28:A:C6	1:A:29:U:C2	3.01	0.48
1:A:1663:G:C6	1:A:1992:G:N7	2.81	0.48
8:H:24:GLY:O	8:H:26:ALA:O	2.31	0.48
1:A:2748:A:C2	1:A:2749:A:C4	3.02	0.48
1:A:183:C:N4	1:A:184:C:C4	2.81	0.48
1:A:54:G:C5	1:A:55:G:C8	3.02	0.48
1:A:1609:A:C6	1:A:1616:A:C4	3.00	0.48
2:B:42:C:C2'	2:B:43:C:C6	2.96	0.48
1:A:1865:U:C4	1:A:1875:G:C2	3.01	0.48
1:A:2209:G:C2	1:A:2216:G:C2	3.02	0.48
1:A:2217:G:C4	1:A:2218:G:C8	3.01	0.48
20:T:85:VAL:O	20:T:86:THR:OG1	2.31	0.48
25:Y:44:LYS:NZ	25:Y:48:ARG:NE	2.61	0.48
1:A:2331:G:C2	1:A:2385:C:N3	2.81	0.48
1:A:55:G:C2	1:A:116:C:C2	3.01	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:379:G:N1	1:A:380:G:C4	2.82	0.48
10:J:44:TYR:C	10:J:44:TYR:CD2	2.86	0.48
1:A:192:C:C4	1:A:193:U:C2	3.01	0.48
1:A:46:G:N2	1:A:47:C:C2	2.82	0.48
1:A:1275:A:C5	14:N:16:HIS:CD2	3.00	0.48
1:A:575:A:C2	1:A:576:U:C5	3.01	0.48
1:A:1267:U:O2'	1:A:1268:A:O5'	2.30	0.48
1:A:2201:G:C5	1:A:2202:U:C5	3.01	0.48
1:A:543:G:N2	1:A:551:G:C4	2.81	0.48
12:L:117:THR:CG2	12:L:118:THR:N	2.76	0.48
1:A:1490:A:C8	3:C:73:ILE:CD1	2.97	0.48
1:A:370:G:C6	1:A:424:G:N7	2.81	0.48
1:A:185:G:C5	1:A:212:G:N2	2.81	0.48
1:A:1737:G:C6	1:A:1738:G:N1	2.82	0.48
1:A:1526:C:N4	1:A:1527:G:C6	2.81	0.48
1:A:204:A:C5	1:A:206:U:O4	2.66	0.48
1:A:2371:G:C2	1:A:2372:U:C6	3.02	0.48
1:A:2653:U:OP2	1:A:2654:A:O2'	2.32	0.48
1:A:996:A:OP2	17:Q:91:ARG:NH1	2.47	0.48
1:A:1099:G:C6	1:A:1100:C:C2	3.01	0.48
1:A:2886:A:N7	27:O:39:ARG:NE	2.61	0.48
21:U:3:LYS:O	21:U:4:ILE:C	2.52	0.48
1:A:53:A:C8	1:A:54:G:C8	3.01	0.48
7:G:91:VAL:N	7:G:93:TYR:CD2	2.81	0.48
1:A:301:G:C2	1:A:317:G:C4	3.01	0.48
1:A:2285:C:O4'	1:A:2288:A:C2	2.66	0.48
1:A:254:G:N7	30:3:4:LYS:CE	2.77	0.48
30:3:5:THR:O	30:3:7:ARG:N	2.47	0.48
3:C:257:ARG:NH2	3:C:263:ASP:OD2	2.46	0.48
1:A:2138:G:C8	1:A:2138:G:OP2	2.67	0.48
1:A:226:A:C6	1:A:227:A:N6	2.82	0.48
1:A:1649:G:O2'	14:N:106:ASP:OD2	2.31	0.48
1:A:303:G:C6	1:A:315:G:C6	3.01	0.48
1:A:2808:G:N2	1:A:2891:U:C6	2.81	0.48
1:A:1716:U:C6	1:A:1743:G:N2	2.82	0.48
1:A:728:G:C2	1:A:730:A:C4	3.01	0.48
1:A:233:A:O2'	1:A:234:U:O4'	2.32	0.48
1:A:1379:U:O2	1:A:1379:U:C2'	2.61	0.48
31:4:2:LYS:O	31:4:36:ARG:N	2.47	0.48
1:A:1821:A:OP1	3:C:199:HIS:NE2	2.46	0.48
1:A:1754:A:C6	1:A:1755:A:C6	3.01	0.48
4:D:10:GLY:O	4:D:11:MET:CB	2.62	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:63:C:C4	2:B:64:G:N7	2.82	0.48
2:B:29:A:C6	2:B:30:C:N4	2.82	0.48
2:B:16:G:O6	2:B:69:G:C6	2.66	0.48
1:A:868:U:C4	1:A:869:G:N7	2.81	0.48
1:A:49:A:C8	1:A:51:G:N2	2.82	0.48
1:A:962:G:O2'	1:A:963:U:C6	2.67	0.48
1:A:39:G:C2	1:A:40:U:C4	3.02	0.48
1:A:204:A:C4	1:A:206:U:O4	2.67	0.48
1:A:237:C:N3	1:A:238:C:C5	2.82	0.48
1:A:2700:A:C2	1:A:2708:G:C2	3.02	0.48
1:A:2298:A:N1	1:A:2321:U:C5	2.82	0.48
1:A:1612:C:C2'	1:A:1613:G:O5'	2.62	0.48
1:A:1385:A:C6	1:A:1403:A:C5	3.01	0.48
1:A:1387:A:C4	1:A:1388:G:N7	2.81	0.48
1:A:1439:A:N7	1:A:1440:U:N1	2.62	0.48
1:A:1568:G:O2'	1:A:1569:A:OP2	2.32	0.48
2:B:52:A:N6	15:O:33:ARG:NE	2.62	0.48
2:B:109:A:C2	2:B:110:C:N3	2.82	0.48
1:A:1339:G:O2'	1:A:1340:U:OP1	2.31	0.48
1:A:1737:G:N7	1:A:1738:G:O6	2.46	0.48
1:A:1798:U:C5	3:C:270:ARG:NH1	2.82	0.48
1:A:503:A:N3	1:A:506:G:C8	2.82	0.48
1:A:1884:G:C8	1:A:1884:G:OP2	2.67	0.48
1:A:2443:C:C2	1:A:2444:G:C8	3.02	0.48
1:A:301:G:O5'	21:U:81:ARG:NH1	2.46	0.48
1:A:76:C:N4	1:A:111:A:C6	2.82	0.48
1:A:3:U:C4	1:A:4:U:C4	3.02	0.48
1:A:1930:G:O2'	1:A:1968:G:N1	2.47	0.48
1:A:1695:G:C8	3:C:7:PRO:O	2.67	0.48
1:A:1638:C:O2	1:A:2698:U:O2'	2.31	0.48
1:A:1519:G:N1	1:A:1520:U:C2	2.82	0.47
1:A:963:U:O2'	1:A:964:C:P	2.72	0.47
1:A:2550:G:N2	1:A:2559:C:O2	2.47	0.47
1:A:478:A:N6	1:A:480:A:C6	2.82	0.47
1:A:1865:U:O4	1:A:1875:G:C2	2.67	0.47
1:A:583:G:C6	1:A:584:C:C4	3.02	0.47
1:A:1060:U:O4'	1:A:1061:U:C2'	2.62	0.47
12:L:3:LEU:O	12:L:4:ASN:C	2.52	0.47
1:A:2319:G:O2'	1:A:2320:U:O5'	2.32	0.47
1:A:389:G:C6	1:A:2413:G:O2'	2.66	0.47
1:A:2506:U:C6	1:A:2506:U:C3'	2.96	0.47
1:A:335:C:O2'	1:A:336:C:O5'	2.32	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1307:A:N6	1:A:1606:C:C6	2.82	0.47
1:A:53:A:N7	1:A:54:G:C5	2.82	0.47
1:A:1649:G:N1	1:A:2009:A:C6	2.82	0.47
1:A:492:A:N1	19:S:49:LYS:CE	2.77	0.47
1:A:273:G:N2	1:A:365:U:O2	2.45	0.47
20:T:29:THR:CB	20:T:86:THR:N	2.77	0.47
24:X:33:HIS:O	24:X:34:SER:O	2.32	0.47
1:A:671:C:O2'	1:A:672:C:P	2.72	0.47
1:A:98:G:O2'	1:A:103:A:C8	2.67	0.47
1:A:1606:C:O2'	1:A:1607:C:P	2.72	0.47
1:A:1633:G:C5	1:A:1635:A:C5	3.02	0.47
1:A:1441:G:C2	1:A:1551:A:C2	3.02	0.47
1:A:2744:G:N2	1:A:2745:C:C2	2.82	0.47
23:W:23:LYS:CD	23:W:24:ARG:N	2.77	0.47
5:E:79:ARG:CG	5:E:80:SER:N	2.77	0.47
1:A:1833:C:C4	1:A:1834:U:C4	3.02	0.47
13:M:19:GLY:N	13:M:38:ARG:NH2	2.62	0.47
1:A:2683:C:OP1	16:P:55:HIS:CB	2.62	0.47
1:A:2250:G:OP1	1:A:2275:C:O2'	2.32	0.47
1:A:1682:G:C2	1:A:1757:A:O4'	2.68	0.47
1:A:1313:U:OP2	1:A:1314:C:C5	2.67	0.47
1:A:185:G:N1	1:A:212:G:C2	2.82	0.47
4:D:12:THR:CG2	4:D:13:ARG:N	2.77	0.47
1:A:1126:A:C4'	1:A:1127:A:O5'	2.62	0.47
23:W:37:VAL:C	23:W:39:GLN:N	2.67	0.47
12:L:29:LYS:O	12:L:30:THR:OG1	2.32	0.47
1:A:347:A:N6	1:A:348:A:N6	2.62	0.47
1:A:219:A:N7	1:A:220:G:C5	2.82	0.47
10:J:19:ASP:O	10:J:23:LYS:NZ	2.47	0.47
1:A:500:G:N2	1:A:503:A:C8	2.83	0.47
1:A:1326:U:O2'	1:A:1327:A:O5'	2.31	0.47
1:A:1616:A:C8	1:A:1616:A:OP1	2.68	0.47
1:A:2809:A:OP2	1:A:2890:G:N1	2.47	0.47
1:A:1553:A:C8	1:A:1555:G:O6	2.67	0.47
1:A:2429:G:OP2	1:A:2430:A:OP2	2.31	0.47
1:A:1339:G:C5'	1:A:1393:A:N1	2.78	0.47
2:B:8:C:O3'	15:O:25:ARG:NH1	2.48	0.47
28:1:38:PHE:CD2	28:1:39:ASP:N	2.82	0.47
13:M:1:MET:O	13:M:2:LEU:O	2.32	0.47
1:A:740:C:O2'	1:A:741:U:C5'	2.63	0.47
2:B:24:G:C6	2:B:56:G:C2	3.01	0.47
1:A:116:C:C4	1:A:117:G:C5	3.03	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:971:G:OP2	1:A:974:G:N2	2.48	0.47
1:A:2060:A:N6	5:E:69:ARG:NH1	2.63	0.47
1:A:241:A:C4	1:A:243:U:O4	2.68	0.47
1:A:607:U:O2	1:A:622:G:C6	2.67	0.47
1:A:2286:G:C4'	1:A:2287:A:O4'	2.62	0.47
1:A:1251:C:C6	17:Q:5:ARG:NH1	2.82	0.47
1:A:1456:G:C5	1:A:1457:U:C5	3.02	0.47
1:A:9:G:C6	1:A:2629:U:C5	3.03	0.47
17:Q:87:VAL:O	17:Q:88:GLU:O	2.32	0.47
26:Z:40:THR:C	26:Z:42:ALA:N	2.67	0.47
1:A:1135:C:N4	1:A:1139:G:O6	2.47	0.47
1:A:51:G:N3	1:A:119:A:C2	2.82	0.47
1:A:118:A:N3	1:A:178:G:C1'	2.77	0.47
1:A:1596:A:N6	1:A:1597:A:C6	2.83	0.47
1:A:675:A:C8	1:A:802:A:N6	2.83	0.47
1:A:2627:G:N2	1:A:2777:G:OP2	2.47	0.47
1:A:1312:U:O2	1:A:1603:A:C2	2.68	0.47
1:A:1733:G:C6	1:A:1734:G:N7	2.82	0.47
2:B:51:G:C8	15:O:64:TYR:CE2	3.03	0.47
24:X:1:SER:C	24:X:3:VAL:N	2.68	0.47
1:A:39:G:C6	1:A:40:U:O4	2.68	0.47
1:A:2748:A:N1	1:A:2757:A:N7	2.62	0.47
1:A:2083:G:C5	1:A:2084:C:C5	3.03	0.47
1:A:475:C:C2'	1:A:476:G:C8	2.98	0.47
16:P:65:ASN:ND2	16:P:65:ASN:N	2.63	0.47
4:D:193:VAL:O	4:D:194:PRO:O	2.33	0.47
1:A:579:G:C2	1:A:1262:A:C5	3.03	0.47
15:O:26:LEU:O	15:O:28:VAL:N	2.48	0.47
1:A:1068:G:C8	1:A:1069:A:N7	2.83	0.47
1:A:500:G:C2	1:A:503:A:N7	2.83	0.47
1:A:455:C:N3	1:A:473:G:C4'	2.78	0.47
1:A:302:C:O2'	1:A:303:G:O5'	2.33	0.47
1:A:1722:A:C6	1:A:1739:A:C8	3.03	0.47
1:A:1358:G:N7	34:A:3256:HOH:O	2.46	0.47
1:A:1737:G:C5'	1:A:1738:G:OP2	2.63	0.47
20:T:17:SER:N	20:T:21:SER:OG	2.48	0.47
1:A:828:U:C5	1:A:829:A:N6	2.83	0.47
5:E:85:PHE:O	5:E:86:ALA:C	2.53	0.47
1:A:1341:G:C2	20:T:84:TYR:CE2	3.03	0.47
1:A:425:G:C2	1:A:426:C:C4	3.03	0.47
1:A:1597:A:O3'	1:A:1598:A:C8	2.68	0.47
1:A:1716:U:C4	1:A:1745:A:N6	2.83	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:607:U:C5	1:A:619:G:C2	3.03	0.47
1:A:2816:G:C2	1:A:2831:G:C2	3.03	0.47
1:A:2740:A:N6	1:A:2764:A:C8	2.83	0.47
21:U:35:VAL:CG1	21:U:36:GLU:N	2.77	0.47
1:A:1394:U:C4	1:A:1395:A:C6	3.03	0.47
1:A:2336:A:N7	23:W:40:ARG:NE	2.63	0.47
1:A:2093:G:C6	1:A:2225:A:C8	3.03	0.47
1:A:616:A:N3	1:A:617:G:C8	2.83	0.47
1:A:379:G:C6	1:A:380:G:N7	2.83	0.47
1:A:141:G:C2'	1:A:142:A:O4'	2.63	0.47
1:A:962:G:O2'	1:A:963:U:O5'	2.32	0.47
1:A:857:G:O2'	23:W:19:ARG:CZ	2.63	0.47
1:A:2345:G:C5	1:A:2347:C:C5	3.02	0.47
10:J:45:THR:C	10:J:47:HIS:N	2.68	0.47
1:A:1255:U:O2'	1:A:1256:G:P	2.72	0.47
1:A:2265:U:OP2	1:A:2266:A:O2'	2.33	0.47
1:A:1455:G:O2'	1:A:1456:G:O5'	2.32	0.47
1:A:2078:C:C4	1:A:2079:U:C4	3.02	0.47
1:A:475:C:O2'	1:A:476:G:C5'	2.63	0.47
1:A:1709:U:C2	1:A:1750:G:N2	2.82	0.47
1:A:321:U:O2'	1:A:340:A:N3	2.46	0.47
1:A:1308:A:N6	1:A:1309:G:C2	2.83	0.47
1:A:2675:A:C2	1:A:2676:C:C2	3.02	0.47
1:A:1549:A:C6	1:A:1550:C:N3	2.83	0.47
1:A:1753:G:C2	1:A:1756:G:C2	3.04	0.47
1:A:861:A:N3	2:B:79:G:O2'	2.48	0.46
1:A:2235:G:C5	1:A:2236:U:C5	3.04	0.46
1:A:2415:G:C4	1:A:2416:C:C5	3.03	0.46
1:A:2330:G:C2	1:A:2386:A:N1	2.83	0.46
1:A:627:A:O4'	1:A:637:A:N6	2.48	0.46
1:A:1244:A:O2'	5:E:29:HIS:NE2	2.48	0.46
1:A:1436:G:N2	1:A:1557:C:C2	2.83	0.46
1:A:1801:A:C4	1:A:2203:U:C5	3.03	0.46
1:A:2497:A:O2'	1:A:2498:C:OP2	2.33	0.46
1:A:1387:A:C4	1:A:1388:G:C8	3.03	0.46
1:A:1341:G:C4	20:T:84:TYR:CE2	3.03	0.46
1:A:971:G:O2'	1:A:983:A:N3	2.48	0.46
2:B:18:G:C6	2:B:19:C:C4	3.03	0.46
1:A:1286:A:C5	1:A:1289:C:N4	2.83	0.46
1:A:483:A:C2'	1:A:484:C:C6	2.98	0.46
2:B:99:A:C5	2:B:100:G:C5	3.03	0.46
1:A:635:C:OP2	12:L:126:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1753:G:N2	1:A:1756:G:OP2	2.49	0.46
19:S:36:LEU:C	19:S:38:TYR:N	2.69	0.46
1:A:333:G:C4	1:A:334:C:C5	3.03	0.46
1:A:333:G:O2'	1:A:334:C:C6	2.68	0.46
1:A:1387:A:C5'	1:A:1469:A:C1'	2.93	0.46
1:A:2750:A:C4'	1:A:2751:G:OP2	2.62	0.46
1:A:2496:C:N4	34:A:3402:HOH:O	2.49	0.46
1:A:774:G:O2'	1:A:775:G:C8	2.68	0.46
1:A:245:G:O2'	1:A:384:A:N1	2.49	0.46
1:A:2322:A:C8	1:A:2323:G:C8	3.03	0.46
1:A:332:A:C5	1:A:335:C:N4	2.83	0.46
1:A:2571:U:N3	1:A:2574:G:C8	2.84	0.46
1:A:1324:G:N2	1:A:1328:A:C6	2.84	0.46
1:A:1551:A:C5	1:A:1552:A:C8	3.03	0.46
1:A:483:A:O2'	1:A:484:C:C5'	2.64	0.46
1:A:235:U:N3	1:A:236:C:C5	2.83	0.46
1:A:1265:A:C4	1:A:1267:U:C4	3.04	0.46
1:A:1394:U:C6	1:A:1394:U:C3'	2.99	0.46
1:A:1801:A:C5	1:A:2203:U:C5	3.03	0.46
1:A:1693:U:OP2	1:A:1694:C:N4	2.48	0.46
1:A:1420:A:N3	1:A:2211:A:N7	2.63	0.46
1:A:2037:A:C6	1:A:2038:G:C6	3.04	0.46
8:H:50:ARG:C	8:H:52:ALA:N	2.69	0.46
1:A:75:G:O2'	1:A:76:C:O5'	2.34	0.46
1:A:1033:U:O2'	1:A:2750:A:N6	2.48	0.46
1:A:2307:G:O2'	1:A:2308:G:C8	2.69	0.46
1:A:1410:G:N2	1:A:1593:A:C4	2.83	0.46
14:N:16:HIS:CE1	14:N:20:MET:CE	2.99	0.46
1:A:40:U:C4	1:A:41:C:C4	3.04	0.46
1:A:186:G:N2	1:A:211:C:C2	2.83	0.46
1:A:1706:C:C4'	1:A:1707:G:OP2	2.62	0.46
16:P:19:PHE:CD2	16:P:19:PHE:N	2.83	0.46
1:A:587:C:N3	12:L:33:ARG:NH2	2.63	0.46
4:D:94:GLN:O	4:D:95:SER:C	2.53	0.46
3:C:35:LYS:O	3:C:36:ASN:CB	2.62	0.46
1:A:482:A:N6	1:A:506:G:C5	2.83	0.46
1:A:406:G:O2'	1:A:407:G:O5'	2.34	0.46
1:A:1378:A:N7	1:A:1380:G:C6	2.83	0.46
1:A:478:A:C2	1:A:480:A:N9	2.84	0.46
1:A:1179:G:C4	1:A:1180:U:C5	3.04	0.46
1:A:204:A:C8	1:A:206:U:C4	3.03	0.46
1:A:533:G:N2	17:Q:44:TYR:CE1	2.83	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1799:G:O2'	3:C:179:GLU:OE2	2.34	0.46
1:A:1512:C:C4	1:A:1513:U:C4	3.03	0.46
1:A:2097:A:C4	1:A:2098:U:C5	3.04	0.46
1:A:2686:G:C5	1:A:2687:U:C4	3.03	0.46
1:A:1611:C:O2'	1:A:1612:C:O5'	2.32	0.46
1:A:1341:G:O2'	1:A:1398:C:C5'	2.64	0.46
1:A:223:A:N1	1:A:407:G:O2'	2.48	0.46
1:A:617:G:N2	1:A:618:G:C4	2.83	0.46
1:A:2444:G:C6	1:A:2445:G:C5	3.04	0.46
1:A:1289:C:O2'	1:A:1290:C:O5'	2.33	0.46
1:A:1022:G:O6	10:J:68:LYS:NZ	2.48	0.46
1:A:1171:G:C4	1:A:1179:G:N2	2.84	0.46
1:A:638:G:O2'	1:A:639:U:O4'	2.33	0.46
6:F:93:GLU:O	6:F:95:MET:N	2.49	0.46
16:P:24:THR:O	16:P:25:VAL:C	2.54	0.46
1:A:1344:U:O2	1:A:1384:A:O2'	2.34	0.46
1:A:1056:G:C1'	1:A:1103:A:N6	2.79	0.46
30:3:50:SER:O	30:3:52:GLY:N	2.49	0.46
1:A:1483:G:C6	1:A:1484:U:C4	3.04	0.46
1:A:2157:G:N2	1:A:2157:G:OP2	2.49	0.46
1:A:2298:A:N6	1:A:2321:U:O4	2.49	0.46
1:A:2067:G:O6	1:A:2444:G:C6	2.69	0.46
1:A:2574:G:N2	4:D:147:GLY:O	2.49	0.46
1:A:647:G:N7	1:A:648:G:N7	2.63	0.46
1:A:58:G:OP1	20:T:78:SER:OG	2.33	0.46
12:L:58:TYR:O	30:3:12:ARG:CZ	2.64	0.46
1:A:945:A:C5	1:A:2448:A:C2	3.04	0.46
17:Q:51:GLN:O	17:Q:54:ARG:N	2.49	0.46
1:A:172:A:C2	1:A:173:A:C5	3.04	0.46
5:E:98:LYS:O	5:E:99:LYS:CB	2.63	0.46
1:A:323:C:OP1	1:A:339:U:O2'	2.32	0.46
1:A:1324:G:O2'	1:A:1616:A:N1	2.49	0.46
1:A:287:G:N1	1:A:354:A:C6	2.84	0.46
2:B:81:G:C5	2:B:82:U:C5	3.05	0.46
1:A:1734:G:C2'	1:A:1735:A:C8	2.99	0.46
1:A:568:U:C2'	1:A:570:G:OP2	2.64	0.46
1:A:1526:C:C4	1:A:1527:G:C5	3.03	0.46
1:A:973:A:C8	1:A:973:A:OP1	2.69	0.46
7:G:88:LEU:N	7:G:128:THR:O	2.49	0.46
17:Q:6:GLY:C	17:Q:8:ILE:N	2.69	0.46
21:U:14:THR:CG2	21:U:15:GLY:N	2.79	0.46
1:A:599:A:N3	1:A:659:G:C2	2.84	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:28:GLY:O	9:I:29:GLN:C	2.53	0.46
1:A:2697:G:C2	1:A:2711:A:C2	3.04	0.46
19:S:62:ASP:OD1	19:S:62:ASP:N	2.48	0.46
1:A:1388:G:O6	1:A:1400:U:O4	2.34	0.45
2:B:66:A:C2	2:B:108:A:C6	3.04	0.45
1:A:2266:A:N6	1:A:2273:A:OP2	2.49	0.45
29:2:28:ARG:C	29:2:30:VAL:N	2.69	0.45
20:T:62:VAL:CG1	20:T:63:VAL:N	2.79	0.45
1:A:2422:C:O2'	1:A:2424:C:OP1	2.34	0.45
6:F:45:ASP:C	6:F:47:LYS:N	2.69	0.45
1:A:1000:A:N1	1:A:1001:A:C2	2.84	0.45
1:A:333:G:O2'	1:A:334:C:O5'	2.34	0.45
1:A:228:C:C5'	1:A:229:C:C5	2.98	0.45
1:A:1611:C:O2'	1:A:1612:C:C6	2.69	0.45
1:A:35:G:C5	1:A:454:A:C2	3.05	0.45
1:A:140:C:O2'	1:A:141:G:OP2	2.34	0.45
1:A:2468:A:O2'	1:A:2469:A:O5'	2.35	0.45
1:A:1019:U:C2'	1:A:1021:A:N1	2.79	0.45
1:A:1363:C:C2	1:A:1364:G:C8	3.04	0.45
1:A:2431:U:N3	1:A:2434:A:OP2	2.49	0.45
1:A:1695:G:O2'	1:A:1696:G:O5'	2.34	0.45
16:P:67:GLU:OE1	16:P:68:GLY:N	2.50	0.45
5:E:40:ARG:NH2	5:E:92:HIS:NE2	2.65	0.45
1:A:99:U:O4'	1:A:99:U:O2	2.33	0.45
1:A:698:C:C4	1:A:762:U:O4	2.69	0.45
14:N:92:GLY:N	14:N:94:TYR:CE1	2.85	0.45
1:A:510:C:C4	1:A:511:U:C4	3.05	0.45
10:J:94:ALA:O	10:J:95:ARG:CG	2.65	0.45
1:A:627:A:C2'	12:L:78:ARG:NH1	2.79	0.45
1:A:668:A:C5	1:A:670:A:N7	2.84	0.45
1:A:1501:G:C4	1:A:1502:A:C8	3.04	0.45
1:A:476:G:O2'	1:A:477:A:C5'	2.65	0.45
1:A:2353:G:N3	23:W:30:VAL:CG1	2.78	0.45
16:P:89:GLY:O	16:P:112:ARG:NH1	2.48	0.45
1:A:358:U:N3	1:A:359:G:N7	2.63	0.45
21:U:94:PHE:O	21:U:94:PHE:CD2	2.70	0.45
4:D:118:PHE:CE1	4:D:119:ALA:O	2.69	0.45
1:A:324:A:N6	1:A:338:G:O2'	2.49	0.45
18:R:81:LYS:O	18:R:82:HIS:C	2.55	0.45
1:A:1260:A:C2	1:A:1261:C:C2	3.04	0.45
1:A:1651:G:C2	1:A:2007:U:N3	2.85	0.45
14:N:14:SER:C	14:N:16:HIS:N	2.69	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1275:A:C4	14:N:16:HIS:CD2	3.05	0.45
1:A:2013:A:C2	19:S:88:ARG:NH1	2.85	0.45
1:A:2748:A:C2	1:A:2757:A:C5	3.04	0.45
1:A:586:A:N1	1:A:809:G:O2'	2.49	0.45
1:A:991:C:C6	1:A:991:C:O5'	2.69	0.45
27:0:38:LEU:N	27:0:41:HIS:CE1	2.83	0.45
1:A:876:C:O4'	1:A:876:C:O2	2.32	0.45
1:A:482:A:N6	1:A:506:G:C8	2.85	0.45
1:A:2234:G:C6	1:A:2235:G:N7	2.85	0.45
1:A:2314:A:N1	1:A:2315:G:C6	2.85	0.45
1:A:489:G:C4'	1:A:490:C:OP1	2.65	0.45
1:A:510:C:OP1	1:A:511:U:OP2	2.35	0.45
17:Q:57:ARG:O	17:Q:59:LEU:N	2.49	0.45
1:A:579:G:N2	1:A:1262:A:C4	2.85	0.45
3:C:8:THR:O	3:C:9:SER:CB	2.65	0.45
1:A:2743:U:OP1	31:4:34:LYS:NZ	2.49	0.45
3:C:76:VAL:O	3:C:93:VAL:O	2.34	0.45
1:A:125:A:OP2	29:2:19:ARG:NH2	2.49	0.45
10:J:97:PRO:C	10:J:99:ARG:N	2.69	0.45
21:U:80:ASP:OD1	21:U:80:ASP:N	2.50	0.45
1:A:310:A:C2	1:A:330:A:C5	3.04	0.45
1:A:1087:G:C4	1:A:1089:A:C2	3.04	0.45
1:A:617:G:O2'	1:A:618:G:O5'	2.35	0.45
1:A:447:A:C8	1:A:473:G:C6	3.04	0.45
1:A:732:C:C4	1:A:733:G:C5	3.05	0.45
14:N:16:HIS:O	14:N:20:MET:CB	2.65	0.45
1:A:785:G:C6	1:A:786:C:C4	3.04	0.45
1:A:1867:G:O6	1:A:1875:G:N2	2.50	0.45
14:N:84:GLY:N	14:N:85:PRO:CD	2.79	0.45
1:A:1014:A:C2	1:A:1149:G:C2	3.05	0.45
1:A:180:G:O6	1:A:213:A:N6	2.50	0.45
1:A:2466:C:OP1	31:4:4:ARG:CB	2.64	0.45
1:A:486:C:O2	1:A:495:G:N2	2.50	0.45
1:A:2889:C:C4	1:A:2890:G:C6	3.04	0.45
1:A:1744:A:N6	1:A:1745:A:C2	2.85	0.45
1:A:1392:A:N6	1:A:1393:A:C6	2.85	0.45
1:A:46:G:N1	1:A:47:C:C4	2.85	0.45
1:A:570:G:C4	1:A:2030:A:N7	2.85	0.45
1:A:2831:G:C8	4:D:59:ARG:NH1	2.84	0.45
12:L:118:THR:O	12:L:120:VAL:N	2.49	0.45
1:A:2887:A:C4	27:0:39:ARG:NH1	2.85	0.45
22:V:56:PHE:C	22:V:56:PHE:CD1	2.90	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:181:ASP:C	4:D:183:GLU:N	2.70	0.45
1:A:1914:C:O2'	1:A:1915:U:C5'	2.64	0.45
1:A:2067:G:C6	1:A:2444:G:N1	2.84	0.45
1:A:1973:G:C5	1:A:1974:C:C5	3.05	0.45
1:A:764:A:C2	1:A:781:A:C4	3.05	0.45
1:A:860:U:O4	1:A:2268:A:C4	2.70	0.45
1:A:200:U:O4	1:A:248:G:C2	2.70	0.45
1:A:508:A:C3'	1:A:509:C:C5'	2.95	0.45
19:S:8:ARG:O	19:S:9:HIS:CB	2.65	0.45
1:A:94:A:C6	1:A:95:A:C6	3.05	0.45
1:A:1544:A:C6	1:A:1545:A:C6	3.05	0.45
1:A:758:C:O2	1:A:759:G:C8	2.69	0.45
16:P:88:ARG:NH1	16:P:112:ARG:NH2	2.65	0.45
4:D:184:ARG:NH2	16:P:6:GLN:NE2	2.65	0.45
9:I:20:SER:N	9:I:21:PRO:CD	2.80	0.45
1:A:121:G:N2	1:A:131:A:C4	2.85	0.45
1:A:1090:A:C6	1:A:1102:C:O2	2.70	0.45
1:A:1352:U:C5	1:A:1377:G:O6	2.70	0.45
1:A:1300:G:O2'	1:A:1635:A:OP1	2.34	0.45
1:A:1716:U:C5	1:A:1743:G:N2	2.84	0.45
1:A:1047:G:C2'	1:A:1048:A:OP2	2.64	0.45
1:A:2531:A:C4	1:A:2532:G:C8	3.05	0.45
1:A:1570:A:C6	1:A:1571:A:C6	3.05	0.45
1:A:1827:U:O4'	1:A:1970:A:O2'	2.34	0.45
1:A:1223:G:N1	1:A:1227:G:C6	2.85	0.45
1:A:1364:G:OP2	24:X:1:SER:N	2.50	0.45
1:A:2043:C:C2	1:A:2044:C:C5	3.05	0.45
1:A:672:C:C3'	1:A:672:C:C6	3.00	0.45
1:A:348:A:C6	1:A:349:U:C4	3.04	0.45
29:2:18:PHE:O	29:2:21:ARG:N	2.50	0.45
11:K:14:SER:OG	11:K:51:LYS:N	2.49	0.45
1:A:642:U:O2'	1:A:644:A:N7	2.49	0.45
21:U:58:VAL:CG1	21:U:59:GLU:N	2.79	0.45
1:A:2056:G:N2	1:A:2057:G:C8	2.85	0.45
1:A:1601:G:C5	1:A:1602:U:C4	3.05	0.45
1:A:249:C:C4'	1:A:250:G:O5'	2.65	0.45
1:A:1019:U:C4	1:A:1020:A:N6	2.85	0.45
17:Q:46:TYR:CE1	17:Q:50:ARG:NH2	2.85	0.45
24:X:52:ALA:O	24:X:53:LYS:CB	2.64	0.45
1:A:219:A:N6	1:A:220:G:N1	2.65	0.45
1:A:2361:G:C6	1:A:2362:C:C4	3.05	0.45
1:A:1775:U:C2'	1:A:1776:G:O5'	2.65	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:685:A:C8	1:A:773:U:O4	2.70	0.45
3:C:30:ALA:N	3:C:31:PRO:CD	2.80	0.45
1:A:804:A:C2'	1:A:806:C:C4	3.00	0.44
1:A:1327:A:N6	1:A:1328:A:C6	2.85	0.44
23:W:17:ALA:O	23:W:18:LYS:CB	2.64	0.44
17:Q:63:ARG:O	17:Q:64:ILE:C	2.54	0.44
1:A:2234:G:C5	1:A:2235:G:N7	2.85	0.44
1:A:2307:G:N7	1:A:2312:U:C5	2.85	0.44
1:A:571:U:C6	1:A:575:A:N6	2.85	0.44
2:B:95:U:O4	34:B:593:HOH:O	2.15	0.44
1:A:271:G:C2	1:A:367:G:N3	2.86	0.44
10:J:43:GLU:O	10:J:44:TYR:C	2.56	0.44
2:B:81:G:C5	2:B:82:U:C4	3.05	0.44
1:A:1499:C:C4	1:A:1500:G:N7	2.85	0.44
1:A:146:A:C2	1:A:147:C:C2	3.05	0.44
13:M:11:LYS:NZ	13:M:86:LYS:O	2.50	0.44
1:A:609:A:N7	1:A:610:C:C2	2.86	0.44
2:B:38:C:C4'	15:O:100:HIS:NE2	2.80	0.44
11:K:17:ARG:O	11:K:18:ARG:O	2.36	0.44
1:A:1485:U:C2	1:A:1505:A:C2	3.05	0.44
1:A:1677:A:C8	34:A:3591:HOH:O	2.70	0.44
8:H:104:THR:O	8:H:104:THR:CG2	2.65	0.44
1:A:2258:C:C4'	1:A:2259:U:OP2	2.65	0.44
1:A:1681:G:O2'	1:A:1762:A:N3	2.50	0.44
1:A:845:A:C6	1:A:932:U:N3	2.85	0.44
1:A:197:A:N6	1:A:2430:A:C2'	2.80	0.44
1:A:648:G:N3	1:A:649:G:C8	2.86	0.44
1:A:491:G:O2'	1:A:492:A:O4'	2.34	0.44
1:A:48:G:N2	1:A:177:G:C2	2.85	0.44
2:B:99:A:N6	2:B:100:G:C6	2.86	0.44
1:A:1670:C:C4	1:A:1671:U:C2	3.05	0.44
1:A:1350:C:C2	1:A:1382:G:N7	2.85	0.44
1:A:2373:G:C2	1:A:2374:C:C2	3.04	0.44
1:A:2650:U:C2	1:A:2671:G:N2	2.85	0.44
5:E:102:ARG:O	5:E:104:ALA:N	2.50	0.44
20:T:47:VAL:O	20:T:53:VAL:O	2.35	0.44
1:A:1064:C:C4	1:A:1065:U:C5	3.05	0.44
1:A:1109:C:C4	1:A:1110:G:C6	3.06	0.44
1:A:1312:U:C4'	1:A:1313:U:O5'	2.66	0.44
1:A:2234:G:C4	1:A:2235:G:C8	3.06	0.44
1:A:2307:G:O2'	1:A:2308:G:O4'	2.36	0.44
1:A:2287:A:C8	1:A:2289:G:C8	3.06	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1935:G:N2	1:A:1964:G:OP2	2.51	0.44
1:A:1251:C:O2'	34:A:3125:HOH:O	2.21	0.44
1:A:2474:U:C2'	1:A:2475:C:O5'	2.65	0.44
1:A:600:G:C5	1:A:601:C:C4	3.05	0.44
8:H:27:ARG:NH1	24:X:59:ASP:CA	2.80	0.44
1:A:2204:G:C2	1:A:2205:A:C8	3.05	0.44
13:M:58:LYS:O	13:M:60:GLN:N	2.51	0.44
1:A:2706:A:N6	34:A:3512:HOH:O	2.49	0.44
1:A:323:C:OP2	5:E:163:ASN:ND2	2.51	0.44
1:A:1080:A:O2'	9:I:126:ARG:O	2.35	0.44
1:A:1608:A:C5	1:A:1611:C:C4	3.05	0.44
1:A:410:G:C2	1:A:2407:A:C6	3.05	0.44
1:A:1626:A:O2'	1:A:1627:G:OP2	2.35	0.44
1:A:1485:U:N3	1:A:1505:A:C2	2.85	0.44
1:A:252:G:N2	1:A:253:C:C2	2.85	0.44
7:G:60:GLY:O	7:G:62:ALA:N	2.51	0.44
4:D:166:GLY:O	4:D:167:ASN:CB	2.65	0.44
1:A:229:C:O2'	1:A:230:G:C5'	2.66	0.44
7:G:91:VAL:O	7:G:93:TYR:N	2.51	0.44
1:A:241:A:C5	1:A:243:U:O4	2.71	0.44
7:G:154:GLU:C	7:G:156:TYR:N	2.71	0.44
1:A:478:A:C2	1:A:480:A:C8	3.06	0.44
1:A:351:C:N4	1:A:352:A:N6	2.66	0.44
1:A:2143:C:C2	1:A:2148:G:N1	2.85	0.44
1:A:1867:G:C2	1:A:1868:C:C2	3.06	0.44
1:A:1232:G:C4	1:A:1233:C:C5	3.05	0.44
8:H:97:ARG:O	8:H:98:ASP:CB	2.66	0.44
3:C:120:ASP:CG	3:C:121:ALA:N	2.71	0.44
6:F:41:GLU:O	6:F:43:ILE:N	2.51	0.44
1:A:1091:G:C2	1:A:1101:U:N3	2.86	0.44
1:A:2298:A:C6	1:A:2321:U:C4	3.05	0.44
1:A:1400:U:C2'	1:A:1401:G:O4'	2.64	0.44
1:A:425:G:C4	1:A:426:C:C5	3.06	0.44
1:A:2665:A:C2	1:A:2666:C:N3	2.85	0.44
1:A:631:A:N3	1:A:2415:G:O2'	2.51	0.44
1:A:1204:A:O4'	1:A:1206:G:N7	2.51	0.44
1:A:1285:A:C6	1:A:1329:U:C5	3.05	0.44
30:3:28:LEU:O	30:3:29:ARG:CB	2.66	0.44
1:A:2209:G:C6	1:A:2216:G:N1	2.86	0.44
1:A:92:U:C6	1:A:93:G:C8	3.05	0.44
1:A:1680:U:O2'	1:A:1763:G:N7	2.51	0.44
1:A:2253:G:C6	1:A:2254:C:C4	3.06	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:983:A:C6	1:A:984:A:C2	3.05	0.44
1:A:90:U:C4	1:A:91:A:C5	3.06	0.44
1:A:1735:A:C6	1:A:1736:U:C4	3.06	0.44
1:A:2142:A:N3	1:A:2144:G:OP1	2.51	0.44
1:A:1204:A:N1	1:A:1241:A:N1	2.65	0.44
1:A:591:U:C2	1:A:592:A:C8	3.06	0.44
1:A:1833:C:C2	1:A:1834:U:C6	3.06	0.44
23:W:35:ILE:O	23:W:36:ILE:O	2.36	0.44
17:Q:57:ARG:NH1	17:Q:92:LYS:CE	2.81	0.44
1:A:533:G:C5	1:A:534:U:C4	3.06	0.44
1:A:2515:C:N3	1:A:2569:G:N2	2.66	0.44
29:2:43:THR:O	29:2:44:VAL:C	2.56	0.44
22:V:30:ILE:O	22:V:38:LEU:N	2.50	0.44
3:C:149:LYS:CE	3:C:152:GLN:NE2	2.81	0.44
1:A:1661:G:C5	1:A:1662:U:C5	3.06	0.44
1:A:308:G:N1	1:A:309:A:C2	2.86	0.44
1:A:1079:C:N4	1:A:1088:A:C5'	2.81	0.44
1:A:1071:G:O4'	1:A:1088:A:O2'	2.35	0.44
2:B:42:C:N4	6:F:87:LYS:NZ	2.66	0.44
1:A:863:A:C2	1:A:864:G:C4	3.05	0.44
1:A:2744:G:C6	1:A:2761:A:N6	2.86	0.44
1:A:2142:A:C2'	1:A:2144:G:P	3.06	0.44
1:A:1670:C:N4	1:A:1671:U:N3	2.66	0.44
6:F:45:ASP:O	6:F:47:LYS:N	2.50	0.44
1:A:2004:G:C5	1:A:2005:A:C8	3.06	0.44
1:A:981:A:N1	1:A:2027:G:O2'	2.51	0.44
1:A:2349:G:OP1	30:3:44:ARG:NH2	2.51	0.44
1:A:2297:A:C2	1:A:2298:A:N7	2.86	0.43
1:A:1304:A:C6	1:A:1305:C:C4	3.06	0.43
1:A:858:G:C5	1:A:2268:A:N1	2.86	0.43
2:B:42:C:O2	6:F:89:THR:N	2.50	0.43
23:W:25:PHE:CD1	23:W:25:PHE:C	2.92	0.43
1:A:1779:U:C5	1:A:1784:A:N7	2.86	0.43
1:A:61:C:C2	1:A:94:A:C2	3.06	0.43
3:C:203:VAL:O	3:C:205:GLY:N	2.51	0.43
1:A:2201:G:C5	1:A:2223:G:C2	3.06	0.43
1:A:237:C:C4	1:A:238:C:C5	3.06	0.43
22:V:32:GLY:O	22:V:33:GLY:C	2.56	0.43
1:A:1907:G:C2	1:A:1924:C:O2	2.71	0.43
1:A:2461:A:C2	1:A:2490:G:N2	2.86	0.43
7:G:72:ASN:OD1	7:G:73:SER:N	2.51	0.43
10:J:30:THR:CG2	10:J:31:GLU:N	2.81	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:229:C:O2'	1:A:230:G:C4'	2.66	0.43
1:A:1388:G:N3	1:A:1389:G:C8	2.86	0.43
1:A:301:G:N1	1:A:302:C:N4	2.65	0.43
1:A:1286:A:C8	1:A:1289:C:N4	2.85	0.43
1:A:2347:C:O2'	1:A:2348:U:C6	2.71	0.43
1:A:2314:A:N1	1:A:2315:G:C5	2.86	0.43
1:A:2519:U:C2	1:A:2542:A:C6	3.06	0.43
1:A:56:A:C6	1:A:57:C:N3	2.86	0.43
18:R:49:ILE:C	18:R:51:VAL:N	2.71	0.43
1:A:2838:G:C1'	14:N:45:ARG:NH2	2.81	0.43
9:I:35:MET:C	9:I:37:PHE:N	2.70	0.43
16:P:92:ARG:CG	16:P:92:ARG:O	2.66	0.43
2:B:11:C:C5	2:B:12:C:C5	3.07	0.43
1:A:311:A:O2'	1:A:312:G:P	2.76	0.43
1:A:226:A:N6	1:A:409:G:N2	2.66	0.43
1:A:1343:G:N2	1:A:1344:U:C2	2.86	0.43
1:A:141:G:O2'	1:A:142:A:O5'	2.37	0.43
1:A:1437:C:C2	1:A:1438:U:C5	3.05	0.43
13:M:1:MET:O	13:M:2:LEU:C	2.55	0.43
16:P:102:ARG:O	16:P:103:THR:CB	2.66	0.43
6:F:36:ASN:O	6:F:37:MET:CB	2.66	0.43
1:A:724:U:O4	1:A:725:G:N1	2.51	0.43
5:E:115:GLN:O	5:E:117:ARG:N	2.51	0.43
7:G:115:GLN:CG	7:G:116:LEU:N	2.82	0.43
1:A:2791:G:O4'	1:A:2791:G:OP1	2.37	0.43
2:B:58:A:C8	2:B:59:A:C8	3.07	0.43
1:A:1401:G:C4	1:A:1402:U:C5	3.07	0.43
1:A:303:G:C2	1:A:304:U:O2	2.71	0.43
1:A:82:U:C2	1:A:83:A:C8	3.07	0.43
1:A:265:A:C6	1:A:428:A:O4'	2.71	0.43
1:A:1179:G:C2	1:A:1180:U:C2	3.06	0.43
1:A:1534:U:C6	1:A:1538:G:N1	2.87	0.43
1:A:1627:G:C2	1:A:1628:G:C8	3.06	0.43
1:A:2209:G:C4	1:A:2216:G:N2	2.86	0.43
29:2:18:PHE:O	29:2:19:ARG:C	2.57	0.43
1:A:1091:G:C2	1:A:1092:C:C2	3.06	0.43
1:A:2463:C:C2	1:A:2488:G:N2	2.87	0.43
17:Q:96:ASP:C	17:Q:98:ALA:N	2.71	0.43
1:A:2324:U:C5'	1:A:2325:G:C5'	2.96	0.43
1:A:1387:A:O2'	1:A:1388:G:P	2.77	0.43
1:A:1403:A:C6	1:A:1404:C:C4	3.07	0.43
1:A:301:G:N1	1:A:317:G:C5	2.86	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1355:G:C2	1:A:1356:G:C8	3.07	0.43
10:J:45:THR:OG1	10:J:48:VAL:N	2.51	0.43
1:A:1968:G:C5'	34:A:3323:HOH:O	2.67	0.43
1:A:295:G:N2	1:A:296:U:C6	2.87	0.43
1:A:107:G:C2	1:A:108:G:C8	3.05	0.43
1:A:991:C:OP2	1:A:1186:G:OP2	2.35	0.43
1:A:1523:U:O2'	1:A:1524:G:OP1	2.37	0.43
25:Y:22:LEU:O	25:Y:26:PHE:N	2.51	0.43
1:A:1530:G:N2	1:A:1542:U:O2	2.52	0.43
9:I:12:VAL:CG1	9:I:13:ALA:N	2.81	0.43
7:G:58:ALA:O	7:G:59:ASP:C	2.57	0.43
20:T:48:GLN:NE2	20:T:54:GLU:CB	2.82	0.43
2:B:67:G:N3	2:B:68:C:C6	2.87	0.43
1:A:142:A:C2	1:A:143:C:C2	3.06	0.43
1:A:2392:A:OP1	30:3:30:HIS:ND1	2.51	0.43
1:A:858:G:C5	1:A:2268:A:C2	3.07	0.43
1:A:621:A:O2'	1:A:622:G:C4'	2.67	0.43
1:A:571:U:O2	1:A:2030:A:O2'	2.36	0.43
1:A:563:A:N3	17:Q:36:GLN:NE2	2.65	0.43
1:A:2733:A:C5	4:D:208:LYS:NZ	2.87	0.43
12:L:4:ASN:O	12:L:6:LEU:N	2.51	0.43
1:A:1091:G:N2	1:A:1101:U:C2	2.86	0.43
1:A:1435:G:N2	1:A:1558:C:N4	2.67	0.43
1:A:782:A:O2'	3:C:223:ALA:O	2.36	0.43
1:A:2029:G:C2	1:A:2033:A:N7	2.87	0.43
8:H:101:ASP:O	8:H:102:ALA:O	2.36	0.43
1:A:2612:C:C5'	1:A:2613:U:OP1	2.66	0.43
1:A:1611:C:C2	1:A:1612:C:C5	3.06	0.43
1:A:54:G:C6	1:A:55:G:N7	2.87	0.43
1:A:415:A:C2	1:A:2409:G:C6	3.06	0.43
1:A:1287:A:O2'	1:A:1288:G:C5'	2.67	0.43
1:A:1438:U:C5	1:A:1552:A:N1	2.86	0.43
1:A:745:G:C5'	1:A:746:U:OP2	2.66	0.43
1:A:1261:C:OP2	19:S:83:LYS:NZ	2.51	0.43
1:A:233:A:O2'	1:A:234:U:O5'	2.37	0.43
1:A:60:G:O2'	1:A:61:C:O5'	2.36	0.43
1:A:371:A:C4	1:A:373:U:O4	2.72	0.43
1:A:927:A:N1	1:A:928:A:C2	2.87	0.43
1:A:485:C:C2	1:A:496:G:N2	2.87	0.43
1:A:2886:A:N7	27:O:39:ARG:CZ	2.82	0.43
1:A:2031:A:O2'	1:A:2454:G:N2	2.52	0.43
8:H:62:LEU:C	8:H:64:ALA:N	2.72	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:75:SER:O	5:E:78:TRP:N	2.52	0.43
1:A:1590:A:C6	1:A:1591:A:N6	2.86	0.43
6:F:131:VAL:C	6:F:133:GLU:N	2.72	0.43
1:A:1585:C:C2'	1:A:1586:A:O5'	2.66	0.43
1:A:412:A:O2'	1:A:413:C:O4'	2.37	0.43
1:A:36:G:C6	1:A:37:C:C4	3.07	0.43
1:A:2415:G:C4	1:A:2416:C:C6	3.06	0.43
1:A:1733:G:C2	1:A:1734:G:C8	3.07	0.43
1:A:1042:G:C5	1:A:1043:C:C4	3.06	0.43
1:A:2682:A:O2'	1:A:2683:C:O4'	2.37	0.43
1:A:2629:U:C5'	1:A:2630:G:OP1	2.67	0.43
17:Q:38:VAL:O	17:Q:42:GLY:N	2.52	0.43
1:A:266:G:C2'	1:A:267:C:O5'	2.66	0.43
1:A:2677:G:C4	1:A:2731:G:N2	2.86	0.43
1:A:391:A:C2	1:A:411:G:C5	3.07	0.43
1:A:2331:G:C2	1:A:2385:C:C4	3.07	0.43
1:A:1236:G:O2'	1:A:1237:A:C8	2.72	0.43
1:A:2069:G:N2	1:A:2443:C:C2	2.87	0.43
1:A:676:A:N1	1:A:2069:G:O2'	2.52	0.43
1:A:1609:A:N3	1:A:1616:A:O4'	2.51	0.43
1:A:1757:A:N1	1:A:1762:A:C2	2.87	0.43
1:A:1663:G:C2	1:A:1998:A:C5	3.07	0.43
1:A:42:A:C2	1:A:438:G:C2	3.07	0.43
10:J:80:HIS:O	10:J:81:ILE:C	2.57	0.43
22:V:21:ARG:NH2	22:V:87:GLN:O	2.51	0.43
1:A:2200:C:O2	1:A:2226:C:N4	2.52	0.43
1:A:2331:G:C2'	1:A:2332:C:O5'	2.67	0.43
1:A:1095:A:N1	1:A:1096:A:N6	2.66	0.43
1:A:1396:U:C2'	1:A:1397:U:OP1	2.67	0.43
1:A:49:A:C6	1:A:118:A:C6	3.06	0.43
1:A:1238:G:O2'	1:A:1239:G:C5'	2.67	0.43
1:A:616:A:O2'	1:A:617:G:O5'	2.37	0.43
1:A:447:A:C2	1:A:454:A:C8	3.07	0.43
1:A:1290:C:O2'	1:A:1291:C:C6	2.72	0.43
1:A:1633:G:C6	1:A:1635:A:C5	3.07	0.43
1:A:250:G:OP1	12:L:59:ARG:NH1	2.52	0.43
1:A:270:A:N1	1:A:369:U:C1'	2.81	0.43
1:A:671:C:O2'	1:A:672:C:OP2	2.37	0.43
17:Q:86:SER:O	17:Q:87:VAL:C	2.58	0.43
1:A:2253:G:C5	1:A:2254:C:C5	3.07	0.43
6:F:36:ASN:OD1	6:F:86:CYS:N	2.52	0.43
20:T:37:ASP:O	20:T:38:ALA:O	2.36	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:87:GLN:CG	18:R:88:GLY:N	2.82	0.43
1:A:1480:C:C4	1:A:1481:U:C5	3.07	0.43
1:A:2199:A:C6	1:A:2200:C:C2	3.07	0.42
1:A:1079:C:N3	1:A:1088:A:C2	2.87	0.42
1:A:2009:A:N6	34:A:3224:HOH:O	2.52	0.42
1:A:241:A:C8	1:A:243:U:N3	2.87	0.42
1:A:2638:G:C2'	1:A:2639:A:OP2	2.66	0.42
1:A:351:C:C2	1:A:352:A:N7	2.87	0.42
24:X:3:VAL:C	24:X:5:GLN:N	2.73	0.42
1:A:2784:U:C4	1:A:2785:C:N4	2.87	0.42
18:R:35:PHE:N	18:R:59:ILE:O	2.52	0.42
1:A:544:C:C4	1:A:545:U:N3	2.86	0.42
19:S:39:THR:CG2	19:S:40:ASN:N	2.82	0.42
1:A:282:A:C6	1:A:283:G:C5	3.07	0.42
5:E:162:ARG:C	5:E:164:LEU:N	2.72	0.42
17:Q:79:ILE:CD1	17:Q:79:ILE:C	2.87	0.42
1:A:370:G:N1	1:A:424:G:N7	2.66	0.42
1:A:1283:G:N1	1:A:1286:A:OP2	2.52	0.42
1:A:2054:A:C2	1:A:2616:C:N3	2.87	0.42
1:A:607:U:C6	1:A:607:U:C3'	3.02	0.42
1:A:70:G:C4'	1:A:71:A:OP1	2.67	0.42
1:A:58:G:N3	1:A:73:A:C2	2.87	0.42
1:A:1275:A:N3	1:A:1275:A:O2'	2.53	0.42
1:A:586:A:O2'	1:A:671:C:O2	2.36	0.42
1:A:1308:A:N7	1:A:1309:G:C5	2.87	0.42
1:A:2738:A:C2	1:A:2739:U:C2	3.08	0.42
1:A:2552:U:C2	1:A:2554:U:C5'	3.01	0.42
10:J:73:VAL:CG2	10:J:74:TYR:N	2.82	0.42
1:A:2332:C:C4'	23:W:40:ARG:NH2	2.82	0.42
1:A:2574:G:C2	1:A:2575:C:C2	3.07	0.42
1:A:1648:U:OP1	34:A:3238:HOH:O	2.20	0.42
1:A:1056:G:C5'	1:A:1085:A:C2	3.02	0.42
1:A:303:G:N1	1:A:315:G:C6	2.87	0.42
1:A:752:A:O2'	1:A:753:A:C8	2.72	0.42
1:A:1475:G:C2'	1:A:1476:U:OP2	2.67	0.42
21:U:44:HIS:O	21:U:45:GLN:C	2.57	0.42
1:A:729:G:C3'	1:A:730:A:C5'	2.98	0.42
1:A:2576:G:O2'	1:A:2579:C:OP2	2.36	0.42
1:A:1865:U:O2	1:A:1877:A:C6	2.73	0.42
1:A:1349:C:N3	1:A:1382:G:O6	2.52	0.42
19:S:40:ASN:OD1	19:S:41:LYS:N	2.52	0.42
1:A:952:G:C6	1:A:966:G:N1	2.88	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:195:GLN:O	5:E:199:MET:N	2.53	0.42
1:A:2418:A:O2'	28:1:19:PHE:CE2	2.73	0.42
11:K:73:ASP:N	11:K:73:ASP:OD1	2.52	0.42
1:A:2337:G:N3	1:A:2337:G:C2'	2.81	0.42
1:A:335:C:O2'	1:A:336:C:P	2.77	0.42
1:A:425:G:C2	1:A:426:C:C5	3.08	0.42
1:A:36:G:C6	1:A:445:C:N4	2.87	0.42
1:A:675:A:N6	1:A:676:A:N6	2.68	0.42
12:L:68:SER:O	12:L:69:ARG:CB	2.68	0.42
1:A:1359:A:OP1	1:A:1360:G:OP2	2.37	0.42
23:W:27:GLY:CA	23:W:31:LEU:CD1	2.97	0.42
1:A:862:G:C4	1:A:863:A:C8	3.07	0.42
1:A:233:A:O2'	1:A:234:U:C5'	2.67	0.42
1:A:570:G:C5	1:A:2030:A:C5	3.08	0.42
1:A:2760:C:C2'	1:A:2760:C:O2	2.66	0.42
1:A:1171:G:C5	1:A:1179:G:N2	2.87	0.42
1:A:121:G:C2	1:A:131:A:C5	3.07	0.42
24:X:24:THR:O	24:X:25:LYS:C	2.57	0.42
3:C:118:GLY:O	3:C:119:VAL:C	2.57	0.42
1:A:2844:G:N2	1:A:2874:C:N3	2.68	0.42
1:A:1904:G:O2'	1:A:1927:A:N6	2.52	0.42
3:C:44:ASN:C	3:C:46:GLY:N	2.73	0.42
19:S:73:LYS:O	19:S:106:VAL:N	2.53	0.42
11:K:13:ASN:ND2	11:K:13:ASN:N	2.68	0.42
2:B:27:C:C5	2:B:28:C:C5	3.08	0.42
1:A:2335:A:C2	1:A:2337:G:C8	3.07	0.42
1:A:323:C:N4	1:A:333:G:N7	2.68	0.42
2:B:67:G:O2'	2:B:68:C:C6	2.73	0.42
1:A:2346:A:C3'	1:A:2347:C:C5'	2.96	0.42
1:A:498:G:C6	1:A:499:U:C4	3.07	0.42
1:A:873:C:C4'	13:M:64:TRP:CD1	3.03	0.42
2:B:21:G:C2	2:B:63:C:C2	3.07	0.42
1:A:1866:A:C4	1:A:1876:A:N6	2.88	0.42
24:X:65:THR:O	24:X:68:ALA:CB	2.67	0.42
3:C:159:THR:N	3:C:194:VAL:CG1	2.83	0.42
21:U:39:ASN:O	21:U:40:LEU:C	2.57	0.42
1:A:2058:A:N6	1:A:2059:A:N6	2.68	0.42
26:Z:28:LEU:N	26:Z:28:LEU:CD2	2.82	0.42
2:B:13:G:N2	2:B:16:G:N3	2.67	0.42
1:A:370:G:C2	1:A:424:G:C8	3.08	0.42
1:A:444:C:O2'	1:A:445:C:P	2.77	0.42
1:A:1286:A:C5	1:A:1289:C:C4	3.07	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:843:G:C6	1:A:844:A:N6	2.87	0.42
21:U:66:VAL:CG1	21:U:67:SER:N	2.81	0.42
4:D:106:LYS:O	4:D:107:VAL:CB	2.68	0.42
1:A:443:A:OP1	5:E:41:GLN:N	2.53	0.42
1:A:582:A:OP1	17:Q:13:HIS:ND1	2.52	0.42
18:R:45:GLU:OE1	18:R:46:GLU:O	2.38	0.42
1:A:1082:U:N3	1:A:1086:A:C6	2.88	0.42
26:Z:21:ALA:O	26:Z:24:LEU:N	2.52	0.42
1:A:2771:C:O2'	4:D:173:GLN:OE1	2.38	0.42
6:F:111:ARG:NE	6:F:111:ARG:N	2.68	0.42
1:A:216:A:N7	1:A:432:A:C6	2.88	0.42
1:A:2322:A:N7	1:A:2323:G:C5	2.88	0.42
1:A:104:A:C8	1:A:105:C:C5	3.08	0.42
1:A:1342:A:C6	1:A:1397:U:C5	3.07	0.42
1:A:749:A:O2'	1:A:1618:A:OP1	2.37	0.42
1:A:647:G:C2'	1:A:648:G:C8	3.03	0.42
23:W:37:VAL:O	23:W:39:GLN:N	2.52	0.42
1:A:1482:G:C4	1:A:1483:G:C8	3.08	0.42
1:A:125:A:C4'	1:A:126:A:OP2	2.68	0.42
18:R:88:GLY:O	18:R:89:HIS:CB	2.68	0.42
1:A:898:C:C5	1:A:899:A:C5	3.08	0.42
1:A:1419:A:C2	1:A:1579:A:C2	3.08	0.42
1:A:1914:C:O2'	1:A:1915:U:C6	2.72	0.42
4:D:119:ALA:CB	4:D:163:GLY:C	2.88	0.42
1:A:1324:G:N2	1:A:1328:A:N1	2.68	0.42
1:A:1361:G:C6	1:A:1371:G:C2	3.08	0.42
1:A:2836:U:O2'	1:A:2837:A:P	2.78	0.42
2:B:109:A:O2'	2:B:110:C:O5'	2.38	0.42
1:A:204:A:C4	1:A:206:U:C4	3.07	0.42
1:A:204:A:O4'	1:A:206:U:C6	2.73	0.42
1:A:374:A:N6	1:A:401:A:C8	2.87	0.42
1:A:466:A:OP1	29:2:34:ARG:NH2	2.53	0.42
1:A:1350:C:O2	1:A:1382:G:C8	2.73	0.42
1:A:320:A:O2'	1:A:322:A:C8	2.72	0.42
1:A:429:A:N6	1:A:430:A:N6	2.68	0.42
11:K:113:MET:O	11:K:116:ILE:CG1	2.68	0.42
1:A:1791:A:N6	1:A:1828:G:O2'	2.52	0.42
1:A:43:G:N2	1:A:437:U:C6	2.88	0.42
1:A:2526:G:C5	1:A:2527:C:C5	3.07	0.42
1:A:1059:G:C6	1:A:1080:A:N1	2.88	0.42
1:A:2056:G:C2	27:0:1:ALA:N	2.88	0.42
1:A:1388:G:O2'	1:A:1389:G:O4'	2.38	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1953:A:O2'	1:A:2559:C:O2'	2.38	0.42
1:A:749:A:C2	1:A:750:A:C8	3.08	0.42
1:A:622:G:O2'	1:A:623:C:C5'	2.68	0.42
1:A:491:G:O2'	1:A:492:A:C5'	2.68	0.42
28:1:5:ARG:NH2	28:1:23:THR:CB	2.83	0.42
25:Y:52:ARG:C	25:Y:54:LYS:N	2.73	0.42
18:R:54:VAL:O	18:R:55:ASP:C	2.57	0.42
1:A:584:C:C5	1:A:585:G:N7	2.88	0.42
31:4:36:ARG:CG	31:4:37:GLN:N	2.83	0.42
1:A:1262:A:N3	27:0:6:LYS:NZ	2.67	0.42
4:D:169:ARG:O	4:D:170:VAL:CG2	2.68	0.42
1:A:300:A:N6	34:A:3436:HOH:O	2.53	0.42
5:E:55:SER:OG	5:E:56:GLY:N	2.52	0.42
10:J:82:GLY:O	10:J:84:ILE:N	2.53	0.42
1:A:814:C:OP1	18:R:86:GLN:NE2	2.53	0.42
1:A:2283:C:C5	1:A:2389:G:C4	3.07	0.42
1:A:1465:G:C4	1:A:1466:U:C6	3.08	0.42
1:A:2684:U:N3	1:A:2685:G:C8	2.88	0.42
1:A:139:U:C2'	1:A:139:U:O2	2.68	0.42
2:B:16:G:C6	2:B:69:G:C5	3.08	0.42
1:A:1066:U:O2	1:A:1069:A:OP2	2.37	0.42
1:A:1339:G:O4'	1:A:1393:A:C2	2.73	0.42
1:A:2345:G:C4	1:A:2347:C:C5	3.08	0.42
1:A:2311:A:C5'	1:A:2312:U:C5	3.03	0.42
1:A:1593:A:C6	1:A:1594:U:N3	2.88	0.42
1:A:1275:A:N6	14:N:15:SER:O	2.53	0.42
1:A:1168:G:C6	1:A:1182:G:C6	3.07	0.42
1:A:1532:A:N1	1:A:1540:G:C6	2.88	0.42
4:D:94:GLN:CG	4:D:94:GLN:O	2.68	0.42
31:4:3:VAL:O	31:4:4:ARG:CB	2.67	0.42
26:Z:10:ARG:NH2	26:Z:52:PHE:O	2.53	0.42
10:J:25:LEU:C	10:J:27:ARG:N	2.73	0.42
1:A:1235:G:C6	1:A:1236:G:N2	2.88	0.41
1:A:224:U:N3	1:A:225:C:C6	2.88	0.41
1:A:614:A:C4'	1:A:616:A:N6	2.83	0.41
1:A:1509:A:C3'	1:A:1510:G:C5'	2.98	0.41
1:A:1048:A:C5	1:A:1049:C:N4	2.88	0.41
1:A:2301:C:C5	1:A:2302:U:C5	3.08	0.41
1:A:71:A:O4'	1:A:73:A:C5	2.73	0.41
6:F:5:ASP:O	6:F:7:TYR:N	2.52	0.41
7:G:157:LYS:C	7:G:159:LYS:N	2.73	0.41
1:A:1833:C:C2	1:A:1834:U:C5	3.08	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1265:A:C5	1:A:1267:U:C4	3.08	0.41
1:A:2831:G:N7	4:D:59:ARG:NH1	2.67	0.41
1:A:183:C:C5	1:A:184:C:C5	3.08	0.41
1:A:1394:U:C4	1:A:1395:A:N6	2.88	0.41
1:A:1420:A:C4	1:A:2211:A:N7	2.88	0.41
1:A:180:G:P	29:2:35:ARG:NH1	2.93	0.41
14:N:97:ILE:CG1	14:N:98:LEU:N	2.83	0.41
4:D:115:GLY:O	14:N:3:HIS:CE1	2.72	0.41
19:S:31:GLN:O	19:S:33:LEU:N	2.54	0.41
23:W:69:GLU:O	23:W:78:PHE:O	2.38	0.41
5:E:128:ALA:CB	5:E:129:PRO:CD	2.97	0.41
20:T:9:LYS:O	20:T:9:LYS:CG	2.67	0.41
1:A:223:A:C6	1:A:408:G:O4'	2.73	0.41
1:A:410:G:N2	1:A:418:C:O2	2.54	0.41
1:A:1358:G:C8	1:A:1371:G:C6	3.08	0.41
1:A:2503:A:O2'	1:A:2505:G:OP2	2.38	0.41
1:A:2316:G:C2	1:A:2317:A:C4	3.08	0.41
29:2:11:LYS:C	29:2:13:ASN:N	2.72	0.41
2:B:23:G:C2	2:B:61:G:N1	2.89	0.41
1:A:1330:C:O2'	1:A:1331:G:P	2.77	0.41
1:A:1532:A:C2	1:A:1540:G:N1	2.88	0.41
1:A:2718:G:OP1	16:P:97:TYR:CD1	2.73	0.41
1:A:1500:G:C6	1:A:1501:G:C5	3.08	0.41
15:O:39:VAL:N	15:O:49:VAL:O	2.53	0.41
9:I:118:GLY:O	9:I:119:ALA:CB	2.68	0.41
1:A:1712:U:O4	1:A:1713:A:C2	2.72	0.41
2:B:47:C:O2'	15:O:98:GLN:OE1	2.37	0.41
1:A:1087:G:C4	1:A:1089:A:N3	2.88	0.41
1:A:1096:A:C8	1:A:1097:U:C5	3.08	0.41
1:A:502:A:C6	1:A:505:A:N7	2.88	0.41
1:A:117:G:C6	1:A:119:A:C6	3.09	0.41
1:A:532:A:N3	1:A:532:A:C2'	2.83	0.41
1:A:446:G:C4'	1:A:447:A:OP1	2.68	0.41
1:A:2067:G:C6	1:A:2444:G:C6	3.08	0.41
1:A:2235:G:C4	1:A:2236:U:C5	3.08	0.41
14:N:62:ASN:OD1	14:N:62:ASN:N	2.51	0.41
1:A:855:G:N2	1:A:923:G:C4	2.88	0.41
1:A:855:G:N3	23:W:23:LYS:CE	2.83	0.41
28:1:38:PHE:CG	28:1:39:ASP:N	2.88	0.41
3:C:65:ASP:OD1	3:C:67:LYS:O	2.38	0.41
1:A:157:C:C2	1:A:158:U:C6	3.07	0.41
23:W:52:CYS:O	23:W:53:GLY:O	2.39	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:170:U:C2	1:A:171:U:C5	3.08	0.41
26:Z:32:GLY:C	26:Z:34:THR:N	2.74	0.41
3:C:26:GLY:O	3:C:27:LYS:C	2.57	0.41
21:U:33:VAL:O	21:U:34:ILE:CG1	2.68	0.41
1:A:1023:U:C5'	1:A:1023:U:C6	3.03	0.41
1:A:225:C:N4	1:A:419:U:O2'	2.54	0.41
1:A:1740:G:C2	1:A:1741:C:C2	3.09	0.41
1:A:279:A:C8	1:A:279:A:P	3.13	0.41
1:A:2234:G:C6	1:A:2235:G:C5	3.08	0.41
1:A:2519:U:N1	1:A:2542:A:N6	2.68	0.41
22:V:57:TYR:N	22:V:57:TYR:CD1	2.89	0.41
1:A:528:A:C2	1:A:2043:C:C5'	3.04	0.41
1:A:1125:G:OP2	1:A:1126:A:O2'	2.38	0.41
1:A:2461:A:N1	1:A:2490:G:N2	2.68	0.41
23:W:77:LYS:O	23:W:78:PHE:CB	2.68	0.41
5:E:106:LYS:O	5:E:110:SER:N	2.53	0.41
3:C:196:ASN:O	3:C:197:ALA:CB	2.67	0.41
12:L:100:ILE:O	12:L:101:ILE:CB	2.69	0.41
22:V:26:PHE:CD1	22:V:26:PHE:C	2.93	0.41
1:A:1345:C:O2'	1:A:1346:G:P	2.79	0.41
1:A:223:A:O2'	1:A:224:U:P	2.79	0.41
1:A:2807:U:C5'	1:A:2808:G:OP2	2.68	0.41
1:A:1429:G:O2'	1:A:1430:G:P	2.79	0.41
1:A:2190:G:C5'	1:A:2191:A:OP2	2.68	0.41
1:A:1005:C:O2'	10:J:30:THR:OG1	2.37	0.41
18:R:15:SER:OG	18:R:16:GLU:N	2.53	0.41
1:A:1842:G:N2	1:A:1901:A:C4	2.89	0.41
1:A:424:G:C2	1:A:425:G:C8	3.08	0.41
1:A:1520:U:C4	1:A:1521:G:C6	3.08	0.41
1:A:1323:C:C4	1:A:1324:G:N7	2.89	0.41
1:A:684:G:OP1	29:2:16:HIS:ND1	2.53	0.41
1:A:478:A:C6	1:A:480:A:C6	3.09	0.41
1:A:2727:A:C2	1:A:2728:U:N3	2.88	0.41
1:A:234:U:O2'	1:A:235:U:C5'	2.69	0.41
1:A:1180:U:O4	1:A:1181:U:C4	2.74	0.41
1:A:604:G:C2	1:A:605:G:C5	3.09	0.41
1:A:668:A:C4	1:A:670:A:N7	2.89	0.41
11:K:91:SER:O	11:K:92:GLU:C	2.58	0.41
1:A:1452:G:C8	1:A:1457:U:N3	2.88	0.41
1:A:2389:G:C5'	1:A:2390:U:C5'	2.98	0.41
2:B:73:A:C4	2:B:104:A:C2	3.09	0.41
24:X:19:HIS:C	24:X:21:LEU:N	2.73	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:176:ASP:O	4:D:190:LYS:N	2.53	0.41
3:C:66:PHE:CZ	3:C:155:ARG:NH1	2.89	0.41
1:A:715:A:C6	1:A:716:A:C6	3.08	0.41
1:A:2305:U:P	6:F:132:ARG:NE	2.94	0.41
29:2:22:MET:O	29:2:22:MET:CG	2.67	0.41
8:H:86:ASP:CG	8:H:86:ASP:O	2.58	0.41
1:A:2108:A:OP2	1:A:2108:A:C8	2.74	0.41
1:A:103:A:O2'	1:A:104:A:O4'	2.38	0.41
1:A:163:C:O2'	1:A:164:C:C5'	2.69	0.41
1:A:74:A:C4'	1:A:75:G:O5'	2.69	0.41
1:A:2212:A:C8	1:A:2214:C:C4	3.09	0.41
17:Q:46:TYR:CZ	17:Q:50:ARG:CZ	3.04	0.41
1:A:1826:G:O2'	1:A:1971:U:OP2	2.38	0.41
1:A:727:A:O2'	1:A:728:G:O5'	2.38	0.41
1:A:1733:G:C2'	1:A:1734:G:O5'	2.69	0.41
1:A:664:G:C2	1:A:665:U:O2	2.73	0.41
1:A:1317:G:N2	1:A:1336:A:C2	2.88	0.41
1:A:1535:A:C5'	1:A:1536:C:OP2	2.69	0.41
1:A:604:G:C6	1:A:625:G:N1	2.89	0.41
1:A:1865:U:O2	1:A:1877:A:N1	2.54	0.41
1:A:195:A:C5	1:A:198:C:C5	3.08	0.41
1:A:2784:U:C4	1:A:2785:C:C4	3.09	0.41
1:A:2652:C:C4	1:A:2653:U:C4	3.09	0.41
17:Q:89:ILE:O	17:Q:91:ARG:N	2.53	0.41
1:A:1482:G:O2'	1:A:1483:G:OP1	2.38	0.41
1:A:383:C:N3	1:A:391:A:N6	2.68	0.41
25:Y:3:ALA:C	25:Y:5:GLU:N	2.73	0.41
19:S:79:GLY:CA	19:S:100:THR:OG1	2.68	0.41
1:A:2087:G:C2	1:A:2233:U:O2	2.73	0.41
1:A:2093:G:O2'	1:A:2094:A:O5'	2.39	0.41
1:A:449:A:C5	1:A:450:G:C8	3.09	0.41
1:A:1050:A:C2	1:A:2751:G:C2	3.08	0.41
1:A:2638:G:O2'	1:A:2639:A:P	2.79	0.41
1:A:2316:G:C4	1:A:2317:A:C8	3.09	0.41
1:A:459:U:OP1	29:2:40:ALA:N	2.54	0.41
18:R:81:LYS:N	18:R:81:LYS:CD	2.84	0.41
1:A:177:G:OP2	1:A:177:G:N2	2.54	0.41
1:A:2287:A:O2'	1:A:2288:A:C2'	2.69	0.41
1:A:2288:A:C4'	1:A:2289:G:OP2	2.69	0.41
1:A:1267:U:N3	1:A:2013:A:N7	2.69	0.41
16:P:19:PHE:CE1	16:P:58:PHE:CD2	3.08	0.41
1:A:1513:U:O4	1:A:1514:G:O6	2.37	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:121:G:N3	1:A:131:A:N1	2.68	0.41
25:Y:1:MET:N	25:Y:5:GLU:CG	2.84	0.41
1:A:1838:C:C5	1:A:1899:A:C6	3.08	0.41
23:W:20:LEU:N	23:W:20:LEU:CD1	2.84	0.41
2:B:24:G:C1'	2:B:27:C:N4	2.84	0.41
1:A:2331:G:C6	1:A:2385:C:N4	2.89	0.41
1:A:1059:G:OP1	9:I:71:LYS:NZ	2.53	0.41
1:A:1857:G:N3	1:A:1884:G:C2	2.89	0.41
1:A:1281:G:C5	1:A:1282:U:C5	3.08	0.41
1:A:138:U:O2	1:A:140:C:O2'	2.39	0.41
1:A:845:A:N6	1:A:932:U:C2	2.89	0.41
1:A:2345:G:C4	1:A:2381:A:C2	3.08	0.41
1:A:1734:G:N2	1:A:1735:A:C4	2.89	0.41
1:A:1171:G:C6	1:A:1179:G:C2	3.09	0.41
1:A:833:A:C6	1:A:834:G:C6	3.09	0.41
1:A:2144:G:N2	1:A:2148:G:O6	2.53	0.41
1:A:627:A:O2'	1:A:628:G:OP2	2.38	0.41
1:A:1527:G:C2	1:A:1546:G:N1	2.89	0.41
1:A:1670:C:O2	4:D:134:HIS:NE2	2.53	0.41
1:A:1297:C:C2	1:A:1298:C:C5	3.09	0.41
1:A:109:C:N3	1:A:110:G:C8	2.89	0.41
1:A:1262:A:C6	1:A:1263:U:C2	3.08	0.41
1:A:774:G:N2	1:A:787:C:O2'	2.54	0.41
16:P:88:ARG:NE	16:P:112:ARG:NH2	2.69	0.41
19:S:39:THR:O	19:S:40:ASN:CB	2.69	0.41
21:U:64:ILE:O	21:U:65:GLN:O	2.39	0.41
1:A:78:U:O2'	1:A:79:C:C5'	2.68	0.41
10:J:119:PHE:C	10:J:121:LYS:N	2.74	0.41
30:3:63:TYR:O	30:3:64:ALA:O	2.39	0.41
1:A:1652:A:C2	1:A:2006:C:N3	2.89	0.41
18:R:39:LEU:O	18:R:40:MET:CB	2.67	0.41
17:Q:66:ALA:O	17:Q:70:GLN:N	2.54	0.41
11:K:119:ALA:O	11:K:120:PRO:C	2.59	0.41
3:C:24:HIS:ND1	3:C:25:LYS:N	2.69	0.41
12:L:103:ILE:N	12:L:103:ILE:CD1	2.84	0.41
18:R:93:PHE:C	18:R:93:PHE:CD2	2.93	0.41
1:A:1915:U:O2'	1:A:1916:A:C5'	2.69	0.41
1:A:502:A:N6	1:A:505:A:C5	2.89	0.41
1:A:1310:G:N2	1:A:1605:C:C2	2.89	0.41
1:A:163:C:O2'	1:A:164:C:O5'	2.38	0.41
1:A:942:G:C2'	1:A:943:A:C5'	2.99	0.41
1:A:200:U:C5	1:A:201:C:C5	3.09	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2301:C:C2	1:A:2316:G:N2	2.89	0.41
1:A:2308:G:O6	1:A:2311:A:N7	2.54	0.41
1:A:265:A:C6	1:A:428:A:C8	3.09	0.41
2:B:99:A:C6	2:B:100:G:C5	3.09	0.41
1:A:604:G:O2'	1:A:605:G:C5'	2.68	0.41
1:A:470:A:N1	1:A:471:A:C4	2.89	0.41
1:A:2402:U:O2'	1:A:2403:C:P	2.79	0.41
1:A:990:A:O2'	1:A:991:C:C5'	2.69	0.41
1:A:2846:G:P	16:P:51:ASN:CB	3.09	0.41
10:J:88:THR:O	10:J:91:GLU:N	2.54	0.41
20:T:13:ALA:O	20:T:32:LEU:CB	2.69	0.41
1:A:1095:A:C2	1:A:1096:A:C5	3.08	0.40
1:A:1389:G:C2	1:A:1399:C:N3	2.89	0.40
1:A:419:U:C2	1:A:420:C:C5	3.09	0.40
1:A:1324:G:C1'	1:A:1616:A:N6	2.84	0.40
1:A:1568:G:OP1	3:C:62:ARG:NH1	2.54	0.40
1:A:2531:A:C5'	7:G:156:TYR:CZ	3.04	0.40
1:A:2024:G:C2	1:A:2040:G:N3	2.89	0.40
1:A:648:G:C2	1:A:649:G:C5	3.08	0.40
1:A:1826:G:C5	1:A:1827:U:C5	3.09	0.40
1:A:235:U:C4	1:A:236:C:C5	3.09	0.40
25:Y:50:VAL:C	25:Y:52:ARG:N	2.74	0.40
1:A:38:A:C2	1:A:442:G:N1	2.89	0.40
1:A:830:G:C2	1:A:2448:A:N7	2.89	0.40
1:A:2357:G:C2	1:A:2361:G:C6	3.09	0.40
2:B:76:G:OP1	22:V:9:ARG:NH2	2.54	0.40
1:A:14:A:C6	1:A:526:A:C2	3.10	0.40
26:Z:19:HIS:O	26:Z:20:LYS:C	2.60	0.40
1:A:26:G:C5'	1:A:27:G:OP2	2.69	0.40
1:A:285:G:C2	1:A:356:G:C4	3.08	0.40
21:U:73:ASN:CB	21:U:95:PHE:CE2	3.04	0.40
1:A:687:C:C2	1:A:788:A:O4'	2.74	0.40
1:A:81:G:C8	1:A:82:U:C5	3.09	0.40
1:A:2745:C:C4	1:A:2746:U:C4	3.09	0.40
1:A:2759:G:C5	1:A:2760:C:C5	3.08	0.40
1:A:1179:G:C6	1:A:1180:U:C4	3.09	0.40
4:D:113:SER:OG	4:D:114:LYS:N	2.55	0.40
1:A:1532:A:C6	1:A:1533:C:C4	3.09	0.40
23:W:35:ILE:O	23:W:36:ILE:C	2.59	0.40
1:A:296:U:C2	1:A:297:G:C8	3.09	0.40
10:J:84:ILE:CG2	10:J:84:ILE:O	2.69	0.40
1:A:1712:U:OP2	1:A:1713:A:O2'	2.39	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:69:ASN:O	3:C:70:LYS:C	2.58	0.40
25:Y:31:GLN:C	25:Y:33:ALA:N	2.75	0.40
8:H:65:ALA:O	8:H:66:ASN:C	2.59	0.40
1:A:2862:G:C2	1:A:2863:C:C2	3.09	0.40
1:A:291:G:N1	1:A:350:G:C5	2.90	0.40
1:A:190:A:O2'	1:A:679:C:O2'	2.40	0.40
1:A:1069:A:C2	1:A:1097:U:OP1	2.75	0.40
1:A:1342:A:C6	1:A:1345:C:N3	2.90	0.40
1:A:2573:C:OP1	1:A:2575:C:OP2	2.39	0.40
1:A:1048:A:C6	1:A:1049:C:N4	2.89	0.40
1:A:202:U:C2'	1:A:202:U:O2	2.68	0.40
1:A:2330:G:C2	1:A:2386:A:C6	3.10	0.40
2:B:50:A:C2	2:B:51:G:C1'	3.05	0.40
1:A:86:G:O2'	1:A:87:U:C6	2.75	0.40
1:A:2221:G:C6	1:A:2222:C:C4	3.10	0.40
1:A:2209:G:C5	1:A:2210:U:C4	3.09	0.40
8:H:61:VAL:CG1	8:H:62:LEU:N	2.85	0.40
1:A:290:U:C4	1:A:291:G:N7	2.90	0.40
1:A:2187:U:N3	1:A:2188:U:C5	2.89	0.40
3:C:141:HIS:CB	3:C:190:THR:O	2.70	0.40
14:N:13:ASN:O	14:N:17:ARG:NE	2.54	0.40
1:A:2337:G:C6	1:A:2338:C:N4	2.89	0.40
1:A:1341:G:C2'	1:A:1397:U:O2'	2.70	0.40
1:A:1401:G:C6	1:A:1402:U:C4	3.09	0.40
1:A:415:A:C2	1:A:2409:G:N1	2.89	0.40
1:A:1355:G:C6	1:A:1377:G:N2	2.90	0.40
10:J:44:TYR:CD1	17:Q:63:ARG:NH2	2.89	0.40
1:A:816:C:C2	1:A:1192:G:N2	2.90	0.40
1:A:1868:C:N4	1:A:1869:G:C6	2.90	0.40
1:A:374:A:C6	1:A:401:A:C8	3.10	0.40
1:A:2013:A:C6	1:A:2014:A:C2	3.09	0.40
1:A:2256:G:N2	1:A:2275:C:C4	2.90	0.40
3:C:44:ASN:O	3:C:46:GLY:N	2.55	0.40
2:B:71:C:C2	2:B:106:G:N2	2.89	0.40
25:Y:40:SER:C	25:Y:42:LEU:N	2.74	0.40
1:A:826:U:OP1	34:A:3529:HOH:O	2.22	0.40
25:Y:58:ASN:C	25:Y:60:LYS:N	2.74	0.40
1:A:1795:C:O2	3:C:252:LYS:NZ	2.54	0.40
1:A:846:U:O4'	1:A:846:U:O2	2.40	0.40
1:A:2341:G:C5	1:A:2342:C:C5	3.10	0.40
2:B:29:A:C4	2:B:30:C:C5	3.10	0.40
2:B:30:C:C2'	2:B:30:C:O2	2.70	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2324:U:C2	1:A:2385:C:N4	2.89	0.40
1:A:1858:A:N1	1:A:1859:U:C2	2.89	0.40
1:A:52:A:N3	1:A:178:G:N2	2.70	0.40
2:B:18:G:C6	2:B:19:C:N3	2.90	0.40
1:A:1715:G:O2'	1:A:1743:G:O6	2.38	0.40
1:A:647:G:C4	1:A:648:G:N7	2.89	0.40
1:A:458:G:O2'	1:A:469:G:O6	2.40	0.40
12:L:98:ALA:O	12:L:99:ASN:C	2.59	0.40
19:S:68:ASP:OD1	19:S:68:ASP:N	2.55	0.40
1:A:570:G:N7	1:A:2030:A:N6	2.70	0.40
24:X:1:SER:O	24:X:2:ARG:C	2.59	0.40
1:A:833:A:N6	1:A:834:G:O6	2.55	0.40
1:A:1027:A:C6	1:A:1126:A:C4	3.09	0.40
16:P:19:PHE:CE1	16:P:58:PHE:CG	3.10	0.40
1:A:77:G:C6	1:A:78:U:N3	2.90	0.40
1:A:2847:U:OP1	16:P:95:LYS:NZ	2.55	0.40
3:C:245:THR:O	3:C:247:TRP:N	2.55	0.40
3:C:161:VAL:CG1	3:C:162:GLN:N	2.84	0.40
5:E:154:ASP:C	5:E:156:ASN:N	2.75	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	
3	C	269/273 (98%)	180 (67%)	60 (22%)	29 (11%)	1	6
4	D	207/209 (99%)	128 (62%)	45 (22%)	34 (16%)	0	1
5	E	199/201 (99%)	117 (59%)	55 (28%)	27 (14%)	0	3
6	F	176/179 (98%)	102 (58%)	42 (24%)	32 (18%)	0	1
7	G	174/177 (98%)	104 (60%)	36 (21%)	34 (20%)	0	1
8	H	147/149 (99%)	73 (50%)	59 (40%)	15 (10%)	1	7
9	I	139/142 (98%)	85 (61%)	37 (27%)	17 (12%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	140/142 (99%)	98 (70%)	28 (20%)	14 (10%)	1	8
11	K	120/123 (98%)	83 (69%)	20 (17%)	17 (14%)	0	2
12	L	141/144 (98%)	77 (55%)	45 (32%)	19 (14%)	0	3
13	M	134/136 (98%)	92 (69%)	28 (21%)	14 (10%)	1	7
14	N	118/127 (93%)	72 (61%)	30 (25%)	16 (14%)	0	3
15	O	114/117 (97%)	74 (65%)	29 (25%)	11 (10%)	1	9
16	P	112/115 (97%)	70 (62%)	25 (22%)	17 (15%)	0	1
17	Q	115/118 (98%)	77 (67%)	27 (24%)	11 (10%)	1	9
18	R	101/103 (98%)	66 (65%)	22 (22%)	13 (13%)	0	3
19	S	108/110 (98%)	75 (69%)	22 (20%)	11 (10%)	1	7
20	T	91/100 (91%)	42 (46%)	27 (30%)	22 (24%)	0	0
21	U	100/104 (96%)	53 (53%)	23 (23%)	24 (24%)	0	0
22	V	92/94 (98%)	61 (66%)	23 (25%)	8 (9%)	1	11
23	W	77/85 (91%)	30 (39%)	27 (35%)	20 (26%)	0	0
24	X	75/78 (96%)	45 (60%)	22 (29%)	8 (11%)	1	6
25	Y	61/63 (97%)	37 (61%)	20 (33%)	4 (7%)	2	19
26	Z	56/59 (95%)	34 (61%)	16 (29%)	6 (11%)	1	6
27	0	54/57 (95%)	38 (70%)	7 (13%)	9 (17%)	0	1
28	1	48/55 (87%)	33 (69%)	10 (21%)	5 (10%)	1	7
29	2	44/46 (96%)	29 (66%)	9 (20%)	6 (14%)	0	3
30	3	62/65 (95%)	43 (69%)	13 (21%)	6 (10%)	1	8
31	4	36/38 (95%)	22 (61%)	8 (22%)	6 (17%)	0	1
All	All	3310/3409 (97%)	2040 (62%)	815 (25%)	455 (14%)	0	2

All (455) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	9	SER
3	C	28	PRO
3	C	69	ASN
3	C	140	VAL
3	C	141	HIS
3	C	227	VAL
3	C	232	GLY

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Mol	Chain	Res	Type
3	C	269	ARG
4	D	14	ILE
4	D	31	ALA
4	D	48	ILE
4	D	74	GLU
4	D	77	ARG
4	D	95	SER
4	D	102	ALA
4	D	112	THR
4	D	118	PHE
4	D	150	GLN
4	D	162	ALA
4	D	164	GLN
4	D	170	VAL
4	D	175	LEU
4	D	194	PRO
4	D	208	LYS
5	E	55	SER
5	E	69	ARG
5	E	116	ASP
5	E	153	LEU
5	E	165	HIS
6	F	10	GLU
6	F	12	VAL
6	F	32	LYS
6	F	36	ASN
6	F	42	ALA
6	F	114	ARG
6	F	120	SER
6	F	122	ASP
6	F	137	PHE
7	G	49	LEU
7	G	95	ALA
7	G	125	PRO
7	G	164	ALA
7	G	165	ASP
8	H	3	VAL
8	H	9	VAL
8	H	10	ALA
8	H	66	ASN
8	H	72	ILE
8	H	98	ASP

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Mol	Chain	Res	Type
8	H	102	ALA
9	I	22	PRO
9	I	29	GLN
9	I	113	ALA
10	J	45	THR
10	J	95	ARG
11	K	16	ALA
11	K	18	ARG
11	K	49	ARG
11	K	71	ARG
11	K	72	PRO
11	K	110	GLU
11	K	120	PRO
12	L	4	ASN
12	L	41	ARG
12	L	82	LEU
12	L	85	VAL
12	L	89	VAL
12	L	99	ASN
12	L	101	ILE
12	L	111	ILE
13	M	2	LEU
13	M	14	LYS
13	M	72	PRO
13	M	77	PRO
13	M	135	VAL
14	N	104	ALA
15	O	27	VAL
15	O	72	ALA
15	O	90	VAL
16	P	25	VAL
16	P	50	ARG
16	P	83	ILE
16	P	85	VAL
16	P	109	ILE
16	P	112	ARG
18	R	3	ALA
18	R	29	THR
18	R	98	ILE
19	S	28	LYS
19	S	33	LEU
19	S	40	ASN

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Mol	Chain	Res	Type
19	S	72	THR
20	T	14	PRO
20	T	20	ALA
20	T	29	THR
20	T	39	THR
20	T	56	GLU
20	T	88	LYS
21	U	4	ILE
21	U	6	ARG
21	U	54	PRO
21	U	65	GLN
21	U	82	VAL
21	U	92	VAL
21	U	96	LYS
21	U	101	THR
22	V	56	PHE
23	W	9	THR
23	W	34	SER
23	W	35	ILE
23	W	36	ILE
23	W	83	ALA
24	X	2	ARG
24	X	25	LYS
25	Y	9	LYS
25	Y	37	LEU
27	0	54	ILE
27	0	55	ALA
30	3	6	VAL
30	3	29	ARG
30	3	51	LYS
31	4	3	VAL
31	4	8	LYS
31	4	20	ASP
3	C	3	VAL
3	C	59	GLN
3	C	94	LEU
3	C	239	PHE
4	D	93	GLY
4	D	107	VAL
4	D	119	ALA
4	D	136	ASN
4	D	144	GLY

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Mol	Chain	Res	Type
4	D	145	SER
4	D	169	ARG
4	D	174	SER
5	E	24	ASN
5	E	62	GLN
5	E	80	SER
5	E	96	VAL
5	E	99	LYS
5	E	166	LYS
5	E	188	MET
6	F	6	TYR
6	F	41	GLU
6	F	43	ILE
6	F	70	ARG
6	F	86	CYS
6	F	138	PRO
6	F	145	VAL
6	F	148	VAL
7	G	80	GLU
7	G	83	THR
7	G	85	LYS
7	G	86	LEU
7	G	92	GLY
7	G	126	THR
7	G	136	ASP
7	G	149	ALA
7	G	150	TYR
7	G	155	PRO
8	H	76	GLU
8	H	99	ILE
9	I	23	VAL
9	I	30	GLN
9	I	35	MET
9	I	58	ILE
9	I	69	VAL
9	I	119	ALA
9	I	140	GLU
10	J	44	TYR
10	J	81	ILE
11	K	14	SER
11	K	35	VAL
11	K	93	GLN

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Mol	Chain	Res	Type
12	L	65	GLY
12	L	88	GLY
13	M	73	ILE
13	M	83	GLY
14	N	2	ARG
14	N	8	ARG
14	N	10	LEU
14	N	13	ASN
14	N	71	ARG
14	N	82	GLU
15	O	110	ALA
16	P	63	ILE
16	P	108	ARG
17	Q	88	GLU
17	Q	91	ARG
18	R	8	GLY
18	R	57	GLY
18	R	65	ALA
18	R	89	HIS
19	S	32	ALA
19	S	61	ASN
19	S	67	ASP
20	T	4	GLU
20	T	15	HIS
20	T	16	VAL
20	T	38	ALA
20	T	50	LEU
20	T	68	LYS
21	U	8	ASP
21	U	17	ASP
21	U	40	LEU
21	U	87	GLU
21	U	95	PHE
21	U	97	SER
21	U	99	SER
22	V	15	GLY
22	V	33	GLY
23	W	16	GLU
23	W	33	GLY
23	W	46	ALA
23	W	53	GLY
23	W	57	THR

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Mol	Chain	Res	Type
23	W	71	LYS
24	X	34	SER
24	X	69	GLU
25	Y	46	VAL
26	Z	4	ILE
26	Z	13	ILE
26	Z	30	ARG
27	0	21	LEU
27	0	25	THR
27	0	32	THR
29	2	29	GLN
29	2	43	THR
30	3	20	GLY
30	3	22	LYS
3	C	36	ASN
3	C	37	SER
3	C	98	GLY
3	C	121	ALA
3	C	190	THR
3	C	196	ASN
3	C	237	ARG
4	D	11	MET
4	D	44	GLY
4	D	99	GLU
4	D	122	VAL
4	D	167	ASN
4	D	173	GLN
5	E	79	ARG
5	E	123	LYS
5	E	127	GLU
6	F	46	LYS
6	F	67	THR
6	F	69	ALA
6	F	88	VAL
6	F	94	ARG
6	F	112	ASP
7	G	9	VAL
7	G	91	VAL
7	G	93	TYR
7	G	169	ARG
8	H	97	ARG
9	I	19	PRO

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Mol	Chain	Res	Type
10	J	6	ALA
10	J	13	ARG
10	J	83	GLY
10	J	112	GLY
11	K	17	ARG
11	K	48	PRO
12	L	5	THR
12	L	29	LYS
12	L	115	GLU
12	L	117	THR
13	M	110	GLU
13	M	111	GLU
13	M	134	THR
14	N	30	ARG
15	O	23	ALA
15	O	43	ASN
16	P	20	ARG
16	P	42	PHE
17	Q	23	TYR
17	Q	58	GLN
17	Q	86	SER
17	Q	87	VAL
18	R	15	SER
18	R	40	MET
19	S	71	VAL
20	T	66	LYS
20	T	77	ARG
21	U	23	LYS
21	U	88	ASP
23	W	17	ALA
23	W	23	LYS
23	W	24	ARG
24	X	27	ARG
24	X	63	ILE
25	Y	22	LEU
26	Z	2	LYS
27	0	26	SER
28	1	35	LEU
31	4	16	ILE
3	C	123	ILE
3	C	204	LEU
3	C	226	PRO

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Mol	Chain	Res	Type
4	D	53	GLY
4	D	176	ASP
5	E	22	ASP
5	E	60	TRP
5	E	148	ILE
6	F	8	LYS
6	F	31	GLU
6	F	77	LYS
6	F	87	LYS
6	F	104	THR
7	G	8	VAL
7	G	11	PRO
7	G	45	ALA
7	G	46	ASP
7	G	59	ASP
7	G	118	ALA
8	H	121	VAL
8	H	143	ILE
8	H	144	VAL
9	I	51	GLY
9	I	52	LEU
10	J	25	LEU
10	J	96	ARG
10	J	113	PRO
10	J	139	VAL
11	K	46	ALA
11	K	88	ASN
12	L	79	LEU
13	M	69	PRO
15	O	7	ARG
15	O	8	ILE
15	O	42	PRO
16	P	32	VAL
16	P	51	ASN
16	P	56	SER
16	P	93	LYS
17	Q	45	ALA
17	Q	90	ASP
18	R	53	PHE
19	S	64	ALA
20	T	19	LYS
20	T	53	VAL

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Mol	Chain	Res	Type
20	T	70	HIS
21	U	14	THR
22	V	58	SER
22	V	84	PRO
23	W	18	LYS
23	W	26	GLY
24	X	17	ARG
26	Z	9	THR
28	1	18	HIS
28	1	36	LYS
29	2	16	HIS
29	2	39	ARG
29	2	40	ALA
31	4	37	GLN
3	C	38	LYS
3	C	45	ASN
3	C	64	VAL
3	C	106	PRO
4	D	109	VAL
5	E	13	THR
5	E	86	ALA
5	E	103	GLY
5	E	129	PRO
6	F	82	TYR
6	F	136	ILE
6	F	156	THR
7	G	40	VAL
7	G	53	PRO
7	G	138	GLN
8	H	61	VAL
9	I	84	GLY
10	J	5	THR
10	J	23	LYS
11	K	98	ARG
12	L	96	LYS
12	L	100	ILE
13	M	16	ARG
13	M	20	LEU
14	N	15	SER
14	N	29	VAL
14	N	68	ALA
14	N	72	ASP

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Mol	Chain	Res	Type
14	N	85	PRO
15	O	3	LYS
15	O	107	ALA
16	P	65	ASN
16	P	84	SER
16	P	113	LEU
17	Q	29	ARG
18	R	52	PRO
18	R	91	GLN
19	S	29	VAL
20	T	8	LEU
20	T	61	LEU
21	U	81	ARG
22	V	55	GLU
23	W	41	GLY
23	W	76	ARG
24	X	5	GLN
27	0	33	SER
28	1	38	PHE
5	E	73	ILE
5	E	126	VAL
5	E	187	VAL
7	G	117	PRO
7	G	166	GLU
12	L	36	LYS
12	L	139	GLY
14	N	63	ARG
14	N	70	THR
14	N	105	GLY
19	S	99	ARG
20	T	11	LEU
21	U	12	VAL
21	U	41	VAL
21	U	64	ILE
22	V	44	HIS
22	V	57	TYR
23	W	22	VAL
23	W	78	PHE
27	0	7	PRO
27	0	53	VAL
5	E	82	GLY
7	G	16	VAL

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Mol	Chain	Res	Type
7	G	97	VAL
9	I	138	VAL
11	K	103	VAL
18	R	27	ILE
21	U	35	VAL
21	U	89	GLY
30	3	3	ILE
31	4	21	GLY
13	M	36	VAL
28	1	4	ILE
29	2	44	VAL
3	C	147	PRO
3	C	195	GLY
4	D	9	VAL
5	E	81	GLY
7	G	152	ARG
8	H	134	VAL
11	K	119	ALA
17	Q	6	GLY
3	C	2	VAL
6	F	125	GLY
7	G	153	PRO
20	T	47	VAL
20	T	74	ILE
9	I	31	GLY
9	I	121	ILE
17	Q	7	VAL
26	Z	50	VAL

### 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	
3	C	216/218 (99%)	181 (84%)	35 (16%)	3	17
4	D	164/164 (100%)	142 (87%)	22 (13%)	6	27
5	E	165/165 (100%)	140 (85%)	25 (15%)	4	20
6	F	149/150 (99%)	120 (80%)	29 (20%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	137/138 (99%)	119 (87%)	18 (13%)	6	28
8	H	114/114 (100%)	91 (80%)	23 (20%)	2	8
9	I	109/110 (99%)	102 (94%)	7 (6%)	25	69
10	J	116/116 (100%)	99 (85%)	17 (15%)	4	22
11	K	103/104 (99%)	84 (82%)	19 (18%)	2	12
12	L	102/103 (99%)	85 (83%)	17 (17%)	3	16
13	M	109/109 (100%)	98 (90%)	11 (10%)	11	42
14	N	100/103 (97%)	85 (85%)	15 (15%)	4	21
15	O	86/87 (99%)	79 (92%)	7 (8%)	17	58
16	P	99/100 (99%)	89 (90%)	10 (10%)	11	42
17	Q	89/90 (99%)	75 (84%)	14 (16%)	4	19
18	R	84/84 (100%)	67 (80%)	17 (20%)	2	8
19	S	93/93 (100%)	73 (78%)	20 (22%)	1	7
20	T	80/84 (95%)	71 (89%)	9 (11%)	9	36
21	U	83/85 (98%)	68 (82%)	15 (18%)	2	12
22	V	78/78 (100%)	67 (86%)	11 (14%)	5	24
23	W	59/63 (94%)	41 (70%)	18 (30%)	0	1
24	X	67/68 (98%)	52 (78%)	15 (22%)	1	6
25	Y	55/55 (100%)	51 (93%)	4 (7%)	20	63
26	Z	48/49 (98%)	37 (77%)	11 (23%)	1	5
27	0	47/48 (98%)	34 (72%)	13 (28%)	0	2
28	1	45/49 (92%)	41 (91%)	4 (9%)	14	51
29	2	38/38 (100%)	32 (84%)	6 (16%)	4	18
30	3	51/52 (98%)	38 (74%)	13 (26%)	1	3
31	4	34/34 (100%)	27 (79%)	7 (21%)	2	8
All	All	2720/2751 (99%)	2288 (84%)	432 (16%)	4	18

All (432) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	12	ARG
3	C	23	LEU
3	C	35	LYS

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Mol	Chain	Res	Type
3	C	43	ASN
3	C	44	ASN
3	C	51	ARG
3	C	52	HIS
3	C	57	HIS
3	C	71	ASP
3	C	102	TYR
3	C	117	SER
3	C	124	LYS
3	C	134	ILE
3	C	152	GLN
3	C	162	GLN
3	C	172	THR
3	C	173	LEU
3	C	176	ARG
3	C	181	ARG
3	C	183	VAL
3	C	187	CYS
3	C	188	ARG
3	C	190	THR
3	C	196	ASN
3	C	212	TRP
3	C	213	ARG
3	C	227	VAL
3	C	235	GLU
3	C	250	GLN
3	C	251	THR
3	C	256	THR
3	C	258	SER
3	C	260	LYS
3	C	267	VAL
3	C	269	ARG
4	D	16	THR
4	D	32	ASN
4	D	33	ARG
4	D	38	LYS
4	D	55	LYS
4	D	62	LYS
4	D	79	LEU
4	D	84	LEU
4	D	98	VAL
4	D	100	LEU

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Mol	Chain	Res	Type
4	D	106	LYS
4	D	121	THR
4	D	138	LEU
4	D	140	HIS
4	D	141	ARG
4	D	148	GLN
4	D	150	GLN
4	D	159	LYS
4	D	168	GLU
4	D	172	VAL
4	D	193	VAL
4	D	203	VAL
5	E	53	THR
5	E	57	LYS
5	E	61	ARG
5	E	63	LYS
5	E	67	ARG
5	E	69	ARG
5	E	73	ILE
5	E	77	ILE
5	E	78	TRP
5	E	84	THR
5	E	91	ASP
5	E	93	SER
5	E	105	LEU
5	E	108	ILE
5	E	112	LEU
5	E	117	ARG
5	E	126	VAL
5	E	139	LYS
5	E	149	ILE
5	E	157	LEU
5	E	163	ASN
5	E	164	LEU
5	E	166	LYS
5	E	169	VAL
5	E	191	ASP
6	F	5	ASP
6	F	13	LYS
6	F	25	MET
6	F	31	GLU
6	F	48	LEU

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Mol	Chain	Res	Type
6	F	49	LEU
6	F	82	TYR
6	F	87	LYS
6	F	91	ARG
6	F	94	ARG
6	F	97	GLU
6	F	110	ILE
6	F	111	ARG
6	F	113	PHE
6	F	119	LYS
6	F	122	ASP
6	F	133	GLU
6	F	134	GLN
6	F	135	ILE
6	F	139	GLU
6	F	141	ASP
6	F	142	TYR
6	F	147	ARG
6	F	151	LEU
6	F	155	ILE
6	F	160	LYS
6	F	169	LEU
6	F	172	PHE
6	F	177	ARG
7	G	2	ARG
7	G	19	ASN
7	G	34	ARG
7	G	35	THR
7	G	40	VAL
7	G	42	VAL
7	G	51	PHE
7	G	72	ASN
7	G	84	LYS
7	G	91	VAL
7	G	93	TYR
7	G	101	VAL
7	G	120	ILE
7	G	126	THR
7	G	162	ARG
7	G	163	TYR
7	G	166	GLU
7	G	176	LYS

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Mol	Chain	Res	Type
8	H	8	LYS
8	H	22	LYS
8	H	25	TYR
8	H	27	ARG
8	H	28	ASN
8	H	50	ARG
8	H	55	GLU
8	H	57	LYS
8	H	62	LEU
8	H	66	ASN
8	H	68	ARG
8	H	71	LYS
8	H	76	GLU
8	H	86	ASP
8	H	90	LEU
8	H	91	PHE
8	H	98	ASP
8	H	103	VAL
8	H	104	THR
8	H	109	GLU
8	H	132	PHE
8	H	133	GLN
8	H	144	VAL
9	I	7	TYR
9	I	30	GLN
9	I	36	GLU
9	I	58	ILE
9	I	68	PHE
9	I	93	ASN
9	I	106	GLN
10	J	3	THR
10	J	5	THR
10	J	25	LEU
10	J	34	ARG
10	J	43	GLU
10	J	47	HIS
10	J	54	ILE
10	J	57	LEU
10	J	80	HIS
10	J	92	MET
10	J	93	ILE
10	J	95	ARG

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Mol	Chain	Res	Type
10	J	98	GLU
10	J	99	ARG
10	J	106	LYS
10	J	129	GLU
10	J	139	VAL
11	K	3	GLN
11	K	7	MET
11	K	10	VAL
11	K	13	ASN
11	K	24	VAL
11	K	25	LEU
11	K	39	ILE
11	K	41	ILE
11	K	47	ILE
11	K	49	ARG
11	K	54	LYS
11	K	65	THR
11	K	77	ILE
11	K	87	LEU
11	K	105	ARG
11	K	106	GLU
11	K	107	LEU
11	K	111	LYS
11	K	114	LYS
12	L	3	LEU
12	L	4	ASN
12	L	6	LEU
12	L	18	ARG
12	L	47	ARG
12	L	48	ARG
12	L	69	ARG
12	L	79	LEU
12	L	82	LEU
12	L	92	LEU
12	L	99	ASN
12	L	103	ILE
12	L	111	ILE
12	L	112	LEU
12	L	116	VAL
12	L	141	LYS
12	L	143	GLU
13	M	7	THR

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Mol	Chain	Res	Type
13	M	8	LYS
13	M	38	ARG
13	M	47	GLU
13	M	66	ARG
13	M	73	ILE
13	M	78	LEU
13	M	97	GLN
13	M	105	MET
13	M	115	GLU
13	M	126	ILE
14	N	14	SER
14	N	18	GLN
14	N	20	MET
14	N	21	PHE
14	N	33	ILE
14	N	34	ILE
14	N	40	LYS
14	N	62	ASN
14	N	69	ARG
14	N	78	LYS
14	N	94	TYR
14	N	95	THR
14	N	96	ARG
14	N	97	ILE
14	N	114	GLU
15	O	17	LYS
15	O	31	THR
15	O	65	THR
15	O	68	LYS
15	O	90	VAL
15	O	115	LEU
15	O	117	PHE
16	P	6	GLN
16	P	7	LEU
16	P	13	LYS
16	P	15	ASP
16	P	28	LYS
16	P	50	ARG
16	P	67	GLU
16	P	83	ILE
16	P	86	LYS
16	P	101	GLU

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Mol	Chain	Res	Type
17	Q	3	VAL
17	Q	10	ARG
17	Q	12	ARG
17	Q	15	LYS
17	Q	21	LYS
17	Q	35	PHE
17	Q	39	ILE
17	Q	50	ARG
17	Q	54	ARG
17	Q	57	ARG
17	Q	63	ARG
17	Q	69	ARG
17	Q	79	ILE
17	Q	93	ILE
18	R	6	GLN
18	R	10	LYS
18	R	13	ARG
18	R	21	ARG
18	R	22	LEU
18	R	37	GLU
18	R	48	LYS
18	R	49	ILE
18	R	51	VAL
18	R	58	VAL
18	R	75	VAL
18	R	80	ARG
18	R	83	TYR
18	R	86	GLN
18	R	90	ARG
18	R	93	PHE
18	R	95	ASP
19	S	4	ILE
19	S	6	LYS
19	S	9	HIS
19	S	22	ASP
19	S	23	LEU
19	S	31	GLN
19	S	33	LEU
19	S	45	VAL
19	S	46	LEU
19	S	62	ASP
19	S	66	ILE

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Mol	Chain	Res	Type
19	S	70	LYS
19	S	73	LYS
19	S	74	ILE
19	S	76	VAL
19	S	84	ARG
19	S	85	ILE
19	S	86	MET
19	S	88	ARG
19	S	101	SER
20	T	8	LEU
20	T	9	LYS
20	T	18	GLU
20	T	21	SER
20	T	39	THR
20	T	50	LEU
20	T	54	GLU
20	T	67	VAL
20	T	91	GLN
21	U	13	LEU
21	U	20	LYS
21	U	21	ARG
21	U	40	LEU
21	U	45	GLN
21	U	61	GLU
21	U	65	GLN
21	U	71	ILE
21	U	81	ARG
21	U	82	VAL
21	U	85	ARG
21	U	94	PHE
21	U	95	PHE
21	U	98	ASN
21	U	101	THR
22	V	26	PHE
22	V	40	ILE
22	V	41	GLU
22	V	44	HIS
22	V	51	GLN
22	V	56	PHE
22	V	61	LEU
22	V	65	VAL
22	V	69	GLU

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Mol	Chain	Res	Type
22	V	70	ILE
22	V	76	ASP
23	W	11	ASN
23	W	18	LYS
23	W	22	VAL
23	W	23	LYS
23	W	25	PHE
23	W	28	GLU
23	W	30	VAL
23	W	31	LEU
23	W	35	ILE
23	W	38	ARG
23	W	39	GLN
23	W	40	ARG
23	W	44	PHE
23	W	58	LEU
23	W	59	PHE
23	W	68	PHE
23	W	76	ARG
23	W	77	LYS
24	X	5	GLN
24	X	6	VAL
24	X	25	LYS
24	X	26	ARG
24	X	29	LEU
24	X	31	ASN
24	X	33	HIS
24	X	34	SER
24	X	44	ARG
24	X	46	VAL
24	X	47	THR
24	X	53	LYS
24	X	57	VAL
24	X	63	ILE
24	X	73	ARG
25	Y	1	MET
25	Y	4	LYS
25	Y	28	LEU
25	Y	45	GLN
26	Z	3	THR
26	Z	16	LEU
26	Z	24	LEU

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Mol	Chain	Res	Type
26	Z	28	LEU
26	Z	29	ARG
26	Z	30	ARG
26	Z	34	THR
26	Z	51	SER
26	Z	53	MET
26	Z	55	LYS
26	Z	58	GLU
27	0	3	GLN
27	0	5	ASN
27	0	9	ARG
27	0	27	LEU
27	0	33	SER
27	0	37	HIS
27	0	39	ARG
27	0	41	HIS
27	0	42	ILE
27	0	48	TYR
27	0	49	ARG
27	0	53	VAL
27	0	54	ILE
28	1	10	LEU
28	1	20	TYR
28	1	44	GLN
28	1	45	HIS
29	2	8	SER
29	2	22	MET
29	2	26	ASN
29	2	28	ARG
29	2	45	SER
29	2	46	LYS
30	3	12	ARG
30	3	14	LYS
30	3	24	LYS
30	3	25	HIS
30	3	27	ASN
30	3	28	LEU
30	3	29	ARG
30	3	33	THR
30	3	41	ARG
30	3	46	LYS
30	3	48	MET

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Mol	Chain	Res	Type
30	3	51	LYS
30	3	61	LEU
31	4	2	LYS
31	4	3	VAL
31	4	9	LYS
31	4	15	LYS
31	4	17	VAL
31	4	20	ASP
31	4	28	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2837/2904 (97%)	870 (30%)	153 (5%)
2	B	116/120 (96%)	31 (26%)	6 (5%)
All	All	2953/3024 (97%)	901 (30%)	159 (5%)

All (901) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	14	A
1	A	15	G
1	A	27	G
1	A	28	A
1	A	34	U
1	A	35	G
1	A	36	G
1	A	39	G
1	A	41	C
1	A	46	G
1	A	49	A
1	A	50	U
1	A	52	A
1	A	53	A
1	A	55	G
1	A	61	C
1	A	62	U

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Mol	Chain	Res	Type
1	A	64	A
1	A	71	A
1	A	73	A
1	A	74	A
1	A	75	G
1	A	76	C
1	A	77	G
1	A	79	C
1	A	83	A
1	A	84	A
1	A	85	G
1	A	86	G
1	A	87	U
1	A	91	A
1	A	100	U
1	A	101	A
1	A	102	U
1	A	103	A
1	A	104	A
1	A	118	A
1	A	119	A
1	A	120	U
1	A	121	G
1	A	126	A
1	A	128	C
1	A	129	C
1	A	134	G
1	A	139	U
1	A	140	C
1	A	141	G
1	A	142	A
1	A	144	A
1	A	155	A
1	A	156	A
1	A	158	U
1	A	160	A
1	A	163	C
1	A	164	C
1	A	166	U
1	A	177	G
1	A	180	G
1	A	181	A

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Mol	Chain	Res	Type
1	A	196	A
1	A	199	A
1	A	204	A
1	A	205	G
1	A	206	U
1	A	207	A
1	A	215	G
1	A	216	A
1	A	217	A
1	A	221	A
1	A	222	A
1	A	223	A
1	A	224	U
1	A	227	A
1	A	228	C
1	A	229	C
1	A	230	G
1	A	231	A
1	A	233	A
1	A	234	U
1	A	235	U
1	A	241	A
1	A	242	G
1	A	245	G
1	A	248	G
1	A	249	C
1	A	250	G
1	A	251	A
1	A	255	A
1	A	259	G
1	A	264	C
1	A	265	A
1	A	266	G
1	A	271	G
1	A	272	A
1	A	273	G
1	A	277	G
1	A	278	A
1	A	281	C
1	A	284	U
1	A	285	G
1	A	294	A

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Mol	Chain	Res	Type
1	A	295	G
1	A	299	A
1	A	302	C
1	A	303	G
1	A	311	A
1	A	312	G
1	A	314	C
1	A	321	U
1	A	322	A
1	A	323	C
1	A	324	A
1	A	325	G
1	A	329	G
1	A	330	A
1	A	334	C
1	A	335	C
1	A	336	C
1	A	349	U
1	A	351	C
1	A	353	C
1	A	354	A
1	A	362	A
1	A	367	G
1	A	370	G
1	A	371	A
1	A	372	G
1	A	374	A
1	A	383	C
1	A	385	C
1	A	386	G
1	A	387	U
1	A	388	G
1	A	389	G
1	A	390	U
1	A	396	G
1	A	397	U
1	A	399	U
1	A	404	A
1	A	405	U
1	A	406	G
1	A	407	G
1	A	411	G

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Mol	Chain	Res	Type
1	A	412	A
1	A	413	C
1	A	421	C
1	A	423	A
1	A	424	G
1	A	430	A
1	A	436	C
1	A	443	A
1	A	444	C
1	A	445	C
1	A	446	G
1	A	447	A
1	A	451	U
1	A	455	C
1	A	457	A
1	A	461	C
1	A	462	C
1	A	475	C
1	A	477	A
1	A	480	A
1	A	481	G
1	A	482	A
1	A	483	A
1	A	484	C
1	A	489	G
1	A	490	C
1	A	491	G
1	A	492	A
1	A	498	G
1	A	502	A
1	A	503	A
1	A	504	A
1	A	505	A
1	A	507	A
1	A	509	C
1	A	510	C
1	A	512	G
1	A	527	C
1	A	528	A
1	A	529	A
1	A	532	A
1	A	533	G

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Mol	Chain	Res	Type
1	A	544	C
1	A	546	U
1	A	547	A
1	A	548	G
1	A	549	G
1	A	550	C
1	A	563	A
1	A	572	A
1	A	573	U
1	A	575	A
1	A	576	U
1	A	586	A
1	A	587	C
1	A	590	A
1	A	592	A
1	A	603	A
1	A	604	G
1	A	605	G
1	A	609	A
1	A	613	A
1	A	614	A
1	A	616	A
1	A	617	G
1	A	618	G
1	A	620	G
1	A	621	A
1	A	622	G
1	A	623	C
1	A	627	A
1	A	628	G
1	A	631	A
1	A	634	C
1	A	637	A
1	A	638	G
1	A	639	U
1	A	645	C
1	A	646	U
1	A	649	G
1	A	653	U
1	A	654	A
1	A	655	A
1	A	656	G

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Mol	Chain	Res	Type
1	A	662	G
1	A	664	G
1	A	671	C
1	A	672	C
1	A	685	A
1	A	686	U
1	A	695	G
1	A	699	A
1	A	711	G
1	A	717	C
1	A	726	G
1	A	728	G
1	A	729	G
1	A	730	A
1	A	740	C
1	A	745	G
1	A	746	U
1	A	747	U
1	A	748	G
1	A	749	A
1	A	751	A
1	A	753	A
1	A	757	G
1	A	763	G
1	A	764	A
1	A	770	G
1	A	775	G
1	A	776	G
1	A	782	A
1	A	784	G
1	A	785	G
1	A	789	A
1	A	790	U
1	A	791	C
1	A	792	A
1	A	801	G
1	A	805	G
1	A	806	C
1	A	807	U
1	A	812	C
1	A	819	A
1	A	827	U

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Mol	Chain	Res	Type
1	A	828	U
1	A	846	U
1	A	847	U
1	A	858	G
1	A	859	G
1	A	860	U
1	A	861	A
1	A	866	A
1	A	867	C
1	A	868	U
1	A	873	C
1	A	875	G
1	A	877	A
1	A	878	A
1	A	902	C
1	A	905	A
1	A	910	A
1	A	911	A
1	A	912	C
1	A	914	G
1	A	915	C
1	A	916	G
1	A	919	U
1	A	922	C
1	A	931	U
1	A	932	U
1	A	933	A
1	A	941	A
1	A	946	C
1	A	953	G
1	A	958	U
1	A	961	C
1	A	963	U
1	A	964	C
1	A	973	A
1	A	974	G
1	A	976	G
1	A	981	A
1	A	983	A
1	A	985	C
1	A	990	A
1	A	991	C

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Mol	Chain	Res	Type
1	A	996	A
1	A	1005	C
1	A	1009	A
1	A	1010	A
1	A	1012	U
1	A	1013	C
1	A	1020	A
1	A	1021	A
1	A	1022	G
1	A	1023	U
1	A	1024	G
1	A	1025	G
1	A	1026	G
1	A	1027	A
1	A	1033	U
1	A	1034	G
1	A	1044	C
1	A	1045	C
1	A	1046	A
1	A	1047	G
1	A	1048	A
1	A	1050	A
1	A	1055	G
1	A	1056	G
1	A	1057	A
1	A	1060	U
1	A	1063	G
1	A	1068	G
1	A	1069	A
1	A	1070	A
1	A	1071	G
1	A	1072	C
1	A	1073	A
1	A	1074	G
1	A	1076	C
1	A	1077	A
1	A	1079	C
1	A	1080	A
1	A	1083	U
1	A	1086	A
1	A	1088	A
1	A	1089	A

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Mol	Chain	Res	Type
1	A	1090	A
1	A	1091	G
1	A	1097	U
1	A	1100	C
1	A	1103	A
1	A	1110	G
1	A	1111	A
1	A	1112	G
1	A	1114	C
1	A	1115	G
1	A	1116	G
1	A	1119	U
1	A	1127	A
1	A	1128	G
1	A	1129	A
1	A	1130	U
1	A	1132	U
1	A	1133	A
1	A	1134	A
1	A	1135	C
1	A	1136	G
1	A	1139	G
1	A	1142	A
1	A	1155	A
1	A	1157	G
1	A	1158	C
1	A	1169	A
1	A	1170	C
1	A	1172	C
1	A	1174	U
1	A	1176	U
1	A	1195	G
1	A	1204	A
1	A	1205	A
1	A	1206	G
1	A	1207	C
1	A	1211	C
1	A	1227	G
1	A	1231	U
1	A	1235	G
1	A	1236	G
1	A	1237	A

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Mol	Chain	Res	Type
1	A	1238	G
1	A	1241	A
1	A	1242	U
1	A	1246	A
1	A	1247	A
1	A	1249	U
1	A	1253	A
1	A	1255	U
1	A	1256	G
1	A	1262	A
1	A	1266	G
1	A	1267	U
1	A	1268	A
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1274	A
1	A	1275	A
1	A	1276	A
1	A	1278	C
1	A	1286	A
1	A	1287	A
1	A	1288	G
1	A	1290	C
1	A	1291	C
1	A	1300	G
1	A	1301	A
1	A	1304	A
1	A	1311	G
1	A	1312	U
1	A	1313	U
1	A	1317	G
1	A	1321	A
1	A	1324	G
1	A	1325	U
1	A	1326	U
1	A	1327	A
1	A	1330	C
1	A	1331	G
1	A	1332	G
1	A	1336	A
1	A	1337	G

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Mol	Chain	Res	Type
1	A	1340	U
1	A	1341	G
1	A	1342	A
1	A	1343	G
1	A	1344	U
1	A	1345	C
1	A	1346	G
1	A	1349	C
1	A	1352	U
1	A	1355	G
1	A	1360	G
1	A	1365	A
1	A	1368	G
1	A	1374	G
1	A	1376	C
1	A	1379	U
1	A	1380	G
1	A	1382	G
1	A	1383	A
1	A	1386	C
1	A	1387	A
1	A	1388	G
1	A	1389	G
1	A	1397	U
1	A	1398	C
1	A	1399	C
1	A	1400	U
1	A	1401	G
1	A	1403	A
1	A	1404	C
1	A	1416	G
1	A	1417	C
1	A	1418	G
1	A	1419	A
1	A	1420	A
1	A	1421	G
1	A	1424	G
1	A	1426	G
1	A	1427	A
1	A	1428	C
1	A	1430	G
1	A	1437	C

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Mol	Chain	Res	Type
1	A	1440	U
1	A	1444	G
1	A	1452	G
1	A	1453	A
1	A	1455	G
1	A	1456	G
1	A	1459	G
1	A	1460	U
1	A	1461	C
1	A	1470	A
1	A	1478	G
1	A	1481	U
1	A	1482	G
1	A	1483	G
1	A	1489	C
1	A	1490	A
1	A	1491	G
1	A	1493	C
1	A	1494	A
1	A	1498	C
1	A	1504	A
1	A	1507	C
1	A	1508	A
1	A	1509	A
1	A	1510	G
1	A	1511	G
1	A	1520	U
1	A	1522	A
1	A	1523	U
1	A	1524	G
1	A	1531	C
1	A	1532	A
1	A	1534	U
1	A	1535	A
1	A	1536	C
1	A	1537	G
1	A	1538	G
1	A	1539	U
1	A	1541	C
1	A	1555	G
1	A	1556	C
1	A	1559	U

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Mol	Chain	Res	Type
1	A	1560	G
1	A	1565	C
1	A	1567	G
1	A	1568	G
1	A	1569	A
1	A	1583	A
1	A	1584	U
1	A	1585	C
1	A	1586	A
1	A	1587	G
1	A	1600	C
1	A	1601	G
1	A	1602	U
1	A	1603	A
1	A	1606	C
1	A	1607	C
1	A	1608	A
1	A	1610	A
1	A	1612	C
1	A	1613	G
1	A	1616	A
1	A	1618	A
1	A	1626	A
1	A	1633	G
1	A	1635	A
1	A	1636	U
1	A	1640	A
1	A	1646	C
1	A	1647	U
1	A	1648	U
1	A	1649	G
1	A	1655	A
1	A	1661	G
1	A	1663	G
1	A	1674	G
1	A	1683	U
1	A	1695	G
1	A	1696	G
1	A	1699	G
1	A	1700	A
1	A	1701	A
1	A	1707	G

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Mol	Chain	Res	Type
1	A	1714	U
1	A	1715	G
1	A	1717	A
1	A	1722	A
1	A	1723	G
1	A	1728	C
1	A	1729	U
1	A	1730	C
1	A	1731	G
1	A	1732	C
1	A	1733	G
1	A	1734	G
1	A	1735	A
1	A	1738	G
1	A	1750	G
1	A	1758	U
1	A	1764	C
1	A	1773	A
1	A	1776	G
1	A	1782	U
1	A	1787	A
1	A	1800	C
1	A	1802	A
1	A	1808	A
1	A	1809	A
1	A	1810	A
1	A	1811	G
1	A	1817	G
1	A	1818	U
1	A	1820	U
1	A	1821	A
1	A	1822	C
1	A	1823	G
1	A	1824	G
1	A	1829	A
1	A	1834	U
1	A	1847	A
1	A	1848	A
1	A	1857	G
1	A	1865	U
1	A	1866	A
1	A	1867	G

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Mol	Chain	Res	Type
1	A	1869	G
1	A	1870	C
1	A	1873	G
1	A	1875	G
1	A	1876	A
1	A	1877	A
1	A	1884	G
1	A	1889	A
1	A	1903	G
1	A	1906	G
1	A	1913	A
1	A	1914	C
1	A	1915	U
1	A	1916	A
1	A	1927	A
1	A	1929	G
1	A	1930	G
1	A	1931	U
1	A	1937	A
1	A	1938	A
1	A	1939	U
1	A	1941	C
1	A	1944	U
1	A	1945	G
1	A	1955	U
1	A	1956	U
1	A	1963	U
1	A	1964	G
1	A	1966	A
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1975	G
1	A	1981	A
1	A	1982	U
1	A	1993	U
1	A	1997	C
1	A	2018	G
1	A	2020	A
1	A	2022	U
1	A	2023	C

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Mol	Chain	Res	Type
1	A	2024	G
1	A	2031	A
1	A	2033	A
1	A	2034	U
1	A	2035	G
1	A	2043	C
1	A	2049	G
1	A	2055	C
1	A	2056	G
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2068	U
1	A	2069	G
1	A	2079	U
1	A	2080	A
1	A	2092	U
1	A	2093	G
1	A	2094	A
1	A	2104	C
1	A	2105	U
1	A	2108	A
1	A	2109	U
1	A	2110	G
1	A	2134	A
1	A	2135	A
1	A	2136	G
1	A	2138	G
1	A	2139	U
1	A	2143	C
1	A	2144	G
1	A	2145	C
1	A	2146	C
1	A	2147	A
1	A	2148	G
1	A	2150	C
1	A	2152	G
1	A	2153	C
1	A	2154	A
1	A	2156	G
1	A	2157	G
1	A	2181	U

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Mol	Chain	Res	Type
1	A	2183	A
1	A	2187	U
1	A	2191	A
1	A	2192	U
1	A	2194	U
1	A	2199	A
1	A	2203	U
1	A	2204	G
1	A	2210	U
1	A	2211	A
1	A	2212	A
1	A	2213	U
1	A	2216	G
1	A	2225	A
1	A	2238	G
1	A	2239	G
1	A	2250	G
1	A	2267	A
1	A	2268	A
1	A	2279	G
1	A	2283	C
1	A	2286	G
1	A	2289	G
1	A	2297	A
1	A	2298	A
1	A	2299	U
1	A	2305	U
1	A	2306	C
1	A	2308	G
1	A	2309	A
1	A	2310	C
1	A	2311	A
1	A	2312	U
1	A	2313	C
1	A	2314	A
1	A	2320	U
1	A	2321	U
1	A	2322	A
1	A	2325	G
1	A	2332	C
1	A	2334	U
1	A	2335	A

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Mol	Chain	Res	Type
1	A	2337	G
1	A	2338	C
1	A	2339	C
1	A	2345	G
1	A	2347	C
1	A	2348	U
1	A	2358	A
1	A	2361	G
1	A	2379	G
1	A	2382	G
1	A	2383	G
1	A	2385	C
1	A	2386	A
1	A	2387	U
1	A	2388	A
1	A	2390	U
1	A	2392	A
1	A	2401	U
1	A	2402	U
1	A	2403	C
1	A	2405	G
1	A	2407	A
1	A	2409	G
1	A	2423	U
1	A	2424	C
1	A	2425	A
1	A	2426	A
1	A	2427	C
1	A	2428	G
1	A	2429	G
1	A	2430	A
1	A	2431	U
1	A	2435	A
1	A	2441	U
1	A	2447	G
1	A	2448	A
1	A	2469	A
1	A	2475	C
1	A	2476	A
1	A	2491	U
1	A	2494	G
1	A	2498	C

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Mol	Chain	Res	Type
1	A	2502	G
1	A	2505	G
1	A	2506	U
1	A	2513	A
1	A	2514	U
1	A	2518	A
1	A	2520	C
1	A	2529	G
1	A	2534	A
1	A	2535	G
1	A	2541	A
1	A	2542	A
1	A	2543	G
1	A	2544	G
1	A	2547	A
1	A	2554	U
1	A	2555	U
1	A	2566	A
1	A	2567	G
1	A	2573	C
1	A	2574	G
1	A	2576	G
1	A	2578	G
1	A	2579	C
1	A	2586	U
1	A	2602	A
1	A	2603	G
1	A	2606	C
1	A	2609	U
1	A	2612	C
1	A	2613	U
1	A	2614	A
1	A	2615	U
1	A	2616	C
1	A	2618	G
1	A	2620	C
1	A	2629	U
1	A	2630	G
1	A	2632	A
1	A	2638	G
1	A	2639	A
1	A	2645	G

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Mol	Chain	Res	Type
1	A	2646	C
1	A	2656	U
1	A	2657	A
1	A	2666	C
1	A	2667	C
1	A	2681	C
1	A	2682	A
1	A	2683	C
1	A	2689	U
1	A	2690	U
1	A	2714	G
1	A	2718	G
1	A	2726	A
1	A	2727	A
1	A	2728	U
1	A	2729	G
1	A	2732	G
1	A	2736	A
1	A	2744	G
1	A	2748	A
1	A	2751	G
1	A	2752	C
1	A	2753	A
1	A	2757	A
1	A	2758	A
1	A	2761	A
1	A	2765	A
1	A	2766	A
1	A	2777	G
1	A	2778	A
1	A	2791	G
1	A	2798	U
1	A	2799	A
1	A	2808	G
1	A	2820	A
1	A	2822	G
1	A	2832	U
1	A	2834	G
1	A	2835	A
1	A	2836	U
1	A	2837	A
1	A	2850	A

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Mol	Chain	Res	Type
1	A	2851	A
1	A	2861	U
1	A	2867	G
1	A	2872	A
1	A	2874	C
1	A	2875	C
1	A	2876	G
1	A	2879	A
1	A	2880	C
1	A	2883	A
1	A	2894	G
1	A	2895	G
2	B	11	C
2	B	13	G
2	B	15	A
2	B	16	G
2	B	24	G
2	B	25	U
2	B	30	C
2	B	35	C
2	B	36	C
2	B	40	U
2	B	41	G
2	B	42	C
2	B	43	C
2	B	44	G
2	B	45	A
2	B	48	U
2	B	57	A
2	B	58	A
2	B	60	C
2	B	64	G
2	B	65	U
2	B	66	A
2	B	67	G
2	B	68	C
2	B	87	U
2	B	89	U
2	B	90	C
2	B	91	C
2	B	99	A
2	B	109	A

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Mol	Chain	Res	Type
2	B	110	C

All (159) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	14	A
1	A	33	C
1	A	35	G
1	A	49	A
1	A	52	A
1	A	73	A
1	A	86	G
1	A	103	A
1	A	121	G
1	A	140	C
1	A	179	C
1	A	196	A
1	A	204	A
1	A	206	U
1	A	215	G
1	A	221	A
1	A	223	A
1	A	227	A
1	A	234	U
1	A	249	C
1	A	311	A
1	A	324	A
1	A	329	G
1	A	386	G
1	A	388	G
1	A	389	G
1	A	406	G
1	A	412	A
1	A	422	A
1	A	423	A
1	A	443	A
1	A	454	A
1	A	474	G
1	A	479	A
1	A	483	A
1	A	489	G
1	A	491	G

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Mol	Chain	Res	Type
1	A	503	A
1	A	575	A
1	A	604	G
1	A	617	G
1	A	621	A
1	A	622	G
1	A	638	G
1	A	648	G
1	A	670	A
1	A	727	A
1	A	740	C
1	A	746	U
1	A	762	U
1	A	763	G
1	A	800	A
1	A	806	C
1	A	915	C
1	A	931	U
1	A	984	A
1	A	990	A
1	A	1009	A
1	A	1011	G
1	A	1021	A
1	A	1023	U
1	A	1026	G
1	A	1079	C
1	A	1129	A
1	A	1135	C
1	A	1157	G
1	A	1204	A
1	A	1206	G
1	A	1210	G
1	A	1267	U
1	A	1274	A
1	A	1275	A
1	A	1312	U
1	A	1325	U
1	A	1339	G
1	A	1385	A
1	A	1388	G
1	A	1398	C
1	A	1399	C

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Mol	Chain	Res	Type
1	A	1400	U
1	A	1417	C
1	A	1427	A
1	A	1455	G
1	A	1482	G
1	A	1489	C
1	A	1510	G
1	A	1537	G
1	A	1555	G
1	A	1612	C
1	A	1635	A
1	A	1648	U
1	A	1654	A
1	A	1682	G
1	A	1695	G
1	A	1700	A
1	A	1706	C
1	A	1713	A
1	A	1731	G
1	A	1733	G
1	A	1734	G
1	A	1775	U
1	A	1799	G
1	A	1810	A
1	A	1816	C
1	A	1817	G
1	A	1828	G
1	A	1866	A
1	A	1913	A
1	A	1915	U
1	A	1941	C
1	A	1943	U
1	A	1965	C
1	A	1981	A
1	A	2068	U
1	A	2143	C
1	A	2148	G
1	A	2214	C
1	A	2282	G
1	A	2286	G
1	A	2288	A
1	A	2310	C

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Mol	Chain	Res	Type
1	A	2311	A
1	A	2337	G
1	A	2344	U
1	A	2347	C
1	A	2391	G
1	A	2406	A
1	A	2425	A
1	A	2427	C
1	A	2428	G
1	A	2468	A
1	A	2497	A
1	A	2543	G
1	A	2566	A
1	A	2613	U
1	A	2615	U
1	A	2638	G
1	A	2656	U
1	A	2666	C
1	A	2681	C
1	A	2682	A
1	A	2727	A
1	A	2750	A
1	A	2752	C
1	A	2756	U
1	A	2757	A
1	A	2776	A
1	A	2777	G
1	A	2798	U
1	A	2850	A
1	A	2866	U
1	A	2874	C
1	A	2875	C
2	B	12	C
2	B	13	G
2	B	16	G
2	B	56	G
2	B	90	C
2	B	110	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 138 ligands modelled in this entry, 138 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	2841/2904 (97%)	0.58	204 (7%) 15 4	64, 141, 260, 408	0
2	B	117/120 (97%)	0.89	19 (16%) 2 1	111, 185, 242, 277	0
3	C	271/273 (99%)	0.42	9 (3%) 44 10	64, 107, 154, 181	0
4	D	209/209 (100%)	0.33	13 (6%) 20 5	71, 122, 174, 236	0
5	E	201/201 (100%)	0.68	20 (9%) 8 2	91, 214, 335, 378	0
6	F	178/179 (99%)	0.79	25 (14%) 3 1	154, 229, 270, 299	0
7	G	176/177 (99%)	0.74	18 (10%) 7 2	129, 198, 270, 312	0
8	H	149/149 (100%)	0.36	11 (7%) 14 4	100, 197, 252, 272	0
9	I	141/142 (99%)	1.27	29 (20%) 1 1	231, 317, 353, 360	0
10	J	142/142 (100%)	0.40	8 (5%) 24 5	75, 127, 168, 193	0
11	K	122/123 (99%)	0.28	1 (0%) 83 39	66, 107, 155, 228	0
12	L	143/144 (99%)	0.98	23 (16%) 2 1	86, 169, 242, 284	0
13	M	136/136 (100%)	0.55	9 (6%) 18 4	78, 131, 175, 208	0
14	N	120/127 (94%)	0.92	18 (15%) 3 1	88, 136, 190, 237	0
15	O	116/117 (99%)	1.07	23 (19%) 2 1	134, 182, 227, 252	0
16	P	114/115 (99%)	0.51	9 (7%) 13 4	82, 121, 160, 197	0
17	Q	117/118 (99%)	0.83	11 (9%) 9 3	88, 126, 203, 287	0
18	R	103/103 (100%)	0.47	9 (8%) 10 3	98, 154, 219, 274	0
19	S	110/110 (100%)	1.10	23 (20%) 1 1	86, 141, 208, 266	0
20	T	93/100 (93%)	1.39	24 (25%) 1 1	133, 215, 282, 315	0
21	U	102/104 (98%)	1.10	20 (19%) 2 1	151, 251, 347, 416	0
22	V	94/94 (100%)	0.38	6 (6%) 19 5	107, 157, 199, 222	0
23	W	79/85 (92%)	1.02	11 (13%) 4 1	108, 163, 232, 250	0
24	X	77/78 (98%)	1.00	12 (15%) 3 1	88, 134, 182, 237	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	63/63 (100%)	1.22	14 (22%) 1 1	167, 286, 366, 383	0
26	Z	58/59 (98%)	0.61	5 (8%) 11 3	104, 143, 200, 247	0
27	0	56/57 (98%)	0.63	6 (10%) 6 2	87, 161, 210, 255	0
28	1	50/55 (90%)	0.16	0 100 100	106, 161, 203, 255	0
29	2	46/46 (100%)	1.15	7 (15%) 3 1	95, 128, 162, 176	0
30	3	64/65 (98%)	2.10	25 (39%) 1 0	96, 140, 173, 212	0
31	4	38/38 (100%)	1.50	11 (28%) 1 1	94, 155, 195, 203	0
All	All	6326/6433 (98%)	0.67	623 (9%) 8 2	64, 149, 286, 416	0

All (623) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	9	LYS	16.9
5	E	128	ALA	12.3
1	A	1537	G	11.7
25	Y	1	MET	11.6
9	I	8	VAL	11.3
5	E	127	GLU	11.1
1	A	1420	A	9.6
1	A	1095	A	9.4
12	L	16	GLY	9.2
30	3	20	GLY	9.0
9	I	2	LYS	8.7
1	A	1067	A	8.2
1	A	1535	A	7.6
21	U	31	GLY	7.4
9	I	56	VAL	7.3
9	I	10	LEU	7.1
7	G	171	LYS	6.9
31	4	21	GLY	6.9
9	I	3	LYS	6.8
1	A	914	G	6.8
1	A	145	C	6.8
1	A	2295	C	6.7
1	A	1396	U	6.6
30	3	19	GLY	6.6
25	Y	32	ALA	6.6
15	O	56	LYS	6.6
1	A	1643	G	6.4
30	3	45	PRO	6.4

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Mol	Chain	Res	Type	RSRZ
20	T	56	GLU	6.4
20	T	65	GLY	6.3
7	G	170	THR	6.2
20	T	83	ALA	6.1
5	E	98	LYS	6.1
1	A	1640	A	6.1
21	U	17	ASP	6.0
1	A	2402	U	6.0
5	E	155	GLU	5.9
30	3	22	LYS	5.9
1	A	2110	G	5.8
1	A	2585	U	5.8
15	O	60	GLU	5.8
1	A	345	A	5.7
23	W	31	LEU	5.7
23	W	32	ALA	5.7
10	J	1	MET	5.7
29	2	22	MET	5.7
6	F	129	MET	5.7
6	F	43	ILE	5.7
7	G	57	TYR	5.6
1	A	1590	A	5.5
31	4	1	MET	5.4
1	A	1094	U	5.4
31	4	9	LYS	5.4
1	A	106	C	5.3
1	A	1205	A	5.3
7	G	166	GLU	5.3
5	E	24	ASN	5.3
30	3	21	PHE	5.2
12	L	82	LEU	5.2
23	W	18	LYS	5.1
1	A	1642	G	5.1
21	U	29	SER	5.1
3	C	1	ALA	5.0
14	N	73	ASN	5.0
30	3	28	LEU	4.9
25	Y	3	ALA	4.9
1	A	1730	C	4.9
4	D	197	THR	4.9
27	0	36	LYS	4.9
1	A	389	G	4.9

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Mol	Chain	Res	Type	RSRZ
18	R	73	LYS	4.9
19	S	93	ALA	4.9
15	O	61	GLN	4.9
1	A	1302	A	4.8
6	F	44	ALA	4.8
1	A	1497	U	4.8
1	A	1523	U	4.8
1	A	1093	G	4.8
1	A	1641	A	4.7
1	A	137	U	4.7
15	O	12	THR	4.7
21	U	32	LYS	4.7
22	V	34	LYS	4.6
6	F	83	PRO	4.6
1	A	1460	U	4.6
9	I	11	GLN	4.6
1	A	613	A	4.6
6	F	105	ILE	4.5
30	3	46	LYS	4.5
30	3	14	LYS	4.5
1	A	1807	G	4.5
1	A	138	U	4.4
2	B	70	C	4.4
15	O	28	VAL	4.4
1	A	1073	A	4.4
1	A	2334	U	4.4
1	A	867	C	4.4
1	A	1554	U	4.4
12	L	92	LEU	4.4
18	R	23	GLU	4.3
30	3	15	LYS	4.3
1	A	2296	U	4.3
21	U	40	LEU	4.2
19	S	27	LYS	4.2
25	Y	29	ARG	4.2
30	3	18	LYS	4.2
1	A	1099	G	4.2
30	3	34	LYS	4.2
22	V	94	ALA	4.2
27	O	24	VAL	4.2
19	S	94	ASP	4.2
7	G	52	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	2104	C	4.2
25	Y	2	LYS	4.2
5	E	25	GLU	4.1
20	T	64	LYS	4.1
1	A	1207	C	4.1
18	R	8	GLY	4.1
21	U	38	ILE	4.1
19	S	85	ILE	4.1
21	U	69	VAL	4.1
1	A	2438	U	4.1
6	F	75	GLY	4.1
1	A	1559	U	4.0
1	A	1413	A	4.0
1	A	1116	G	4.0
10	J	2	LYS	4.0
5	E	130	LYS	4.0
13	M	41	LEU	4.0
6	F	155	ILE	4.0
6	F	78	ILE	4.0
21	U	30	SER	4.0
14	N	69	ARG	4.0
18	R	22	LEU	4.0
30	3	39	ARG	4.0
19	S	34	ASP	3.9
2	B	72	G	3.9
19	S	95	ARG	3.9
9	I	1	ALA	3.9
2	B	20	G	3.9
9	I	6	ALA	3.9
1	A	1808	A	3.9
27	0	23	ALA	3.9
29	2	33	ARG	3.9
1	A	619	G	3.8
4	D	198	GLY	3.8
7	G	168	VAL	3.8
12	L	45	GLY	3.8
21	U	59	GLU	3.8
8	H	1	MET	3.8
1	A	1299	G	3.8
1	A	1984	G	3.8
19	S	70	LYS	3.8
30	3	36	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
14	N	76	VAL	3.8
6	F	175	PRO	3.8
9	I	5	GLN	3.8
25	Y	5	GLU	3.8
1	A	2799	A	3.8
12	L	2	ARG	3.8
12	L	17	LYS	3.7
9	I	95	ASP	3.7
1	A	915	C	3.7
7	G	122	ALA	3.7
1	A	866	A	3.7
20	T	43	ILE	3.7
5	E	133	LEU	3.6
6	F	74	ALA	3.6
16	P	100	ARG	3.6
1	A	1536	C	3.6
19	S	92	ARG	3.6
1	A	2297	A	3.6
15	O	9	ARG	3.6
20	T	88	LYS	3.6
9	I	21	PRO	3.6
12	L	96	LYS	3.6
1	A	1552	A	3.6
20	T	89	GLU	3.6
24	X	53	LYS	3.6
25	Y	37	LEU	3.6
27	O	25	THR	3.6
5	E	34	ALA	3.6
12	L	5	THR	3.5
15	O	11	ALA	3.5
1	A	1938	A	3.5
30	3	16	THR	3.5
22	V	35	GLU	3.5
31	4	8	LYS	3.5
9	I	72	THR	3.5
21	U	28	LEU	3.5
1	A	816	C	3.5
19	S	26	GLY	3.5
15	O	19	GLN	3.4
17	Q	20	ALA	3.4
1	A	1644	C	3.4
2	B	41	G	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	102	G	3.4
16	P	6	GLN	3.4
14	N	66	ALA	3.4
9	I	30	GLN	3.4
14	N	72	ASP	3.4
1	A	2147	A	3.4
6	F	111	ARG	3.4
6	F	80	GLN	3.4
9	I	96	LYS	3.3
7	G	9	VAL	3.3
1	A	2179	C	3.3
12	L	12	SER	3.3
1	A	1298	C	3.3
1	A	1453	A	3.3
18	R	72	VAL	3.3
1	A	12	U	3.3
7	G	150	TYR	3.3
1	A	2712	C	3.3
12	L	19	LEU	3.3
1	A	146	A	3.3
9	I	115	ASP	3.3
17	Q	99	VAL	3.3
1	A	995	C	3.3
1	A	2084	C	3.3
6	F	156	THR	3.3
1	A	2820	A	3.3
9	I	4	VAL	3.2
9	I	31	GLY	3.2
15	O	58	ILE	3.2
24	X	52	ALA	3.2
1	A	93	G	3.2
1	A	1303	G	3.2
1	A	308	G	3.2
24	X	23	ALA	3.2
22	V	33	GLY	3.2
1	A	1538	G	3.2
1	A	317	G	3.2
19	S	71	VAL	3.2
7	G	121	THR	3.2
26	Z	12	ALA	3.2
19	S	84	ARG	3.1
1	A	136	G	3.1

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Mol	Chain	Res	Type	RSRZ
14	N	43	GLU	3.1
1	A	318	C	3.1
29	2	26	ASN	3.1
19	S	86	MET	3.1
15	O	62	LEU	3.1
1	A	1058	U	3.1
8	H	140	ALA	3.1
1	A	236	C	3.1
20	T	34	VAL	3.1
1	A	2873	A	3.1
20	T	2	ILE	3.1
16	P	98	TYR	3.1
20	T	79	ASP	3.1
20	T	37	ASP	3.1
1	A	2184	A	3.1
29	2	19	ARG	3.1
6	F	157	THR	3.1
1	A	974	G	3.1
30	3	48	MET	3.1
18	R	88	GLY	3.1
9	I	111	THR	3.1
6	F	174	PHE	3.1
1	A	440	C	3.1
8	H	106	ALA	3.1
19	S	39	THR	3.1
25	Y	43	LEU	3.0
1	A	2667	C	3.0
7	G	118	ALA	3.0
1	A	1070	A	3.0
15	O	57	ALA	3.0
8	H	81	ALA	3.0
30	3	10	ALA	3.0
1	A	139	U	3.0
1	A	1583	A	3.0
17	Q	105	PHE	3.0
23	W	19	ARG	3.0
1	A	124	G	3.0
16	P	113	LEU	3.0
30	3	27	ASN	3.0
12	L	67	THR	3.0
5	E	9	GLN	3.0
1	A	1406	U	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1215	G	3.0
1	A	1985	C	3.0
1	A	1096	A	2.9
1	A	1100	C	2.9
26	Z	51	SER	2.9
12	L	11	GLY	2.9
1	A	1390	U	2.9
17	Q	98	ALA	2.9
1	A	1553	A	2.9
19	S	64	ALA	2.9
1	A	1193	G	2.9
7	G	106	LEU	2.9
24	X	76	LYS	2.9
1	A	235	U	2.9
8	H	39	ALA	2.9
1	A	436	C	2.9
1	A	2463	C	2.9
21	U	70	ALA	2.9
20	T	68	LYS	2.9
19	S	31	GLN	2.9
3	C	30	ALA	2.9
1	A	549	G	2.9
1	A	1639	C	2.9
1	A	2305	U	2.9
15	O	13	ARG	2.9
1	A	1016	G	2.9
1	A	92	U	2.9
1	A	1297	C	2.9
2	B	9	G	2.9
14	N	63	ARG	2.8
21	U	16	LYS	2.8
14	N	46	ARG	2.8
11	K	33	ALA	2.8
26	Z	55	LYS	2.8
2	B	14	U	2.8
20	T	55	VAL	2.8
1	A	1097	U	2.8
1	A	935	C	2.8
1	A	2666	C	2.8
21	U	20	LYS	2.8
29	2	46	LYS	2.8
31	4	10	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	329	G	2.8
1	A	2689	U	2.8
1	A	2690	U	2.8
1	A	698	C	2.8
1	A	2380	C	2.8
1	A	2180	U	2.8
17	Q	13	HIS	2.8
1	A	508	A	2.8
1	A	1075	C	2.8
1	A	1806	C	2.8
1	A	2105	U	2.8
4	D	8	LYS	2.8
30	3	40	LYS	2.8
21	U	12	VAL	2.8
15	O	82	ALA	2.8
6	F	107	VAL	2.7
18	R	71	LYS	2.7
1	A	102	U	2.7
6	F	158	THR	2.7
13	M	129	THR	2.7
17	Q	58	GLN	2.7
9	I	26	ALA	2.7
20	T	38	ALA	2.7
1	A	2428	G	2.7
5	E	198	GLU	2.7
15	O	76	LYS	2.7
23	W	67	LYS	2.7
13	M	52	ALA	2.7
10	J	97	PRO	2.7
1	A	1548	A	2.7
6	F	32	LYS	2.7
19	S	32	ALA	2.7
1	A	492	A	2.7
24	X	7	THR	2.7
2	B	88	C	2.7
15	O	69	ASP	2.7
30	3	47	ALA	2.7
1	A	1312	U	2.7
1	A	1627	G	2.7
1	A	2439	A	2.7
10	J	98	GLU	2.7
21	U	13	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
30	3	57	VAL	2.7
9	I	67	THR	2.7
22	V	93	ARG	2.7
1	A	282	A	2.7
17	Q	55	GLN	2.7
2	B	59	A	2.7
4	D	140	HIS	2.7
1	A	228	C	2.7
1	A	2145	C	2.7
3	C	2	VAL	2.7
31	4	33	HIS	2.7
1	A	1414	C	2.6
6	F	76	PHE	2.6
1	A	2603	G	2.6
8	H	87	GLU	2.6
14	N	54	LEU	2.6
25	Y	4	LYS	2.6
27	0	1	ALA	2.6
8	H	12	LEU	2.6
10	J	96	ARG	2.6
2	B	71	C	2.6
6	F	45	ASP	2.6
13	M	88	ASN	2.6
22	V	3	THR	2.6
7	G	169	ARG	2.6
1	A	2379	G	2.6
9	I	27	LEU	2.6
1	A	1135	C	2.6
9	I	116	MET	2.6
19	S	91	GLY	2.6
30	3	13	PHE	2.6
4	D	57	ALA	2.6
8	H	13	GLY	2.6
2	B	10	G	2.6
1	A	268	C	2.6
29	2	29	GLN	2.6
16	P	101	GLU	2.6
17	Q	28	SER	2.5
20	T	76	ARG	2.5
30	3	11	LYS	2.5
1	A	2309	A	2.5
12	L	62	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1395	A	2.5
1	A	1415	U	2.5
12	L	6	LEU	2.5
7	G	53	PRO	2.5
1	A	822	G	2.5
1	A	1028	A	2.5
4	D	14	ILE	2.5
5	E	56	GLY	2.5
1	A	89	A	2.5
1	A	876	C	2.5
1	A	2085	U	2.5
5	E	13	THR	2.5
5	E	140	ASP	2.5
12	L	20	GLY	2.5
14	N	8	ARG	2.5
24	X	42	GLU	2.5
1	A	1002	G	2.5
14	N	37	THR	2.5
14	N	38	LEU	2.5
31	4	32	LYS	2.5
14	N	39	PRO	2.5
1	A	493	G	2.5
1	A	938	G	2.5
12	L	63	LYS	2.5
1	A	1031	G	2.5
1	A	961	C	2.5
4	D	10	GLY	2.5
1	A	1738	G	2.4
2	B	21	G	2.4
31	4	20	ASP	2.4
6	F	89	THR	2.4
16	P	7	LEU	2.4
1	A	2339	C	2.4
10	J	3	THR	2.4
29	2	13	ASN	2.4
20	T	51	PHE	2.4
1	A	88	G	2.4
1	A	283	G	2.4
1	A	2106	U	2.4
31	4	2	LYS	2.4
12	L	64	PHE	2.4
17	Q	89	ILE	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
20	T	74	ILE	2.4
14	N	12	ARG	2.4
1	A	1551	A	2.4
7	G	123	GLU	2.4
6	F	56	LEU	2.4
7	G	71	LEU	2.4
1	A	2341	G	2.4
1	A	1729	U	2.4
1	A	2800	A	2.4
12	L	86	GLU	2.4
14	N	59	SER	2.4
15	O	88	LYS	2.4
4	D	1	MET	2.4
1	A	2191	A	2.4
1	A	2676	C	2.3
1	A	411	G	2.3
5	E	129	PRO	2.3
9	I	79	LEU	2.3
1	A	105	C	2.3
1	A	1870	C	2.3
2	B	60	C	2.3
1	A	388	G	2.3
1	A	1068	G	2.3
1	A	1459	G	2.3
1	A	2742	G	2.3
12	L	49	GLY	2.3
12	L	75	ALA	2.3
30	3	50	SER	2.3
3	C	4	LYS	2.3
12	L	66	PHE	2.3
17	Q	14	LYS	2.3
7	G	77	GLY	2.3
14	N	51	LEU	2.3
1	A	2610	C	2.3
1	A	1645	G	2.3
5	E	59	PRO	2.3
19	S	88	ARG	2.3
1	A	2031	A	2.3
2	B	12	C	2.3
16	P	19	PHE	2.3
23	W	20	LEU	2.3
1	A	325	G	2.3

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Mol	Chain	Res	Type	RSRZ
4	D	199	SER	2.3
25	Y	33	ALA	2.3
3	C	35	LYS	2.3
20	T	66	LYS	2.3
3	C	227	VAL	2.3
24	X	6	VAL	2.3
30	3	43	LEU	2.3
1	A	1407	G	2.3
1	A	2885	G	2.3
23	W	24	ARG	2.3
27	0	2	VAL	2.3
1	A	2602	A	2.3
1	A	390	U	2.3
19	S	69	LEU	2.3
1	A	2083	G	2.3
20	T	67	VAL	2.3
21	U	89	GLY	2.3
1	A	2589	A	2.3
13	M	54	THR	2.3
14	N	82	GLU	2.3
13	M	124	LEU	2.3
12	L	93	ASN	2.3
9	I	97	VAL	2.2
4	D	154	LYS	2.2
20	T	70	HIS	2.2
1	A	2363	G	2.2
1	A	980	A	2.2
1	A	1076	C	2.2
9	I	7	TYR	2.2
1	A	2135	A	2.2
13	M	96	ILE	2.2
3	C	70	LYS	2.2
8	H	10	ALA	2.2
15	O	4	LYS	2.2
9	I	66	PHE	2.2
3	C	36	ASN	2.2
12	L	65	GLY	2.2
24	X	75	GLU	2.2
13	M	114	ARG	2.2
1	A	1421	G	2.2
1	A	2677	G	2.2
1	A	599	A	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	2062	A	2.2
1	A	546	U	2.2
1	A	1547	C	2.2
1	A	2001	C	2.2
4	D	179	ARG	2.2
24	X	71	ARG	2.2
1	A	1090	A	2.2
13	M	16	ARG	2.2
19	S	110	ARG	2.2
15	O	59	ALA	2.2
23	W	60	ALA	2.2
6	F	110	ILE	2.2
7	G	90	GLY	2.2
10	J	87	ALA	2.2
1	A	229	C	2.2
1	A	1061	U	2.2
2	B	107	G	2.2
20	T	11	LEU	2.2
5	E	201	ALA	2.1
24	X	74	GLY	2.1
15	O	87	ILE	2.1
15	O	93	ASP	2.1
1	A	2340	A	2.1
1	A	2399	G	2.1
19	S	82	MET	2.1
1	A	2065	C	2.1
18	R	19	THR	2.1
1	A	1132	U	2.1
1	A	858	G	2.1
19	S	48	LYS	2.1
1	A	509	C	2.1
21	U	85	ARG	2.1
26	Z	32	GLY	2.1
1	A	1546	G	2.1
20	T	49	LYS	2.1
25	Y	30	MET	2.1
4	D	55	LYS	2.1
15	O	63	LYS	2.1
30	3	56	LEU	2.1
2	B	77	U	2.1
6	F	79	ARG	2.1
23	W	54	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1591	A	2.1
31	4	18	LYS	2.1
5	E	26	ALA	2.1
1	A	517	C	2.1
5	E	76	PRO	2.1
16	P	3	ILE	2.1
15	O	49	VAL	2.1
16	P	91	VAL	2.1
18	R	87	GLN	2.1
1	A	1057	A	2.1
6	F	22	ASN	2.1
26	Z	9	THR	2.1
1	A	1056	G	2.1
8	H	3	VAL	2.1
2	B	90	C	2.1
1	A	1434	A	2.1
19	S	65	ASP	2.1
1	A	41	C	2.1
17	Q	3	VAL	2.1
14	N	70	THR	2.0
21	U	37	GLY	2.0
1	A	2397	G	2.0
15	O	21	LEU	2.0
25	Y	49	ASP	2.0
5	E	126	VAL	2.0
9	I	68	PHE	2.0
24	X	77	TYR	2.0
23	W	46	ALA	2.0
10	J	70	THR	2.0
21	U	49	PRO	2.0
1	A	631	A	2.0
1	A	833	A	2.0
20	T	81	LYS	2.0
21	U	2	ALA	2.0
23	W	47	GLY	2.0
4	D	196	ALA	2.0
31	4	14	CYS	2.0
24	X	24	THR	2.0
25	Y	14	LEU	2.0
1	A	1029	A	2.0
2	B	73	A	2.0
3	C	237	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
9	I	55	PRO	2.0
25	Y	62	GLY	2.0
1	A	267	C	2.0
1	A	965	C	2.0
2	B	105	G	2.0
8	H	19	VAL	2.0
20	T	33	LYS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
32	MG	A	3036	1/1	0.32	181.00	240,240,240,240	0
32	MG	A	2962	1/1	0.81	68.56	249,249,249,249	0
32	MG	A	2961	1/1	1.29	55.32	205,205,205,205	0
32	MG	J	747	1/1	1.29	35.40	319,319,319,319	0
32	MG	A	2967	1/1	0.97	32.68	273,273,273,273	0
32	MG	A	3031	1/1	1.07	29.05	248,248,248,248	0
32	MG	A	3001	1/1	0.94	20.74	159,159,159,159	0
32	MG	A	2966	1/1	1.06	20.69	190,190,190,190	0
32	MG	A	2923	1/1	0.77	19.47	278,278,278,278	0
32	MG	A	2919	1/1	0.70	17.02	219,219,219,219	0
32	MG	A	2983	1/1	1.23	15.54	225,225,225,225	0
32	MG	A	2937	1/1	1.10	12.85	151,151,151,151	0
32	MG	A	2930	1/1	1.24	12.62	242,242,242,242	0
32	MG	A	3013	1/1	0.39	12.30	227,227,227,227	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	2992	1/1	0.44	11.94	222,222,222,222	0
32	MG	A	2979	1/1	0.58	10.75	209,209,209,209	0
32	MG	A	2909	1/1	1.02	7.80	282,282,282,282	0
32	MG	A	3012	1/1	0.80	6.70	217,217,217,217	0
32	MG	C	722	1/1	0.89	6.30	201,201,201,201	0
32	MG	A	2995	1/1	0.72	6.18	184,184,184,184	0
32	MG	A	2964	1/1	0.58	6.00	235,235,235,235	0
32	MG	A	2933	1/1	0.44	5.95	178,178,178,178	0
32	MG	A	3002	1/1	0.39	5.23	183,183,183,183	0
32	MG	A	2996	1/1	0.40	5.07	169,169,169,169	0
32	MG	A	3027	1/1	0.60	5.06	217,217,217,217	0
32	MG	A	3034	1/1	1.06	3.98	271,271,271,271	0
32	MG	A	2942	1/1	0.69	3.93	234,234,234,234	0
32	MG	A	2915	1/1	0.45	3.91	150,150,150,150	0
32	MG	A	2925	1/1	0.30	3.78	183,183,183,183	0
32	MG	A	2913	1/1	0.33	3.50	157,157,157,157	0
32	MG	A	3019	1/1	0.25	3.46	176,176,176,176	0
32	MG	A	2982	1/1	0.36	3.41	214,214,214,214	0
32	MG	A	2906	1/1	0.31	3.17	231,231,231,231	0
32	MG	A	2960	1/1	0.31	3.04	85,85,85,85	0
32	MG	A	2917	1/1	0.54	2.24	241,241,241,241	0
32	MG	A	2936	1/1	0.28	2.17	162,162,162,162	0
32	MG	A	2938	1/1	0.43	2.15	88,88,88,88	0
32	MG	A	2968	1/1	0.31	1.93	256,256,256,256	0
32	MG	A	2991	1/1	0.25	1.88	199,199,199,199	0
32	MG	A	2973	1/1	0.39	1.55	267,267,267,267	0
32	MG	A	2949	1/1	0.34	1.54	206,206,206,206	0
32	MG	A	3003	1/1	0.25	1.51	188,188,188,188	0
32	MG	A	2986	1/1	0.32	1.45	164,164,164,164	0
32	MG	A	2990	1/1	0.31	1.38	109,109,109,109	0
32	MG	A	3026	1/1	0.28	1.38	104,104,104,104	0
32	MG	A	2912	1/1	0.25	1.30	147,147,147,147	0
32	MG	A	3029	1/1	0.44	1.27	200,200,200,200	0
32	MG	A	2932	1/1	0.38	1.27	222,222,222,222	0
32	MG	A	3018	1/1	0.43	1.13	182,182,182,182	0
32	MG	A	3015	1/1	0.33	1.04	202,202,202,202	0
32	MG	A	2998	1/1	0.41	1.01	145,145,145,145	0
32	MG	A	3025	1/1	0.23	0.93	168,168,168,168	0
32	MG	A	2907	1/1	0.35	0.79	238,238,238,238	0
32	MG	A	3033	1/1	0.28	0.70	261,261,261,261	0
32	MG	A	2954	1/1	0.25	0.55	154,154,154,154	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3032	1/1	0.37	0.34	163,163,163,163	0
32	MG	B	590	1/1	0.24	0.34	111,111,111,111	0
32	MG	A	2987	1/1	0.23	0.32	214,214,214,214	0
32	MG	A	2963	1/1	0.20	0.30	233,233,233,233	0
32	MG	A	2934	1/1	0.31	0.25	130,130,130,130	0
32	MG	A	2945	1/1	0.26	0.23	119,119,119,119	0
32	MG	A	3009	1/1	0.25	0.16	97,97,97,97	0
32	MG	A	2918	1/1	0.27	0.11	113,113,113,113	0
32	MG	A	2988	1/1	0.25	0.10	168,168,168,168	0
32	MG	A	2929	1/1	0.29	0.07	162,162,162,162	0
32	MG	A	2953	1/1	0.27	0.05	243,243,243,243	0
32	MG	A	3020	1/1	0.24	0.04	84,84,84,84	0
32	MG	A	2997	1/1	0.26	0.01	189,189,189,189	0
32	MG	A	2989	1/1	0.30	-0.01	158,158,158,158	0
32	MG	A	3037	1/1	0.36	-0.02	220,220,220,220	0
32	MG	A	2978	1/1	0.20	-0.32	260,260,260,260	0
32	MG	A	2952	1/1	0.26	-0.34	103,103,103,103	0
32	MG	A	2921	1/1	0.25	-0.34	185,185,185,185	0
32	MG	A	2928	1/1	0.24	-0.36	102,102,102,102	0
32	MG	A	2985	1/1	0.25	-0.60	83,83,83,83	0
32	MG	A	3006	1/1	0.25	-0.68	118,118,118,118	0
32	MG	A	3005	1/1	0.21	-0.75	96,96,96,96	0
32	MG	A	3010	1/1	0.18	-0.81	218,218,218,218	0
32	MG	A	2940	1/1	0.18	-0.84	205,205,205,205	0
32	MG	A	2999	1/1	0.18	-0.84	138,138,138,138	0
32	MG	A	2984	1/1	0.24	-0.88	154,154,154,154	0
32	MG	A	3000	1/1	0.17	-0.91	127,127,127,127	0
32	MG	A	3004	1/1	0.22	-1.00	124,124,124,124	0
32	MG	A	2972	1/1	0.17	-1.08	98,98,98,98	0
32	MG	A	2905	1/1	0.15	-1.10	141,141,141,141	0
32	MG	A	3024	1/1	0.18	-1.11	124,124,124,124	0
32	MG	A	2947	1/1	0.19	-1.12	155,155,155,155	0
32	MG	A	2935	1/1	0.14	-1.18	80,80,80,80	0
32	MG	A	2951	1/1	0.17	-1.19	174,174,174,174	0
32	MG	A	2975	1/1	0.22	-1.19	102,102,102,102	0
32	MG	A	2922	1/1	0.18	-1.23	185,185,185,185	0
32	MG	A	2977	1/1	0.12	-1.32	193,193,193,193	0
32	MG	A	2910	1/1	0.14	-1.35	237,237,237,237	0
32	MG	A	2911	1/1	0.16	-1.41	232,232,232,232	0
32	MG	A	3016	1/1	0.14	-1.74	79,79,79,79	0
32	MG	A	2971	1/1	0.10	-1.82	72,72,72,72	0
32	MG	A	2927	1/1	0.13	-1.83	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
32	MG	A	3030	1/1	0.18	-1.85	120,120,120,120	0
32	MG	A	3035	1/1	0.05	-1.87	94,94,94,94	0
32	MG	A	3014	1/1	0.07	-1.92	120,120,120,120	0
32	MG	A	2931	1/1	0.17	-1.97	194,194,194,194	0
32	MG	A	3011	1/1	0.17	-1.98	91,91,91,91	0
32	MG	A	2957	1/1	0.16	-1.98	127,127,127,127	0
32	MG	A	2969	1/1	0.16	-2.06	88,88,88,88	0
33	ZN	4	781	1/1	0.07	-2.09	169,169,169,169	0
32	MG	A	2976	1/1	0.16	-2.15	183,183,183,183	0
32	MG	A	2994	1/1	0.14	-2.17	112,112,112,112	0
32	MG	A	2956	1/1	0.10	-2.18	72,72,72,72	0
32	MG	A	3028	1/1	0.12	-2.18	82,82,82,82	0
32	MG	A	2944	1/1	0.16	-2.27	72,72,72,72	0
32	MG	A	2981	1/1	0.14	-2.42	109,109,109,109	0
32	MG	A	2943	1/1	0.11	-2.57	105,105,105,105	0
32	MG	A	2941	1/1	0.07	-2.64	81,81,81,81	0
32	MG	A	3022	1/1	0.12	-2.95	100,100,100,100	0
32	MG	A	2974	1/1	0.13	-2.96	91,91,91,91	0
32	MG	A	2908	1/1	0.14	-3.07	134,134,134,134	0
32	MG	A	2993	1/1	0.09	-3.12	101,101,101,101	0
32	MG	A	2916	1/1	0.15	-3.13	72,72,72,72	0
32	MG	A	3021	1/1	0.14	-3.18	73,73,73,73	0
32	MG	A	3008	1/1	0.16	-3.35	52,52,52,52	0
32	MG	A	2920	1/1	0.11	-3.38	60,60,60,60	0
32	MG	E	202	1/1	0.17	-3.40	199,199,199,199	0
32	MG	A	2939	1/1	0.10	-3.47	90,90,90,90	0
32	MG	A	2948	1/1	0.07	-3.59	87,87,87,87	0
32	MG	A	3023	1/1	0.11	-3.63	60,60,60,60	0
32	MG	A	2959	1/1	0.12	-3.71	103,103,103,103	0
32	MG	A	2980	1/1	0.14	-3.82	195,195,195,195	0
32	MG	A	2924	1/1	0.12	-3.94	53,53,53,53	0
32	MG	A	2970	1/1	0.10	-4.24	105,105,105,105	0
32	MG	A	2926	1/1	0.12	-4.40	149,149,149,149	0
32	MG	A	2950	1/1	0.08	-4.92	73,73,73,73	0
32	MG	A	3007	1/1	0.14	-5.08	86,86,86,86	0
32	MG	A	3017	1/1	0.09	-5.60	128,128,128,128	0
32	MG	A	2965	1/1	0.07	-6.44	110,110,110,110	0
32	MG	A	2955	1/1	0.13	-9.11	88,88,88,88	0
32	MG	A	2946	1/1	0.08	-12.79	81,81,81,81	0
32	MG	A	2958	1/1	0.08	-21.80	86,86,86,86	0
32	MG	A	2914	1/1	1.12	-	272,272,272,272	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.