



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:20 am BST

PDB ID : 4WFN  
Title : Crystal structure of the large ribosomal subunit (50S) of *Deinococcus radiodurans* containing a three residue insertion in L22 in complex with erythromycin  
Authors : Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.  
Deposited on : 2014-09-16  
Resolution : 3.54 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

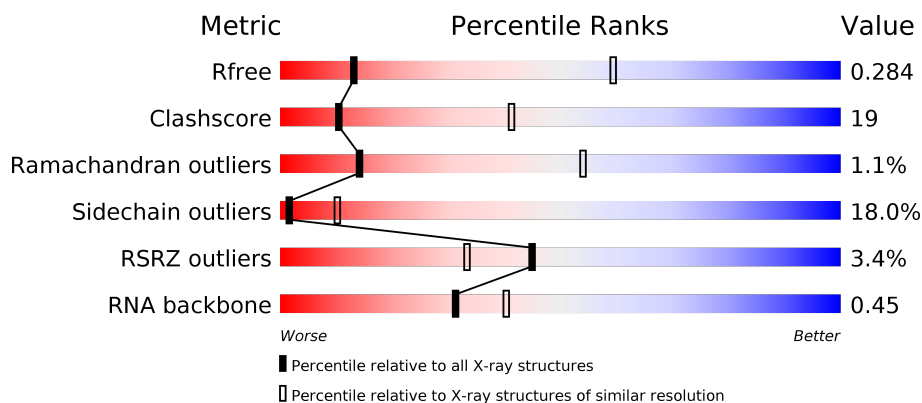
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.54 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))
$R_{free}$	130704	1028 (3.60-3.48)
Clashscore	141614	1109 (3.60-3.48)
Ramachandran outliers	138981	1073 (3.60-3.48)
Sidechain outliers	138945	1074 (3.60-3.48)
RSRZ outliers	127900	1079 (3.62-3.46)
RNA backbone	3102	1003 (4.02-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	275	<div> <div>0%</div> <div> <div>40%</div> <div>45%</div> <div>10%</div> <div>5%</div> </div> </div>
2	B	211	<div> <div>2%</div> <div> <div>45%</div> <div>43%</div> <div>10%</div> <div>•</div> </div> </div>
3	C	205	<div> <div>4%</div> <div> <div>42%</div> <div>44%</div> <div>8%</div> <div>5%</div> </div> </div>
4	D	180	<div> <div>6%</div> <div> <div>48%</div> <div>46%</div> <div>5%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	E	185	
6	G	174	
7	H	134	
8	I	156	
9	J	141	
10	K	116	
11	L	114	
12	M	165	
13	N	118	
14	O	100	
15	P	137	
16	Q	95	
17	R	115	
18	S	237	
19	T	91	
20	U	81	
21	V	67	
22	W	55	
23	Z	60	
24	1	55	
25	2	47	
26	3	65	
27	X	2880	
28	Y	124	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	MG	B	301	-	-	-	X
29	MG	K	202	-	-	-	X

## 2 Entry composition [i](#)

There are 30 unique types of molecules in this entry. The entry contains 84117 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1987	1235	399	350	3			

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	205	Total	C	N	O	S	0	0	0
			1539	965	295	271	8			

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	194	Total	C	N	O	S	0	0	0
			1481	920	284	275	2			

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	177	Total	C	N	O	S	0	0	0
			1400	892	247	254	7			

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

- Molecule 6 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	142	Total	C	N	O	S	0	0	0
			1114	704	209	198	3			

- Molecule 7 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

- Molecule 8 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	134	Total	C	N	O		0	0	0
			1011	619	206	186				

- Molecule 9 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	136	Total	C	N	O	S	0	0	0
			1090	696	202	185	7			

- Molecule 10 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	113	Total	C	N	O	S	0	0	0
			878	541	178	157	2			

- Molecule 11 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	104	Total	C	N	O		0	0	0
			779	476	161	142				

- Molecule 12 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	108	Total	C	N	O		0	0	0
			871	543	172	156				

- Molecule 13 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 14 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	O	94	Total	C	N	O			
			741	465	139	137	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L22,50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	P	130	Total	C	N	O	S		
			1038	655	205	176	2	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	110	VAL	-	linker	UNP Q9RXJ7
P	111	PRO	-	linker	UNP Q9RXJ7
P	112	ARG	-	linker	UNP Q9RXJ7

- Molecule 16 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	Q	93	Total	C	N	O	S		
			726	458	136	130	2	0	0

- Molecule 17 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	R	110	Total	C	N	O	S		
			825	513	160	151	1	0	0

- Molecule 18 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	S	175	Total	C	N	O	S		
			1345	849	236	254	6	0	0

- Molecule 19 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	T	74	Total	C	N	O	S		
			556	351	107	97	1	0	0

- Molecule 20 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	U	72	Total	C	N	O			
			552	341	116	95	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	V	65	Total	C	N	O	S			
			525	322	106	95	2	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	W	55	Total	C	N	O	S			
			424	264	82	76	2	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Z	56	Total	C	N	O	S			
			443	272	91	75	5	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	1	53	Total	C	N	O	S			
			431	274	80	76	1	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	2	46	Total	C	N	O	S			
			383	230	91	60	2	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	3	59	Total	C	N	O	S			
			462	290	95	73	4	0	0	0

- Molecule 27 is a RNA chain called 23S ribosomal RNA.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	X	2680	Total	C	N	O	P	0	0	0
			57533	25663	10626	18564	2680			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	UNK	conflict	GB 11612676

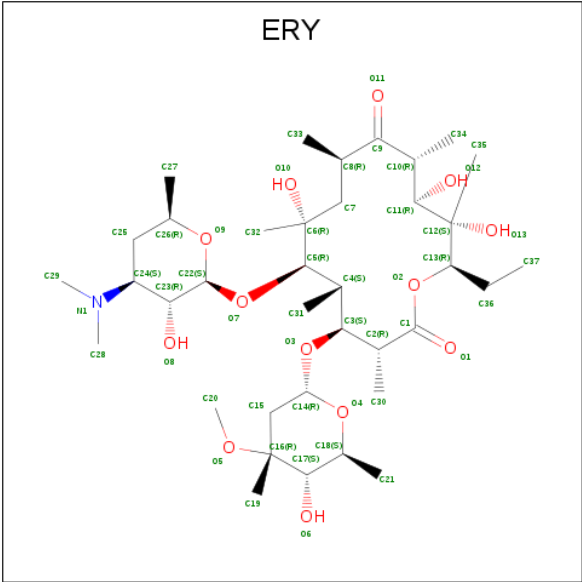
- Molecule 28 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Y	122	Total	C	N	O	P	0	0	0
			2601	1161	476	842	122			

- Molecule 29 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	X	64	Total	Mg	0	0
			64	64		
29	B	1	Total	Mg	0	0
			1	1		
29	A	1	Total	Mg	0	0
			1	1		
29	K	2	Total	Mg	0	0
			2	2		
29	M	2	Total	Mg	0	0
			2	2		

- Molecule 30 is ERYTHROMYCIN A (three-letter code: ERY) (formula: C<sub>37</sub>H<sub>67</sub>NO<sub>13</sub>).

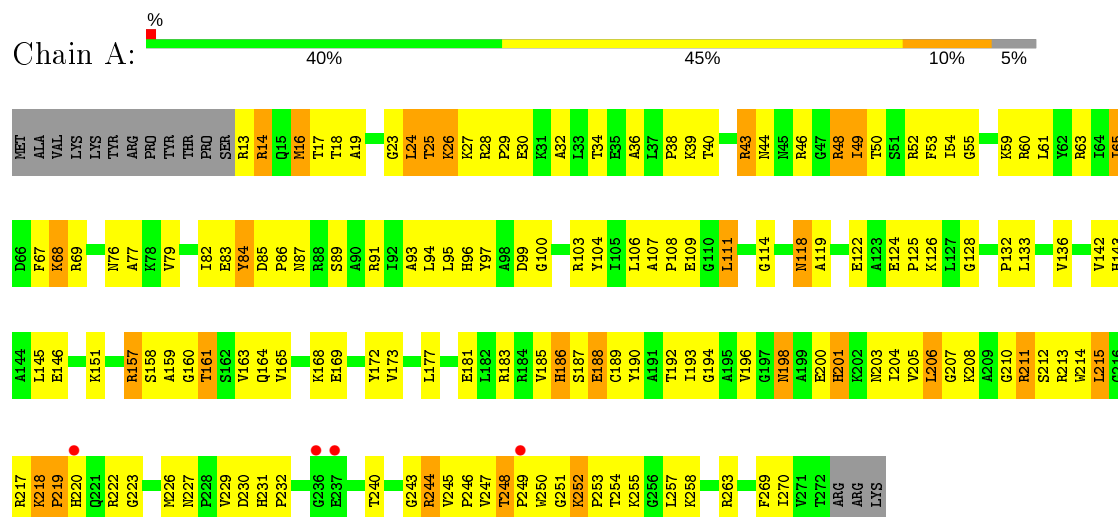


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	X	1	Total	C	N	O	0	0
			51	37	1	13		

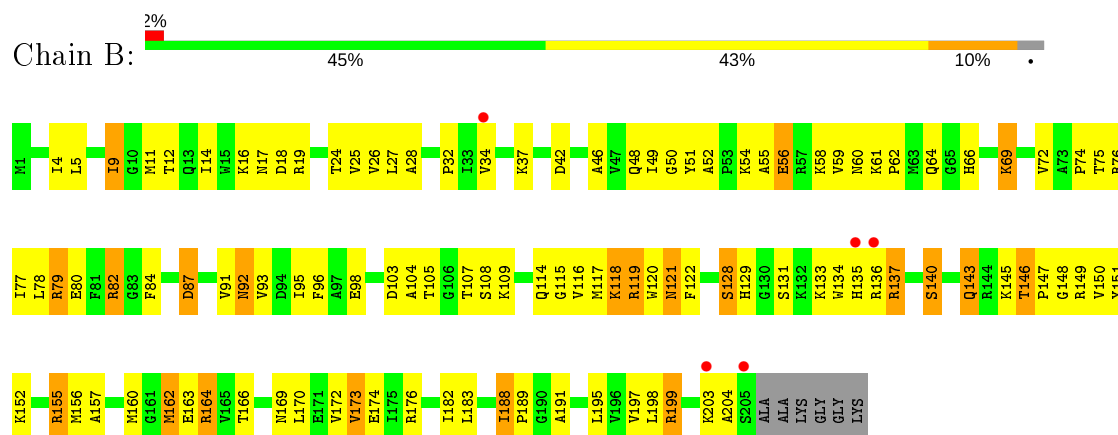
### 3 Residue-property plots

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

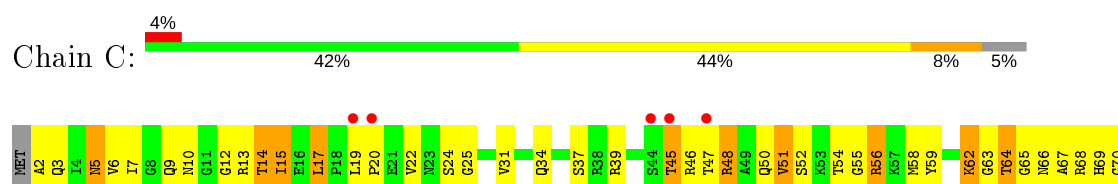
#### • Molecule 1: 50S ribosomal protein L2

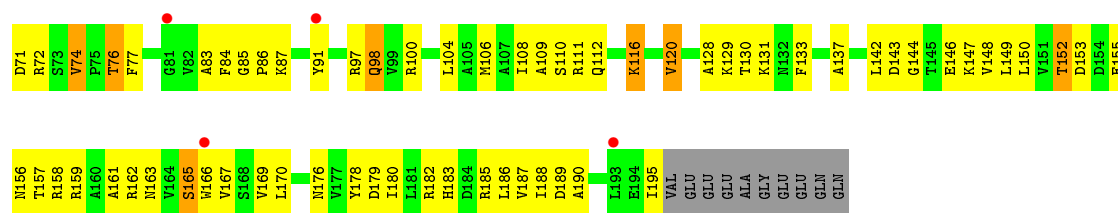


#### • Molecule 2: 50S ribosomal protein L3

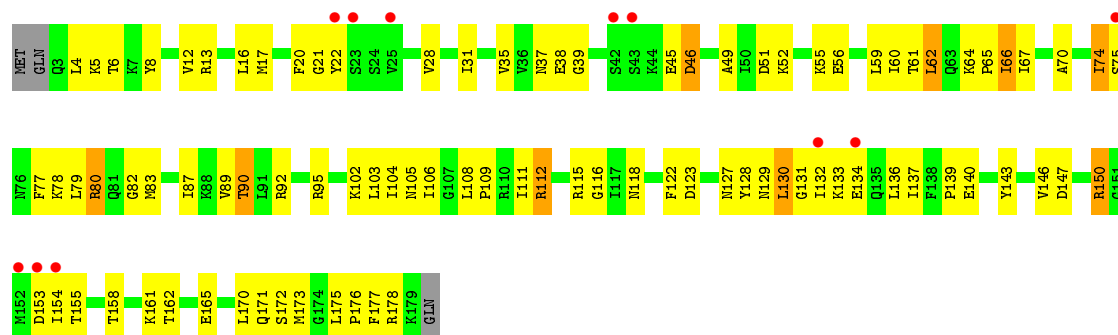


#### • Molecule 3: 50S ribosomal protein L4

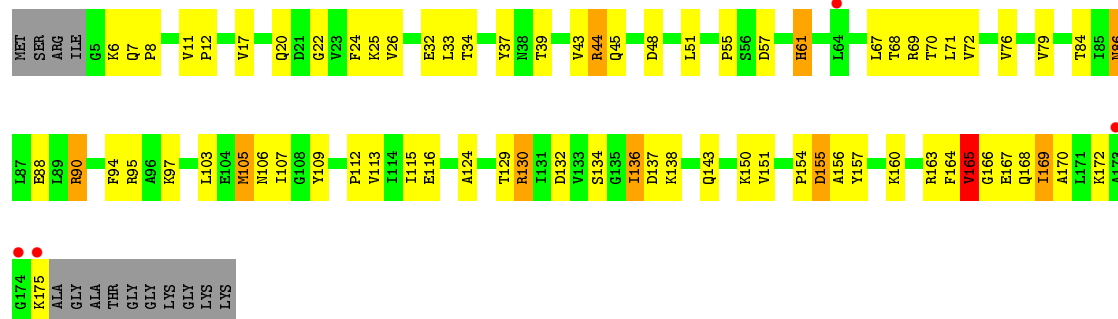




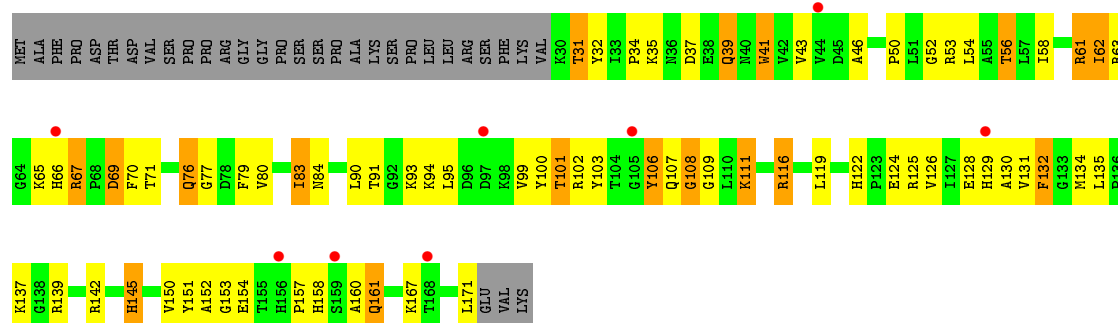
• Molecule 4: 50S ribosomal protein L5



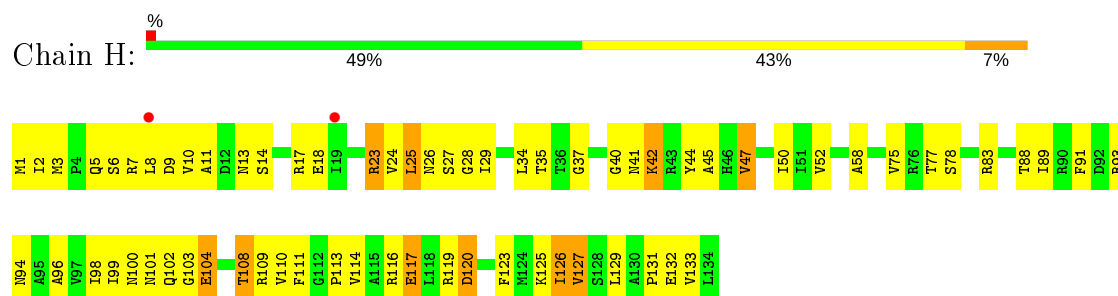
• Molecule 5: 50S ribosomal protein L6



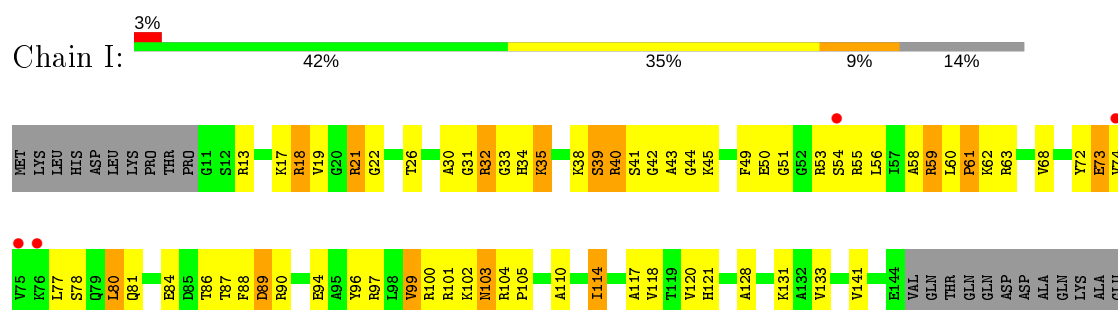
• Molecule 6: 50S ribosomal protein L13



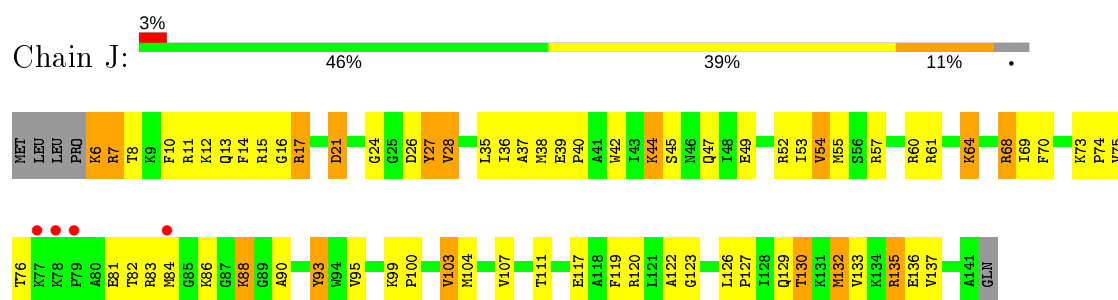
- Molecule 7: 50S ribosomal protein L14



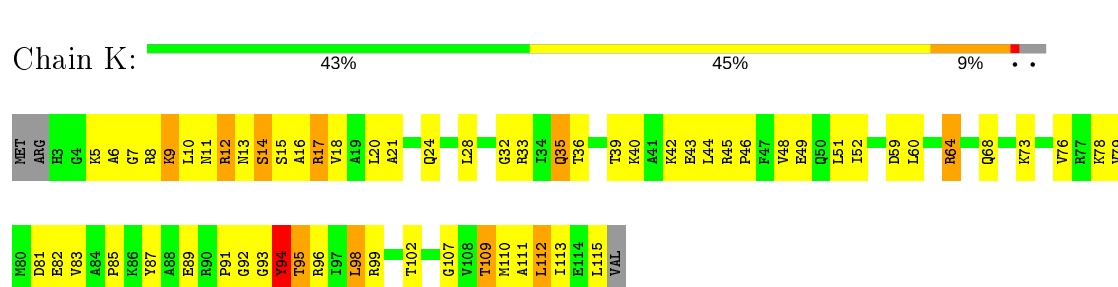
- Molecule 8: 50S ribosomal protein L15



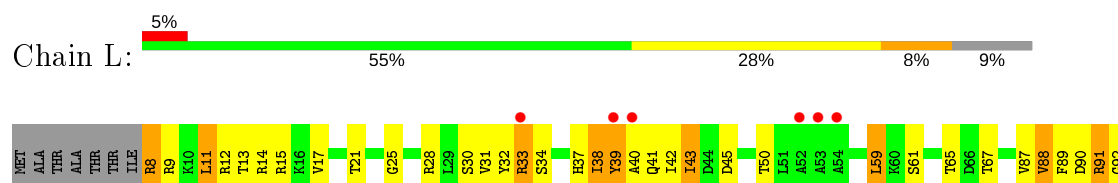
- Molecule 9: 50S ribosomal protein L16

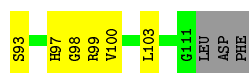


- Molecule 10: 50S ribosomal protein L17



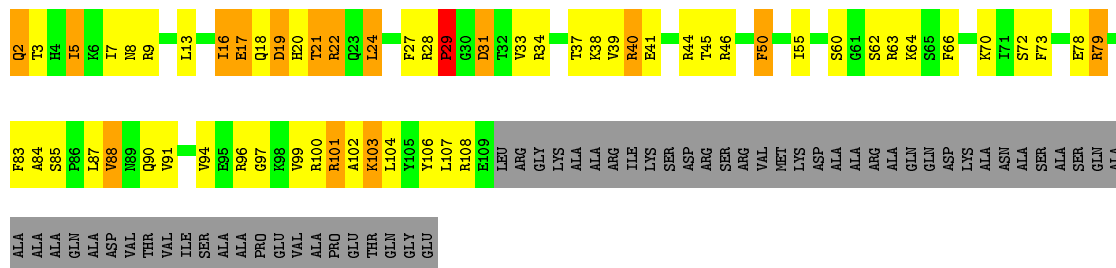
- Molecule 11: 50S ribosomal protein L18





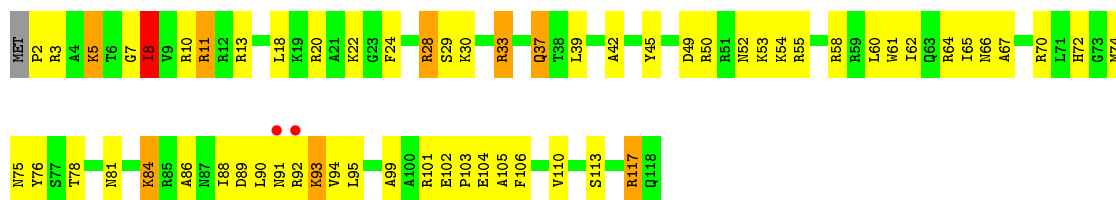
- Molecule 12: 50S ribosomal protein L19

Chain M: 29% 27% 9% 35%



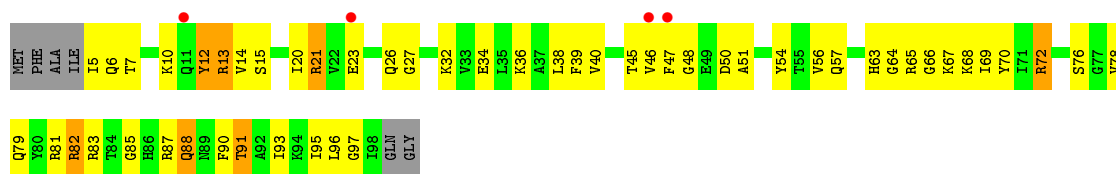
- Molecule 13: 50S ribosomal protein L20

Chain N: 2% 47% 44% 7%



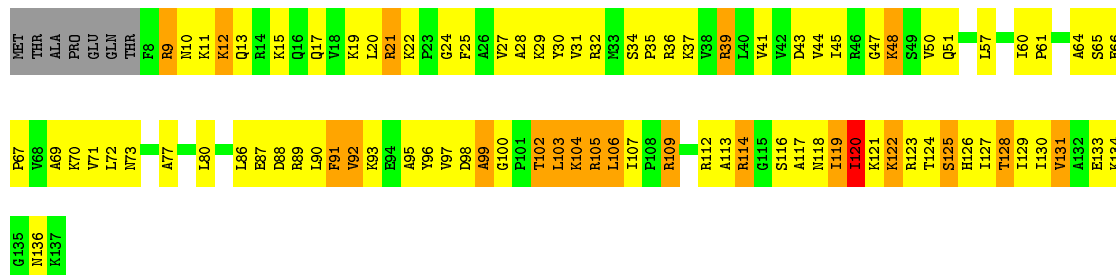
- Molecule 14: 50S ribosomal protein L21

Chain O: 4% 42% 45% 7% 6%

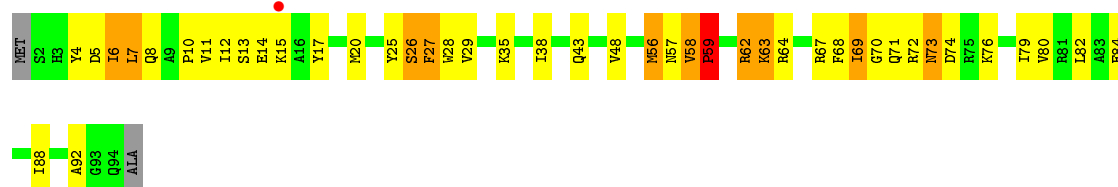


- Molecule 15: 50S ribosomal protein L22, 50S ribosomal protein L22

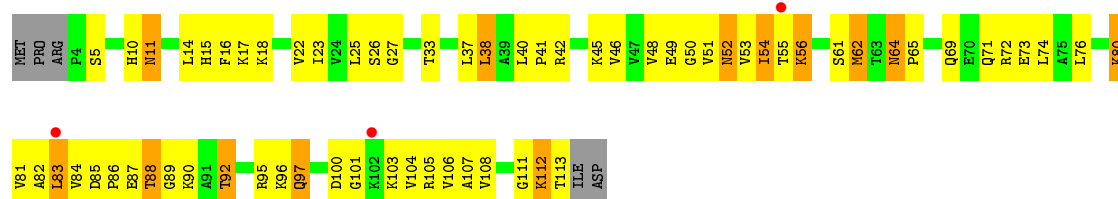
Chain P: 30% 50% 15% 5%



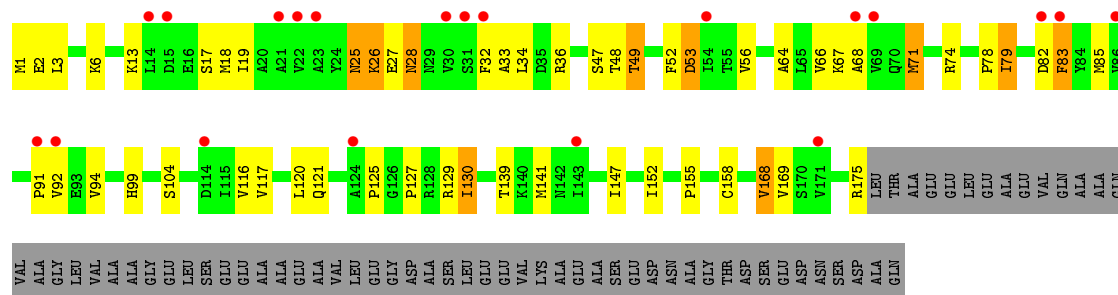
- Molecule 16: 50S ribosomal protein L23



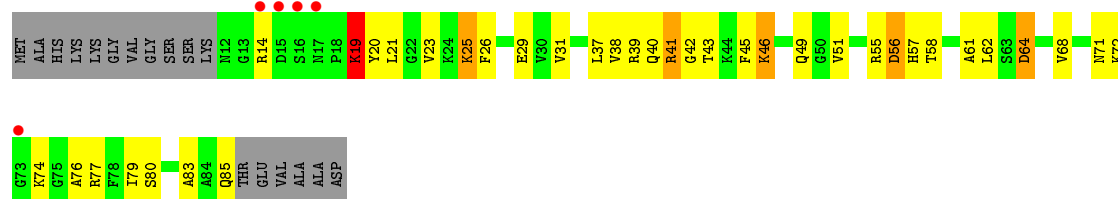
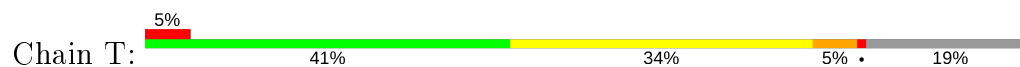
- Molecule 17: 50S ribosomal protein L24



- Molecule 18: 50S ribosomal protein L25

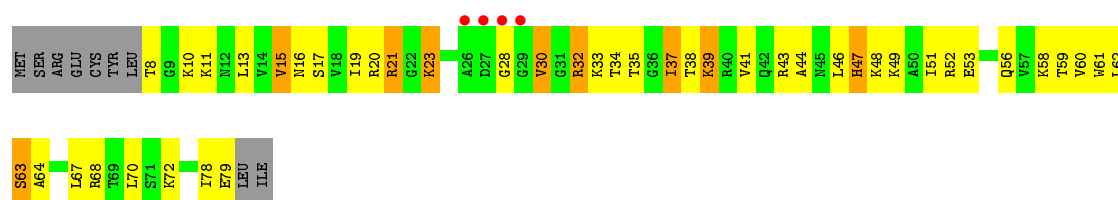


- Molecule 19: 50S ribosomal protein L27



- Molecule 20: 50S ribosomal protein L28





- Molecule 21: 50S ribosomal protein L29



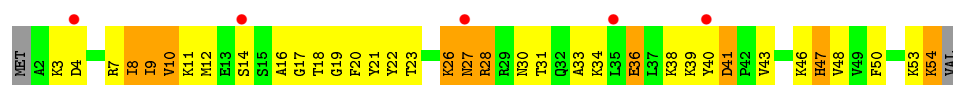
- Molecule 22: 50S ribosomal protein L30



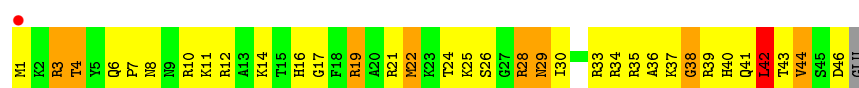
- Molecule 23: 50S ribosomal protein L32



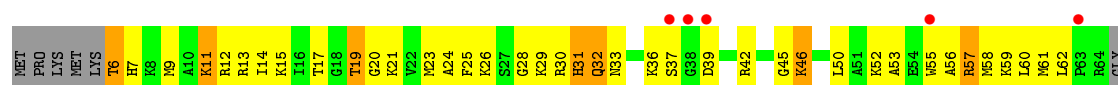
- Molecule 24: 50S ribosomal protein L33



- Molecule 25: 50S ribosomal protein L34

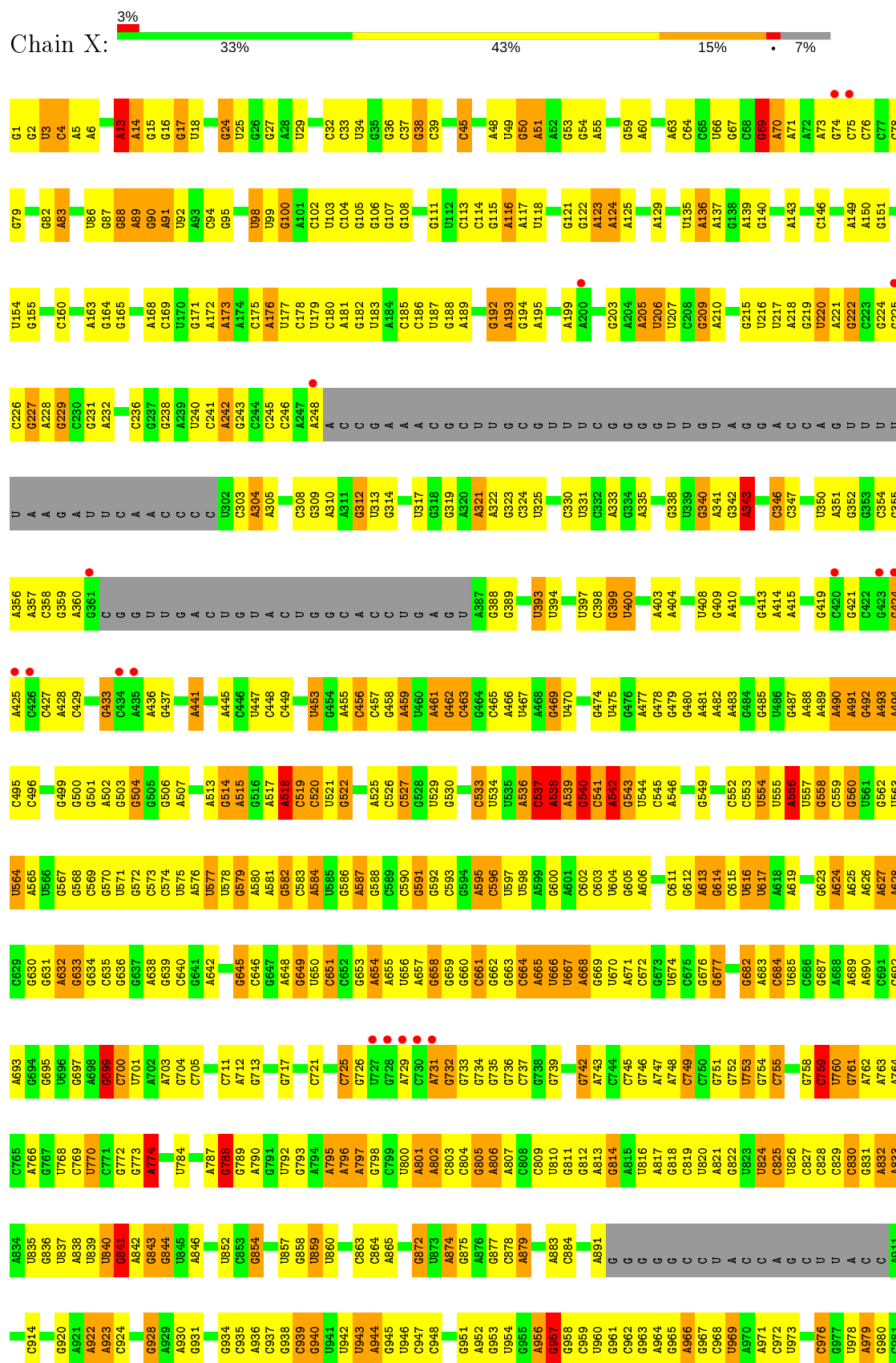


- Molecule 26: 50S ribosomal protein L35





• Molecule 27: 23S ribosomal RNA

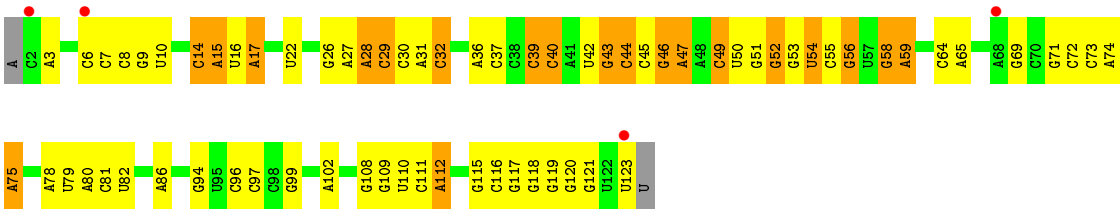




U2838	G2007	U2869	U	A2204	C2273	A2345	G2413	G2484	C2552	G2633	G2698	A2770	U2838
G2839	C2008	G2070	G	C2205	A2278	G2346	A2417	U2495	G2553	G2634	G2699	G2771	G2839
U2840	U2009	U2074	A	G2209	A2280	C2347	U2418	G2488	C2554	G2635	U2700	U2772	U2840
C2845	U2010	U2075	G	U2212	A2281	G2351	A2419	U2490	G2555	G2636	A2701	G2773	C2845
G2846	A2012	G2082	G	G2213	A2282	A2352	C2410	U2491	A2556	G2637	G2702	U	G2846
U2847	A2013	G2083	C	G2217	G2284	C2353	C2421	U2492	C2557	G2638	G2703	U	U2847
A2848	A2014	G2085	A	G2218	U2285	G2354	G2422	U2493	U2558	G2639	U2704	A	A2848
C2849	G2015	U2089	C	G2219	G2286	G2355	G2423	U2494	G2559	G2640	U2705	U	C2849
U2850	A2016	U2090	G	U2221	U2287	A2356	G2424	C2495	G2560	G2641	U2706	C	U2850
G2851	U2017	C	C	G2222	G2288	G2357	G2425	C2496	G2561	G2642	G2707	U	G2851
C2854	G2018	U2090	U	U2223	A2289	U2358	G2426	C2497	U2562	G2643	G2708	A2780	C2854
C2855	C2019	C	G	U2224	U2290	U2359	A2427	U2498	U2563	C2644	C2709	G2781	C2855
U2856	G2020	G	A	U2225	U2291	G2360	U2428	C2499	U2564	G2645	C2710	G2782	U2856
A2858	C2021	U	A	U2226	U2292	G2361	U2429	C2500	C2570	G2646	G2711	A2785	A2858
U2859	C2022	A	A	U2227	U2293	G2362	U2430	C2501	C2571	G2650	G2712	A2786	U2859
C2860	U2023	C	A	A2228	G2294	G2363	A2431	U2502	U2572	A2653	A2713	C2791	C2860
A2861	C2024	U	C	A2229	U2295	G2364	C2432	G2503	G2573	A2654	A2714	C2792	A2861
C2864	A2025	C	C	U2230	U2296	U2365	G2433	G2504	U2574	A2655	G2715	G2793	C2864
G2865	C2026	U	C	U2231	U2297	U2366	G2434	G2505	U2575	A2656	G2716	G2794	G2865
C2867	A2027	C	C	U2232	U2298	G2367	G2435	G2506	G2576	A2657	G2717	A2795	C2867
G2868	C2028	G	A	G2233	U2299	G2368	U2436	G2507	A2577	A2658	G2718	A2796	G2868
U2869	G2029	C	C	G2234	U2300	U2369	U2437	G2508	G2578	A2659	G2719	G2797	U2869
C2870	U2030	C	C	U2235	U2301	G2370	G2438	G2509	U2579	G2660	A2720	C2798	C2870
U2871	A2031	U	C	U2236	U2302	A2371	U2439	G2510	A2580	G2661	G2721	G2799	U2871
U2872	G2032	G	U	C2237	U2303	A2372	C2441	G2511	A2581	G2662	G2722	C2800	G2872
G2873	C2033	U	G	U2238	U2304	G2373	C2442	G2512	G2582	G2663	G2723	A2801	G2873
C2877	G2035	C	U	G2239	U2305	C2374	C2443	G2513	U2583	G2664	G2724	G2804	C2877
U	A2036	A	C	C2240	U2306	G2375	C2444	G2514	G2584	G2665	G2725	G2805	U
C	G2037	C	C	U2241	U2307	G2376	U2445	G2515	U2585	G2666	G2726	G2806	C
U2877	U2038	G	A	U2242	U2308	G2377	G2446	G2516	G2586	G2667	G2727	G2807	U2877
U2878	A2039	C	A	U2243	U2309	G2378	A2447	G2517	U2587	G2668	G2728	U2808	U2878
U2879	G2040	C	C	U2244	U2310	G2379	A2448	G2518	G2588	G2669	G2729	G2809	U2879
U2880	A2041	C	C	U2245	U2311	A2381	A2449	G2519	U2589	C2670	G2730	A2810	U2880
U2881	U2042	C	C	U2246	U2312	G2382	A2450	G2520	C2590	C2671	G2731	G2811	U2881
U2882	A2043	U	C	U2247	U2313	G2383	U2451	G2521	U2591	C2672	G2732	G2812	U2882
U2883	G2044	C	C	U2250	U2314	G2384	U2452	G2522	U2592	C2673	G2733	G2813	U2883
U2884	A2045	C	C	U2251	U2315	G2385	C2453	G2523	G2593	C2674	G2734	G2814	U2884
U2885	C2046	G	A	U2252	U2316	G2386	C2454	G2524	C2594	U2675	G2735	G2815	U2885
U2886	G2047	A	A	A2182	U2317	U2385	A2455	G2525	G2595	U2676	G2736	G2816	U2886
U2887	C2048	C	A	C2183	U2318	U2386	U2456	G2526	C2600	U2677	G2737	G2817	U2887
U2888	C2049	U	C	U2185	U2319	U2387	A2457	G2527	C2601	U2678	G2738	G2818	U2888
U2889	G2050	G	U	G2186	U2320	U2388	G2460	G2528	G2605	U2679	G2739	G2819	U2889
U2890	U2051	C	C	A2187	U2321	G2394	G2463	U2529	G2606	C2682	G2740	G2820	U2890
G2052	G2052	C	G	U2188	U2322	C2395	U2464	U2530	C2607	C2683	U2741	G2821	G2052
A2054	A2054	C	C	A2189	U2323	C2396	U2465	U2531	U2608	A2684	U2742	G2822	A2054
G2055	G2055	U	U	A2190	U2324	A2397	U2466	C2535	G2609	A2685	U2743	G2823	G2055
C2056	C2056	U	U	U2191	U2325	U2398	U2467	G2536	A2614	U2615	U2744	G2824	C2056
U2057	U2057	U	U	C2193	U2326	U2399	G2470	U2541	U2616	U2616	U2745	G2825	U2057
U2058	U2058	U	U	U2196	U2327	G2400	G2471	U2542	U2617	U2617	U2746	G2826	U2058
U2059	U2059	G	U	A2197	U2328	A2401	G2472	U2543	G2624	G2624	U2747	G2827	U2059
C2061	C2061	G	G	U2198	U2329	C2403	U2473	A2544	U2625	U2625	U2748	G2828	C2061
U2062	U2062	G	G	A2267	U2330	G2404	G2474	A2545	U2626	U2626	U2749	G2829	U2062
A2063	A2063	U	U	G2268	U2331	C2406	U2475	C2547	U2627	U2627	U2750	G2830	A2063
U2067	U2067	C	C	G2269	U2332	G2407	U2476	G2548	G2628	G2628	U2751	G2831	U2067
C2068	C2068	G	G	U2270	U2333	G2408	U2477	G2549	U2629	U2629	U2752	G2832	C2068
				U2271	U2334	A2409	U2478	A2482			U2753	U2836	
				U2272	U2344	U2410	U2483				U2754	G2837	

• Molecule 28: 5S ribosomal RNA





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.09 Å   411.59 Å   695.88 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	19.99 – 3.54 49.53 – 3.52	Depositor EDS
% Data completeness (in resolution range)	90.4 (19.99-3.54) 89.6 (49.53-3.52)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.02 (at 3.48 Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.234   ,   0.282 0.235   ,   0.284	Depositor DCC
$R_{free}$ test set	13533 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	100.0	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.16 , 14.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	84117	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.43	0/2025	0.70	0/2726
2	B	0.55	0/1567	0.76	0/2105
3	C	0.47	0/1504	0.72	1/2036 (0.0%)
4	D	0.29	0/1419	0.52	0/1903
5	E	0.29	0/1308	0.51	0/1771
6	G	0.47	0/1138	0.78	1/1539 (0.1%)
7	H	0.61	0/1007	0.80	0/1352
8	I	0.46	0/1022	0.76	0/1366
9	J	0.52	0/1113	0.75	0/1486
10	K	0.67	0/886	0.90	1/1188 (0.1%)
11	L	0.32	0/785	0.60	0/1048
12	M	0.61	0/884	0.87	1/1186 (0.1%)
13	N	0.45	0/994	0.68	0/1323
14	O	0.44	0/750	0.74	1/1000 (0.1%)
15	P	0.58	0/1052	0.79	1/1409 (0.1%)
16	Q	0.42	0/737	0.67	1/988 (0.1%)
17	R	0.45	0/835	0.72	0/1121
18	S	0.30	0/1370	0.53	0/1862
19	T	0.44	0/563	0.70	0/747
20	U	0.41	0/556	0.69	0/741
21	V	0.31	0/529	0.51	0/704
22	W	0.36	0/426	0.61	0/568
23	Z	0.52	0/455	0.87	0/611
24	1	0.47	0/438	0.74	0/583
25	2	0.46	0/387	0.79	1/509 (0.2%)
26	3	0.53	0/468	0.85	0/614
27	X	0.63	3/64429 (0.0%)	1.22	424/100499 (0.4%)
28	Y	0.40	0/2907	0.96	1/4529 (0.0%)
All	All	0.58	3/91554 (0.0%)	1.11	433/137514 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
6	G	0	1
7	H	0	1
8	I	0	3
10	K	0	2
16	Q	0	1
17	R	0	1
19	T	0	1
20	U	0	1
23	Z	0	1
25	2	0	1
26	3	0	1
All	All	0	15

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	X	1	G	OP3-P	-10.37	1.48	1.61
27	X	1981	A	N3-C4	-5.23	1.31	1.34
27	X	774	A	N3-C4	5.08	1.37	1.34

All (433) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	1468	A	C8-N9-C4	-12.74	100.70	105.80
27	X	1746	A	O5'-P-OP1	-12.19	94.73	105.70
27	X	1670	G	C8-N9-C4	11.14	110.86	106.40
27	X	537	C	C6-N1-C2	-10.97	115.91	120.30
27	X	774	A	N7-C8-N9	10.55	119.08	113.80
27	X	2018	G	O5'-P-OP2	-9.92	96.77	105.70
27	X	774	A	C8-N9-C4	-9.89	101.84	105.80
27	X	2544	A	O5'-P-OP1	-9.88	96.80	105.70
27	X	1468	A	N7-C8-N9	9.40	118.50	113.80
27	X	522	G	N1-C6-O6	9.20	125.42	119.90
27	X	2705	A	C5-N7-C8	-9.11	99.35	103.90
27	X	2489	C	C6-N1-C2	-8.98	116.71	120.30
27	X	2478	C	C5-C6-N1	8.96	125.48	121.00
27	X	2705	A	N7-C8-N9	8.93	118.26	113.80
27	X	2815	C	C6-N1-C2	8.84	123.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	1333	G	N3-C4-N9	-8.82	120.71	126.00
27	X	2478	C	C6-N1-C2	-8.79	116.78	120.30
27	X	2488	G	N1-C6-O6	-8.78	114.63	119.90
27	X	2018	G	O4'-C1'-N9	8.78	115.22	108.20
27	X	1668	G	N1-C6-O6	8.74	125.14	119.90
27	X	2018	G	C4-C5-N7	8.71	114.28	110.80
27	X	2705	A	N1-C6-N6	8.61	123.76	118.60
27	X	1670	G	N9-C4-C5	-8.59	101.97	105.40
27	X	538	A	C2-N3-C4	8.56	114.88	110.60
27	X	2542	U	C5-C4-O4	8.55	131.03	125.90
27	X	661	C	C6-N1-C2	-8.55	116.88	120.30
27	X	1812	U	C2-N1-C1'	8.54	127.95	117.70
27	X	2470	U	N1-C2-O2	8.33	128.63	122.80
27	X	2542	U	N1-C2-N3	8.32	119.89	114.90
27	X	2470	U	C2-N1-C1'	8.28	127.64	117.70
27	X	1992	G	C8-N9-C4	8.26	109.70	106.40
27	X	2693	U	C2-N1-C1'	-8.25	107.80	117.70
27	X	542	A	C2-N3-C4	-8.21	106.50	110.60
27	X	2495	G	N3-C4-C5	-7.82	124.69	128.60
27	X	2025	A	C8-N9-C4	-7.74	102.70	105.80
27	X	957	G	N1-C6-O6	-7.72	115.27	119.90
27	X	1467	U	C4-C5-C6	-7.72	115.07	119.70
6	G	106	TYR	N-CA-C	-7.69	90.24	111.00
27	X	774	A	C5-N7-C8	-7.69	100.06	103.90
27	X	2018	G	C5-N7-C8	-7.66	100.47	104.30
27	X	2553	G	N3-C4-C5	7.65	132.43	128.60
27	X	2548	G	C5-C6-N1	-7.56	107.72	111.50
27	X	2687	G	C8-N9-C4	7.53	109.41	106.40
27	X	2705	A	C4-C5-N7	7.49	114.44	110.70
27	X	1664	G	C4-N9-C1'	-7.43	116.83	126.50
27	X	928	G	C5-C6-O6	-7.43	124.14	128.60
27	X	343	A	C8-N9-C4	-7.42	102.83	105.80
27	X	2799	C	C6-N1-C2	-7.41	117.34	120.30
27	X	522	G	C6-C5-N7	-7.41	125.96	130.40
27	X	2690	A	C2-N3-C4	-7.41	106.90	110.60
27	X	1333	G	N3-C4-C5	7.38	132.29	128.60
27	X	860	U	C2-N1-C1'	7.33	126.50	117.70
27	X	2329	C	C5-C6-N1	7.32	124.66	121.00
27	X	774	A	C6-C5-N7	-7.27	127.21	132.30
27	X	2488	G	C5-C6-N1	7.26	115.13	111.50
27	X	1208	A	C8-N9-C4	-7.23	102.91	105.80
27	X	540	G	O4'-C1'-N9	7.23	113.98	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	2857	C	C6-N1-C2	-7.21	117.42	120.30
27	X	527	C	C6-N1-C2	-7.20	117.42	120.30
27	X	2591	C	C6-N1-C2	-7.19	117.42	120.30
27	X	1989	C	C5-C6-N1	7.18	124.59	121.00
27	X	2470	U	C6-N1-C1'	-7.13	111.22	121.20
27	X	2845	C	N3-C4-C5	-7.12	119.05	121.90
27	X	1283	C	N1-C2-O2	-7.11	114.63	118.90
27	X	2705	A	C2-N3-C4	-7.11	107.05	110.60
27	X	343	A	N7-C8-N9	7.09	117.35	113.80
27	X	1682	A	N1-C6-N6	7.08	122.85	118.60
27	X	462	G	C5-C6-N1	-6.96	108.02	111.50
27	X	1468	A	C2-N3-C4	6.95	114.08	110.60
10	K	92	GLY	N-CA-C	-6.94	95.74	113.10
27	X	2485	U	C2-N1-C1'	6.94	126.03	117.70
27	X	983	G	C8-N9-C4	-6.93	103.63	106.40
27	X	1270	C	C6-N1-C2	-6.92	117.53	120.30
27	X	841	G	C8-N9-C4	-6.91	103.64	106.40
27	X	774	A	N1-C6-N6	6.91	122.74	118.60
27	X	796	A	C2-N3-C4	-6.90	107.15	110.60
27	X	1724	C	C6-N1-C2	6.88	123.05	120.30
27	X	579	G	C4-C5-N7	-6.88	108.05	110.80
27	X	1468	A	C5-C6-N1	6.83	121.11	117.70
27	X	1993	G	N1-C6-O6	6.83	124.00	119.90
27	X	1235	C	C6-N1-C2	6.82	123.03	120.30
14	O	38	LEU	CA-CB-CG	6.81	130.97	115.30
27	X	1253	C	C6-N1-C2	-6.79	117.58	120.30
27	X	661	C	C5-C6-N1	6.77	124.39	121.00
27	X	1979	C	N3-C2-O2	-6.77	117.16	121.90
27	X	2815	C	C5-C6-N1	-6.76	117.62	121.00
27	X	2592	U	N3-C4-O4	6.75	124.12	119.40
27	X	2371	A	N7-C8-N9	6.72	117.16	113.80
27	X	2706	U	O5'-P-OP2	-6.72	99.65	105.70
27	X	796	A	C5-C6-N1	-6.70	114.35	117.70
27	X	1982	C	C2-N3-C4	-6.69	116.55	119.90
27	X	2553	G	N3-C4-N9	-6.69	121.98	126.00
27	X	2668	U	N1-C2-N3	6.69	118.92	114.90
27	X	1208	A	N7-C8-N9	6.69	117.15	113.80
27	X	759	C	C6-N1-C2	6.68	122.97	120.30
27	X	816	U	N3-C2-O2	-6.68	117.53	122.20
25	2	38	GLY	N-CA-C	-6.67	96.42	113.10
27	X	2845	C	C6-N1-C2	-6.65	117.64	120.30
27	X	2478	C	C2-N1-C1'	6.63	126.09	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	1682	A	C4-C5-C6	6.63	120.31	117.00
27	X	2607	C	N1-C2-O2	6.62	122.87	118.90
27	X	2434	G	C4-N9-C1'	6.62	135.11	126.50
27	X	1332	G	N1-C6-O6	6.57	123.84	119.90
27	X	2488	G	N3-C4-C5	-6.52	125.34	128.60
27	X	2508	G	N1-C6-O6	6.52	123.81	119.90
27	X	1288	A	O4'-C1'-N9	6.51	113.41	108.20
27	X	957	G	N3-C4-C5	-6.50	125.35	128.60
27	X	1481	U	C2-N1-C1'	-6.49	109.91	117.70
27	X	2542	U	C6-N1-C2	-6.49	117.10	121.00
27	X	1716	G	N1-C6-O6	-6.48	116.01	119.90
27	X	538	A	N1-C2-N3	-6.48	126.06	129.30
27	X	522	G	C5-C6-O6	-6.47	124.72	128.60
27	X	2404	A	P-O3'-C3'	6.46	127.46	119.70
27	X	537	C	N3-C2-O2	-6.41	117.41	121.90
27	X	774	A	C4-C5-N7	6.41	113.91	110.70
27	X	1664	G	C8-N9-C1'	6.41	135.33	127.00
27	X	1812	U	C5-C6-N1	6.40	125.90	122.70
27	X	2705	A	C6-C5-N7	-6.38	127.84	132.30
27	X	699	G	C4-C5-N7	6.38	113.35	110.80
27	X	2670	C	C6-N1-C2	-6.38	117.75	120.30
27	X	522	G	N9-C4-C5	-6.37	102.85	105.40
27	X	2705	A	C8-N9-C4	-6.35	103.26	105.80
27	X	1467	U	C5-C6-N1	6.33	125.86	122.70
27	X	1682	A	C6-C5-N7	-6.32	127.88	132.30
27	X	1481	U	N1-C2-O2	-6.31	118.38	122.80
27	X	2541	U	N3-C2-O2	-6.29	117.80	122.20
27	X	2542	U	N3-C2-O2	-6.26	117.82	122.20
27	X	1975	G	P-O3'-C3'	6.25	127.20	119.70
27	X	1812	U	C6-N1-C1'	-6.23	112.48	121.20
27	X	522	G	C4-C5-N7	6.20	113.28	110.80
27	X	2697	G	C2-N3-C4	6.20	115.00	111.90
27	X	2421	C	C6-N1-C2	-6.19	117.82	120.30
27	X	29	U	N3-C4-O4	6.17	123.72	119.40
27	X	556	A	N1-C6-N6	6.16	122.30	118.60
27	X	928	G	C4-C5-N7	6.16	113.26	110.80
27	X	2587	G	C5-C6-O6	-6.16	124.91	128.60
27	X	346	C	C6-N1-C2	-6.15	117.84	120.30
27	X	1466	C	C6-N1-C2	-6.14	117.84	120.30
27	X	24	G	O4'-C1'-N9	6.14	113.11	108.20
27	X	1250	A	P-O3'-C3'	6.12	127.04	119.70
27	X	923	A	C2-N3-C4	6.11	113.66	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	2508	G	C4-C5-N7	6.11	113.24	110.80
27	X	968	C	C2-N1-C1'	6.10	125.51	118.80
27	X	1674	C	N1-C2-O2	6.10	122.56	118.90
27	X	2795	A	N1-C6-N6	-6.10	114.94	118.60
27	X	841	G	N7-C8-N9	6.10	116.15	113.10
27	X	843	G	C5-C6-O6	-6.10	124.94	128.60
27	X	2767	C	C6-N1-C2	-6.08	117.87	120.30
27	X	2799	C	N1-C2-O2	-6.07	115.26	118.90
27	X	816	U	C6-N1-C2	-6.07	117.36	121.00
27	X	928	G	N9-C4-C5	-6.07	102.97	105.40
27	X	1984	A	C2-N3-C4	-6.07	107.57	110.60
27	X	1305	C	C6-N1-C2	6.05	122.72	120.30
27	X	617	U	N3-C2-O2	-6.04	117.97	122.20
27	X	538	A	C5-C6-N1	6.02	120.71	117.70
27	X	1747	G	C8-N9-C4	-6.02	103.99	106.40
27	X	2867	G	N3-C4-C5	6.01	131.61	128.60
27	X	1668	G	C6-C5-N7	-6.01	126.79	130.40
27	X	1988	A	N1-C6-N6	6.01	122.21	118.60
27	X	2034	A	N1-C6-N6	-6.01	115.00	118.60
27	X	1812	U	N1-C2-O2	6.01	127.00	122.80
27	X	2279	G	N1-C6-O6	6.01	123.50	119.90
27	X	1333	G	C2-N3-C4	-6.00	108.90	111.90
27	X	2668	U	C5-C4-O4	5.99	129.50	125.90
27	X	2638	G	N3-C4-C5	5.99	131.60	128.60
27	X	2410	U	C6-N1-C2	-5.97	117.42	121.00
27	X	2398	U	C6-N1-C2	-5.97	117.42	121.00
27	X	2854	G	C4-C5-N7	5.96	113.19	110.80
27	X	2669	C	N3-C2-O2	-5.96	117.73	121.90
27	X	2806	G	N1-C6-O6	5.96	123.48	119.90
27	X	699	G	N1-C6-O6	5.96	123.47	119.90
27	X	699	G	C5-N7-C8	-5.96	101.32	104.30
27	X	2019	C	C6-N1-C2	-5.96	117.92	120.30
27	X	540	G	N1-C6-O6	-5.95	116.33	119.90
27	X	1286	U	O5'-P-OP1	-5.94	100.36	105.70
27	X	2705	A	P-O3'-C3'	5.93	126.81	119.70
27	X	1975	G	N3-C4-C5	-5.92	125.64	128.60
27	X	2799	C	N1-C2-N3	5.91	123.34	119.20
27	X	2812	A	C8-N9-C4	-5.90	103.44	105.80
27	X	2485	U	C5-C6-N1	5.89	125.65	122.70
27	X	1141	U	P-O3'-C3'	5.88	126.75	119.70
27	X	2478	C	N3-C4-N4	5.88	122.11	118.00
27	X	684	C	N3-C4-C5	-5.87	119.55	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	1674	C	N3-C4-C5	5.87	124.25	121.90
27	X	2495	G	C2-N3-C4	5.87	114.84	111.90
27	X	985	G	C8-N9-C4	-5.86	104.06	106.40
27	X	1481	U	N3-C2-O2	5.86	126.30	122.20
27	X	2049	C	C6-N1-C2	-5.85	117.96	120.30
27	X	1324	G	O4'-C1'-N9	5.83	112.86	108.20
27	X	536	A	N1-C6-N6	5.83	122.10	118.60
27	X	2021	G	C6-C5-N7	-5.82	126.91	130.40
27	X	2409	A	P-O3'-C3'	5.82	126.68	119.70
27	X	1636	G	C8-N9-C4	5.81	108.72	106.40
27	X	1647	U	N3-C4-C5	-5.81	111.11	114.60
27	X	1770	U	C5-C6-N1	-5.81	119.79	122.70
27	X	1979	C	N1-C2-O2	5.81	122.39	118.90
27	X	2508	G	C6-C5-N7	-5.81	126.92	130.40
27	X	699	G	C6-C5-N7	-5.80	126.92	130.40
27	X	1712	G	C4-N9-C1'	5.80	134.04	126.50
27	X	538	A	P-O3'-C3'	5.79	126.65	119.70
27	X	2827	G	N3-C4-N9	5.79	129.47	126.00
27	X	2488	G	C2-N3-C4	5.78	114.79	111.90
27	X	2638	G	N3-C4-N9	-5.78	122.53	126.00
27	X	479	G	N1-C6-O6	5.78	123.37	119.90
27	X	1691	G	N9-C4-C5	-5.78	103.09	105.40
27	X	1142	G	N3-C4-C5	-5.78	125.71	128.60
27	X	1982	C	C5-C6-N1	-5.78	118.11	121.00
27	X	2846	G	C8-N9-C4	5.77	108.71	106.40
12	M	17	GLU	N-CA-C	-5.77	95.43	111.00
27	X	1992	G	N7-C8-N9	-5.77	110.22	113.10
27	X	579	G	C5-C6-O6	5.76	132.06	128.60
27	X	2034	A	C8-N9-C4	-5.76	103.50	105.80
27	X	1315	A	N1-C6-N6	-5.76	115.14	118.60
27	X	2508	G	C5-C6-O6	-5.75	125.15	128.60
27	X	661	C	C2-N1-C1'	5.74	125.11	118.80
27	X	1693	A	C8-N9-C4	-5.71	103.51	105.80
27	X	1712	G	C6-C5-N7	-5.71	126.97	130.40
27	X	2563	U	C2-N1-C1'	5.71	124.55	117.70
27	X	700	C	C6-N1-C2	-5.70	118.02	120.30
27	X	841	G	C5-N7-C8	-5.69	101.46	104.30
27	X	2576	G	N1-C6-O6	5.68	123.31	119.90
27	X	2854	G	C5-N7-C8	-5.68	101.46	104.30
27	X	1934	U	C6-N1-C2	-5.68	117.59	121.00
27	X	2859	U	O5'-P-OP1	-5.68	100.59	105.70
27	X	1746	A	C8-N9-C4	-5.67	103.53	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	2434	G	N3-C4-C5	-5.67	125.76	128.60
27	X	2655	C	C6-N1-C2	5.67	122.57	120.30
27	X	2634	G	O4'-C1'-N9	5.66	112.73	108.20
27	X	29	U	C5-C4-O4	-5.66	122.51	125.90
27	X	1691	G	C5-C6-O6	-5.65	125.21	128.60
27	X	2409	A	OP1-P-O3'	5.64	117.62	105.20
27	X	2587	G	C6-C5-N7	-5.64	127.01	130.40
27	X	684	C	C6-N1-C2	-5.64	118.04	120.30
27	X	2495	G	C5-C6-N1	5.63	114.32	111.50
27	X	2491	C	C6-N1-C2	-5.62	118.05	120.30
27	X	2587	G	N1-C6-O6	5.62	123.27	119.90
27	X	2813	G	C8-N9-C4	5.61	108.65	106.40
27	X	841	G	N3-C4-N9	-5.61	122.63	126.00
27	X	533	C	C2-N1-C1'	-5.61	112.63	118.80
27	X	1712	G	N3-C4-N9	5.61	129.36	126.00
27	X	2806	G	C6-C5-N7	-5.61	127.04	130.40
27	X	2656	G	OP2-P-O3'	5.60	117.52	105.20
27	X	617	U	C4-C5-C6	5.59	123.06	119.70
27	X	822	G	N3-C4-C5	-5.59	125.80	128.60
27	X	2371	A	C8-N9-C4	-5.59	103.56	105.80
27	X	1981	A	N1-C2-N3	5.59	132.10	129.30
27	X	2426	G	OP1-P-O3'	5.59	117.50	105.20
27	X	689	A	O4'-C1'-N9	5.59	112.67	108.20
27	X	1994	U	C5-C6-N1	5.58	125.49	122.70
27	X	2580	C	N1-C2-O2	-5.58	115.55	118.90
27	X	860	U	N1-C2-O2	5.57	126.70	122.80
27	X	2796	A	O5'-P-OP2	-5.57	100.69	105.70
27	X	2806	G	C5-C6-O6	-5.57	125.26	128.60
27	X	1670	G	N7-C8-N9	-5.57	110.31	113.10
27	X	1770	U	C4-C5-C6	5.57	123.04	119.70
27	X	2693	U	C6-N1-C1'	5.53	128.95	121.20
27	X	1692	C	C4-C5-C6	5.53	120.16	117.40
27	X	1713	G	N1-C6-O6	-5.52	116.59	119.90
27	X	2437	G	C8-N9-C4	-5.52	104.19	106.40
27	X	2664	G	N3-C2-N2	-5.51	116.05	119.90
27	X	542	A	N1-C2-N3	5.50	132.05	129.30
27	X	2475	C	C6-N1-C2	-5.50	118.10	120.30
27	X	522	G	C8-N9-C1'	-5.49	119.86	127.00
27	X	2481	G	C8-N9-C4	-5.49	104.20	106.40
28	Y	32	C	C6-N1-C2	-5.49	118.10	120.30
27	X	2398	U	N3-C4-C5	-5.49	111.31	114.60
27	X	1770	U	O4'-C1'-N1	5.49	112.59	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	1780	A	N1-C6-N6	5.48	121.89	118.60
27	X	1982	C	N3-C4-C5	5.48	124.09	121.90
27	X	1208	A	C5-N7-C8	-5.48	101.16	103.90
27	X	1629	G	OP1-P-O3'	5.47	117.24	105.20
27	X	2796	A	N1-C6-N6	-5.47	115.32	118.60
27	X	2812	A	N7-C8-N9	5.46	116.53	113.80
27	X	2579	A	C8-N9-C4	5.46	107.98	105.80
27	X	788	G	P-O3'-C3'	5.46	126.25	119.70
27	X	1664	G	O5'-P-OP1	-5.46	100.79	105.70
27	X	2254	C	C6-N1-C2	-5.46	118.12	120.30
27	X	2382	C	C6-N1-C2	-5.46	118.12	120.30
27	X	2025	A	N9-C4-C5	5.45	107.98	105.80
27	X	1770	U	C5-C4-O4	5.45	129.17	125.90
27	X	1661	C	N3-C2-O2	-5.45	118.08	121.90
27	X	2669	C	N3-C4-C5	-5.45	119.72	121.90
27	X	1691	G	C4-C5-N7	5.45	112.98	110.80
27	X	2607	C	N3-C2-O2	-5.44	118.09	121.90
27	X	577	U	C6-N1-C2	-5.43	117.74	121.00
27	X	928	G	N1-C6-O6	5.43	123.16	119.90
27	X	2798	A	N9-C4-C5	-5.42	103.63	105.80
27	X	1923	U	P-O3'-C3'	5.42	126.21	119.70
27	X	2548	G	C4-C5-N7	-5.42	108.63	110.80
27	X	1240	G	C8-N9-C4	5.42	108.57	106.40
27	X	755	C	O5'-P-OP1	-5.41	100.83	105.70
27	X	2756	A	P-O3'-C3'	5.41	126.20	119.70
27	X	2674	C	N3-C4-N4	5.41	121.79	118.00
27	X	2706	U	C5-C6-N1	5.41	125.40	122.70
27	X	2018	G	N3-C4-C5	5.40	131.30	128.60
27	X	1682	A	C8-N9-C4	-5.39	103.64	105.80
27	X	1664	G	N3-C4-C5	5.39	131.30	128.60
27	X	2820	C	N3-C4-C5	5.39	124.06	121.90
27	X	2246	A	N1-C6-N6	-5.39	115.37	118.60
27	X	2854	G	N7-C8-N9	5.39	115.80	113.10
27	X	2837	G	C8-N9-C4	5.39	108.55	106.40
27	X	2490	U	N3-C2-O2	-5.38	118.43	122.20
27	X	519	C	C6-N1-C2	-5.38	118.15	120.30
27	X	338	G	C8-N9-C4	-5.37	104.25	106.40
27	X	2561	G	C5-C6-N1	5.37	114.19	111.50
27	X	1696	C	N1-C2-O2	-5.36	115.68	118.90
27	X	1468	A	N3-C4-C5	-5.36	123.05	126.80
27	X	2694	G	OP2-P-O3'	5.34	116.94	105.20
27	X	2019	C	C2-N1-C1'	5.34	124.67	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	2023	C	C6-N1-C2	5.34	122.43	120.30
27	X	2019	C	C5-C6-N1	5.33	123.67	121.00
27	X	1657	A	C2-N3-C4	-5.33	107.93	110.60
27	X	2032	G	N3-C4-N9	5.33	129.20	126.00
27	X	2279	G	C6-C5-N7	-5.33	127.20	130.40
27	X	2025	A	N1-C6-N6	-5.32	115.41	118.60
27	X	2434	G	C8-N9-C1'	-5.32	120.08	127.00
27	X	774	A	C2-N3-C4	-5.32	107.94	110.60
27	X	1246	G	N1-C6-O6	-5.32	116.71	119.90
27	X	2470	U	N3-C2-O2	-5.32	118.48	122.20
27	X	1164	C	C6-N1-C2	-5.30	118.18	120.30
27	X	1934	U	N3-C4-O4	5.29	123.11	119.40
27	X	540	G	C8-N9-C4	-5.29	104.28	106.40
27	X	596	C	N3-C4-C5	-5.28	119.79	121.90
27	X	1742	G	N3-C4-N9	5.28	129.17	126.00
27	X	1746	A	N1-C6-N6	-5.28	115.43	118.60
27	X	1313	U	P-O3'-C3'	5.28	126.03	119.70
27	X	1679	U	N3-C2-O2	-5.28	118.50	122.20
27	X	2021	G	N1-C6-O6	5.28	123.07	119.90
27	X	2751	C	N3-C4-C5	5.28	124.01	121.90
27	X	699	G	N7-C8-N9	5.27	115.73	113.10
27	X	2693	U	N3-C4-O4	-5.26	115.72	119.40
27	X	1976	U	N3-C4-O4	-5.25	115.72	119.40
27	X	1747	G	N3-C4-C5	-5.25	125.98	128.60
27	X	833	A	C5-C6-N6	-5.24	119.50	123.70
27	X	1934	U	N3-C4-C5	-5.24	111.45	114.60
27	X	2831	A	C4-C5-C6	-5.24	114.38	117.00
27	X	1310	C	N3-C4-C5	5.24	124.00	121.90
27	X	2321	C	C6-N1-C2	-5.23	118.21	120.30
27	X	923	A	C8-N9-C4	-5.23	103.71	105.80
27	X	2239	C	C6-N1-C2	-5.22	118.21	120.30
27	X	2524	G	C4-C5-N7	5.22	112.89	110.80
27	X	1713	G	C4-C5-N7	-5.21	108.71	110.80
27	X	1993	G	C4-C5-N7	5.21	112.89	110.80
27	X	1278	A	O5'-P-OP2	-5.21	101.01	105.70
27	X	844	G	OP2-P-O3'	5.20	116.65	105.20
27	X	2662	C	C6-N1-C2	-5.20	118.22	120.30
27	X	2791	C	C6-N1-C2	5.20	122.38	120.30
27	X	2712	G	N1-C2-N2	-5.20	111.52	116.20
27	X	742	G	C4-N9-C1'	5.20	133.26	126.50
3	C	56	ARG	N-CA-C	5.20	125.03	111.00
27	X	2560	G	O4'-C1'-N9	5.20	112.36	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	1288	A	N7-C8-N9	5.19	116.40	113.80
27	X	1391	A	P-O3'-C3'	5.19	125.93	119.70
27	X	2524	G	C5-C6-O6	-5.19	125.49	128.60
27	X	1647	U	C6-N1-C2	-5.19	117.89	121.00
27	X	1342	U	O5'-P-OP2	-5.18	101.03	105.70
27	X	2541	U	N1-C2-O2	5.18	126.43	122.80
27	X	874	A	C8-N9-C4	-5.18	103.73	105.80
27	X	2638	G	N3-C2-N2	-5.18	116.27	119.90
27	X	2827	G	N3-C4-C5	-5.18	126.01	128.60
27	X	2338	C	C6-N1-C2	-5.18	118.23	120.30
27	X	2485	U	N1-C2-O2	5.18	126.42	122.80
27	X	24	G	C4-N9-C1'	-5.17	119.78	126.50
27	X	833	A	C4-C5-N7	5.17	113.28	110.70
27	X	1223	G	C6-C5-N7	-5.17	127.30	130.40
27	X	2590	U	C2-N1-C1'	5.17	123.90	117.70
27	X	1885	C	N1-C2-O2	5.16	122.00	118.90
27	X	1712	G	C8-N9-C1'	-5.16	120.29	127.00
27	X	2815	C	N3-C4-C5	5.16	123.96	121.90
27	X	522	G	N3-C4-N9	5.16	129.09	126.00
27	X	2057	U	C6-N1-C2	-5.15	117.91	121.00
27	X	1141	U	N3-C2-O2	-5.15	118.59	122.20
27	X	1694	A	C5-N7-C8	-5.15	101.33	103.90
27	X	1623	C	N1-C2-O2	5.14	121.99	118.90
27	X	2050	G	N9-C4-C5	-5.14	103.34	105.40
27	X	1934	U	C5-C6-N1	5.14	125.27	122.70
27	X	2592	U	N3-C4-C5	-5.14	111.52	114.60
27	X	1326	U	C2-N1-C1'	5.13	123.86	117.70
27	X	593	C	C6-N1-C2	-5.13	118.25	120.30
27	X	2857	C	N3-C4-C5	-5.13	119.85	121.90
27	X	461	A	O5'-P-OP1	-5.13	101.08	105.70
27	X	1625	A	P-O3'-C3'	5.13	125.86	119.70
27	X	1232	U	N1-C2-O2	-5.13	119.21	122.80
27	X	1035	G	N3-C4-C5	-5.12	126.04	128.60
27	X	2410	U	C5-C6-N1	5.12	125.26	122.70
27	X	1992	G	N9-C4-C5	-5.12	103.35	105.40
27	X	2000	U	N3-C2-O2	5.12	125.79	122.20
27	X	2495	G	C6-N1-C2	-5.12	122.03	125.10
27	X	1211	G	N3-C4-N9	5.12	129.07	126.00
27	X	1142	G	C2-N3-C4	5.12	114.46	111.90
27	X	2668	U	N1-C2-O2	-5.12	119.22	122.80
27	X	13	A	OP2-P-O3'	5.12	116.45	105.20
27	X	985	G	N7-C8-N9	5.11	115.66	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	1223	G	C4-N9-C1'	5.11	133.14	126.50
27	X	1975	G	C4-N9-C1'	5.11	133.14	126.50
27	X	2690	A	N1-C6-N6	5.11	121.67	118.60
27	X	968	C	N1-C2-O2	5.10	121.96	118.90
27	X	1222	G	N3-C4-N9	5.10	129.06	126.00
27	X	2576	G	C6-C5-N7	-5.10	127.34	130.40
27	X	2039	G	C8-N9-C4	-5.09	104.36	106.40
27	X	2850	U	O5'-P-OP1	-5.08	101.13	105.70
27	X	537	C	P-O3'-C3'	5.08	125.80	119.70
27	X	518	A	C8-N9-C4	-5.08	103.77	105.80
27	X	1315	A	N1-C2-N3	5.08	131.84	129.30
27	X	2050	G	N1-C6-O6	5.08	122.95	119.90
27	X	2482	A	OP1-P-OP2	-5.07	112.00	119.60
27	X	2837	G	C6-C5-N7	5.07	133.44	130.40
27	X	236	C	C6-N1-C2	-5.07	118.27	120.30
27	X	479	G	C5-C6-O6	-5.06	125.56	128.60
27	X	1662	G	N3-C4-N9	5.06	129.04	126.00
27	X	1141	U	C2-N1-C1'	5.06	123.77	117.70
27	X	558	G	C4-N9-C1'	5.05	133.06	126.50
15	P	120	ILE	N-CA-C	5.04	124.62	111.00
27	X	2795	A	P-O3'-C3'	5.04	125.75	119.70
16	Q	7	LEU	CA-CB-CG	5.04	126.89	115.30
27	X	2026	C	N1-C2-O2	5.03	121.92	118.90
27	X	536	A	C5-C6-N6	-5.03	119.68	123.70
27	X	1467	U	N1-C2-N3	-5.03	111.89	114.90
27	X	1683	G	N3-C4-N9	-5.03	122.98	126.00
27	X	2371	A	C5-N7-C8	-5.03	101.39	103.90
27	X	2596	C	C6-N1-C2	5.03	122.31	120.30
27	X	69	G	C4-N9-C1'	5.02	133.03	126.50
27	X	854	G	N1-C6-O6	5.02	122.91	119.90
27	X	1240	G	N9-C4-C5	-5.02	103.39	105.40
27	X	2792	C	C6-N1-C2	5.02	122.31	120.30
27	X	2682	C	C2-N1-C1'	5.02	124.32	118.80
27	X	2693	U	C5-C6-N1	-5.02	120.19	122.70
27	X	1315	A	C5-C6-N6	5.01	127.71	123.70
27	X	2472	U	O5'-P-OP1	-5.01	101.19	105.70
27	X	770	U	C6-N1-C2	-5.01	118.00	121.00
27	X	1682	A	N7-C8-N9	5.01	116.30	113.80
27	X	1618	U	N3-C4-C5	-5.00	111.60	114.60
27	X	2687	G	N7-C8-N9	-5.00	110.60	113.10

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	2	42	LEU	Peptide
26	3	45	GLY	Peptide
2	B	146	THR	Peptide
6	G	108	GLY	Peptide
7	H	26	ASN	Peptide
8	I	35	LYS	Peptide
8	I	40	ARG	Peptide
8	I	99	VAL	Peptide
10	K	93	GLY	Peptide
10	K	94	TYR	Peptide
16	Q	59	PRO	Peptide
17	R	64	ASN	Peptide
19	T	19	LYS	Peptide
20	U	30	VAL	Peptide
23	Z	4	HIS	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1987	0	2056	145	0
2	B	1539	0	1600	109	0
3	C	1481	0	1504	99	0
4	D	1400	0	1481	55	0
5	E	1286	0	1336	54	0
6	G	1114	0	1144	73	0
7	H	997	0	1046	56	0
8	I	1011	0	1047	72	0
9	J	1090	0	1125	64	0
10	K	878	0	930	45	0
11	L	779	0	820	36	0
12	M	871	0	894	61	0
13	N	978	0	1020	52	0
14	O	741	0	756	51	0
15	P	1038	0	1125	85	0
16	Q	726	0	753	32	0
17	R	825	0	881	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	S	1345	0	1372	37	0
19	T	556	0	579	30	0
20	U	552	0	604	35	0
21	V	525	0	546	19	0
22	W	424	0	470	16	0
23	Z	443	0	444	26	0
24	1	431	0	456	29	0
25	2	383	0	414	26	0
26	3	462	0	506	53	0
27	X	57533	0	28987	1344	0
28	Y	2601	0	1327	62	0
29	A	1	0	0	0	0
29	B	1	0	0	0	0
29	K	2	0	0	0	0
29	M	2	0	0	0	0
29	X	64	0	0	0	0
30	X	51	0	67	9	0
All	All	84117	0	55290	2467	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (2467) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:VAL:HG22	2:B:136:ARG:HG3	1.32	1.11
23:Z:19:ARG:NH2	27:X:1277:G:OP1	1.90	1.04
13:N:66:ASN:HB3	13:N:76:TYR:HB2	1.46	0.97
27:X:854:G:H1	27:X:948:C:H42	1.04	0.96
7:H:40:GLY:HA3	27:X:2545:A:H61	1.29	0.95
8:I:21:ARG:HE	8:I:22:GLY:H	1.08	0.95
6:G:109:GLY:HA2	6:G:111:LYS:HE3	1.46	0.95
27:X:517:A:H5''	27:X:518:A:H5'	1.50	0.94
1:A:250:TRP:O	1:A:255:LYS:NZ	2.01	0.93
27:X:2447:G:HO2'	27:X:2448:A:H8	1.07	0.92
9:J:82:THR:HA	27:X:2474:G:H5''	1.53	0.90
27:X:4:C:H42	27:X:2873:G:H1	1.17	0.89
1:A:55:GLY:H	1:A:217:ARG:HB2	1.38	0.88
27:X:571:U:HO2'	27:X:581:A:H8	1.21	0.87
10:K:60:LEU:HG	10:K:64:ARG:HD2	1.55	0.86
27:X:2281:C:H42	27:X:2293:G:H1	1.23	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:38:THR:HB	27:X:2063:A:H5'	1.58	0.85
15:P:80:LEU:HD11	15:P:87:GLU:HB3	1.58	0.85
24:1:41:ASP:HB2	24:1:46:LYS:HE3	1.56	0.85
8:I:21:ARG:HE	8:I:22:GLY:N	1.75	0.85
27:X:538:A:H62	27:X:2026:C:H5'	1.40	0.84
27:X:832:A:OP2	27:X:1201:G:N2	2.10	0.84
1:A:218:LYS:NZ	1:A:219:PRO:O	2.10	0.84
27:X:2016:A:O2'	27:X:2018:G:OP2	1.95	0.84
27:X:2225:G:H2'	27:X:2226:A:H8	1.41	0.83
27:X:833:A:N3	27:X:954:U:O2'	2.10	0.83
9:J:83:ARG:HH22	27:X:971:A:H61	1.22	0.83
27:X:2757:G:H5''	27:X:2758:A:H5'	1.60	0.83
26:3:13:ARG:HE	26:3:25:PHE:H	1.27	0.83
15:P:100:GLY:HA3	15:P:124:THR:HA	1.58	0.83
2:B:14:ILE:HG12	12:M:20:HIS:HD2	1.43	0.82
27:X:2811:G:H2'	27:X:2812:A:C8	2.13	0.82
2:B:146:THR:HG1	27:X:2550:C:HO2'	1.19	0.82
1:A:252:LYS:HZ2	1:A:252:LYS:H	1.28	0.81
14:O:12:TYR:HB3	14:O:40:VAL:H	1.45	0.81
27:X:649:G:H22	27:X:661:C:H1'	1.45	0.81
22:W:8:SER:HB2	27:X:999:A:H5''	1.62	0.81
27:X:1173:G:H2'	27:X:1174:G:H8	1.46	0.80
6:G:37:ASP:O	6:G:39:GLN:NE2	2.15	0.79
27:X:841:G:H2'	27:X:842:A:C8	2.16	0.79
27:X:2259:G:H4'	27:X:2306:A:H5'	1.65	0.79
27:X:415:A:H61	27:X:436:A:H61	1.30	0.79
15:P:99:ALA:HB2	27:X:24:G:O2'	1.83	0.78
26:3:26:LYS:HD3	26:3:28:GLY:H	1.45	0.78
2:B:82:ARG:NH2	27:X:2617:G:OP2	2.16	0.78
9:J:17:ARG:NH1	27:X:966:A:OP2	2.17	0.78
15:P:30:TYR:H	15:P:126:HIS:HD2	1.32	0.78
14:O:57:GLN:H	14:O:97:GLY:HA3	1.47	0.78
27:X:538:A:O2'	27:X:539:A:O5'	2.00	0.78
2:B:51:TYR:HE2	12:M:3:THR:HG21	1.49	0.77
18:S:125:PRO:O	18:S:129:ARG:NH1	2.18	0.77
1:A:157:ARG:NH1	27:X:1810:U:OP2	2.17	0.77
9:J:100:PRO:HB2	18:S:74:ARG:HG2	1.67	0.77
7:H:23:ARG:NH1	27:X:2526:U:O2	2.17	0.77
27:X:2796:A:H2'	27:X:2797:G:C8	2.19	0.77
27:X:89:A:H4'	27:X:90:G:H5'	1.68	0.76
27:X:1856:U:OP1	27:X:2389:G:O2'	2.02	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:163:ASN:HD21	3:C:167:VAL:H	1.31	0.76
27:X:1882:G:N2	27:X:1885:C:H41	1.83	0.76
27:X:215:G:H21	27:X:632:A:H8	1.30	0.76
20:U:21:ARG:HD3	20:U:23:LYS:HG2	1.66	0.76
3:C:162:ARG:O	3:C:162:ARG:NH1	2.19	0.76
27:X:1329:U:H2'	27:X:1330:G:H8	1.49	0.76
27:X:2002:A:N6	27:X:2018:G:O6	2.19	0.76
1:A:14:ARG:HG3	1:A:24:LEU:HG	1.68	0.76
8:I:40:ARG:NH2	27:X:820:U:OP1	2.18	0.76
3:C:161:ALA:HB1	3:C:167:VAL:HG21	1.69	0.75
2:B:176:ARG:HH21	12:M:16:ILE:HG23	1.51	0.75
27:X:2543:A:H5'	27:X:2627:G:H4'	1.66	0.75
27:X:2761:A:H5''	27:X:2762:G:H5'	1.67	0.75
1:A:243:GLY:C	1:A:244:ARG:HE	1.89	0.75
1:A:24:LEU:HB2	1:A:205:VAL:HG22	1.68	0.75
15:P:45:ILE:HD11	15:P:57:LEU:HD11	1.68	0.75
27:X:965:G:O2'	27:X:2253:A:N1	2.20	0.75
3:C:137:ALA:HB1	3:C:142:LEU:HB2	1.68	0.75
24:1:27:ASN:ND2	24:1:36:GLU:OE1	2.20	0.75
1:A:210:GLY:HA2	1:A:213:ARG:HG2	1.69	0.75
16:Q:14:GLU:OE2	27:X:1405:A:N6	2.18	0.75
17:R:56:LYS:HB3	17:R:69:GLN:HG2	1.69	0.75
27:X:1327:C:H42	27:X:1351:G:H1	1.32	0.75
26:3:32:GLN:HB3	27:X:2400:G:N7	2.02	0.75
27:X:2225:G:H2'	27:X:2226:A:C8	2.20	0.75
27:X:27:G:N2	27:X:522:G:H1'	2.02	0.75
27:X:2796:A:H2'	27:X:2797:G:H8	1.50	0.74
11:L:90:ASP:OD2	11:L:91:ARG:N	2.20	0.74
1:A:91:ARG:HB2	1:A:107:ALA:HB3	1.69	0.74
15:P:30:TYR:H	15:P:126:HIS:CD2	2.05	0.74
2:B:91:VAL:HB	2:B:93:VAL:HG12	1.70	0.74
27:X:1673:C:H2'	27:X:1674:C:H6	1.52	0.74
27:X:1278:A:H2	27:X:1997:A:H62	1.35	0.74
27:X:1922:U:H3'	27:X:1923:U:H5'	1.70	0.74
27:X:591:G:H3'	27:X:592:G:H8	1.51	0.74
6:G:34:PRO:HB3	6:G:71:THR:HG21	1.69	0.74
9:J:117:GLU:OE1	9:J:120:ARG:NH1	2.21	0.74
12:M:60:SER:HA	12:M:64:LYS:HB2	1.69	0.74
27:X:2757:G:OP2	27:X:2761:A:O2'	2.06	0.74
22:W:5:LEU:HB2	22:W:25:LEU:HD13	1.68	0.74
25:2:19:ARG:HG2	27:X:123:A:H5'	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:465:C:O2'	27:X:483:A:N6	2.21	0.74
27:X:2820:C:H2'	27:X:2821:G:H8	1.52	0.73
27:X:1337:G:N2	27:X:1343:C:O2	2.20	0.73
11:L:65:THR:OG1	28:Y:52:G:OP1	2.06	0.73
2:B:137:ARG:NH2	27:X:2034:A:OP1	2.19	0.73
27:X:854:G:N2	27:X:948:C:N3	2.32	0.73
2:B:9:ILE:HD11	2:B:27:LEU:HB2	1.70	0.73
27:X:872:G:O2'	27:X:928:G:O6	2.07	0.73
12:M:100:ARG:HD2	27:X:1744:G:OP1	1.89	0.73
27:X:115:G:OP2	27:X:117:A:O2'	2.07	0.73
2:B:128:SER:HB3	27:X:1976:U:H4'	1.71	0.73
27:X:613:A:N6	27:X:668:A:O2'	2.22	0.73
4:D:116:GLY:HA2	4:D:176:PRO:HB2	1.71	0.73
15:P:35:PRO:HD3	15:P:124:THR:OG1	1.89	0.73
27:X:1963:G:O2'	27:X:1965:U:OP2	2.07	0.73
27:X:2708:U:H2'	27:X:2709:C:C6	2.23	0.73
27:X:2484:G:H22	30:X:2902:ERY:H191	1.54	0.72
17:R:17:LYS:NZ	27:X:83:A:OP2	2.16	0.72
17:R:105:ARG:HH22	17:R:113:THR:H	1.37	0.72
27:X:313:U:H2'	27:X:314:G:H8	1.54	0.72
1:A:63:ARG:HH21	1:A:86:PRO:HD2	1.55	0.72
2:B:152:LYS:HB3	6:G:106:TYR:HB2	1.71	0.72
27:X:1399:C:OP2	27:X:1409:U:N3	2.21	0.72
16:Q:35:LYS:NZ	27:X:1615:C:OP2	2.23	0.72
27:X:2324:G:HO2'	27:X:2360:C:HO2'	1.35	0.72
14:O:68:LYS:NZ	27:X:1238:A:OP1	2.18	0.72
27:X:1744:G:N2	27:X:1747:G:OP2	2.18	0.72
23:Z:16:ARG:NH1	23:Z:17:ASP:OD2	2.22	0.72
24:1:28:ARG:NH1	27:X:2264:C:OP2	2.22	0.72
27:X:1643:A:H61	27:X:1656:U:H3	1.38	0.72
1:A:54:ILE:HA	1:A:217:ARG:H	1.55	0.71
27:X:168:A:H2'	27:X:169:C:C6	2.24	0.71
27:X:209:G:N2	27:X:433:G:OP1	2.22	0.71
3:C:6:VAL:HG13	3:C:7:ILE:HG12	1.72	0.71
14:O:66:GLY:O	14:O:87:ARG:NH2	2.23	0.71
27:X:1030:U:H3	27:X:1153:A:H62	1.38	0.71
26:3:30:ARG:HE	26:3:31:HIS:CE1	2.09	0.71
16:Q:64:ARG:NH2	27:X:1348:C:O2'	2.22	0.71
27:X:2048:C:O2	27:X:2428:U:N3	2.20	0.71
9:J:16:GLY:HA2	9:J:17:ARG:HH11	1.55	0.71
27:X:2020:G:H2'	27:X:2021:G:C8	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ARG:O	1:A:252:LYS:NZ	2.20	0.71
27:X:1551:U:OP2	27:X:1553:G:N2	2.24	0.71
3:C:149:LEU:HD11	3:C:170:LEU:HB2	1.73	0.71
22:W:25:LEU:HD22	22:W:30:ASP:HB3	1.73	0.71
27:X:2354:G:N2	27:X:2357:A:OP2	2.22	0.71
8:I:38:LYS:NZ	27:X:954:U:OP2	2.20	0.71
8:I:31:GLY:O	8:I:32:ARG:NH2	2.23	0.71
27:X:1466:C:H2'	27:X:1467:U:O4'	1.91	0.71
6:G:116:ARG:HA	6:G:119:LEU:HD23	1.73	0.70
8:I:18:ARG:NH2	8:I:18:ARG:O	2.23	0.70
27:X:1845:A:N3	27:X:2212:U:O2'	2.24	0.70
28:Y:51:G:H2'	28:Y:52:G:H8	1.56	0.70
6:G:100:TYR:HB2	6:G:116:ARG:NH1	2.06	0.70
27:X:1361:G:H1	27:X:1614:C:H42	1.39	0.70
7:H:28:GLY:HA3	7:H:35:THR:OG1	1.91	0.70
24:1:41:ASP:N	24:1:41:ASP:OD1	2.24	0.70
8:I:17:LYS:HG3	8:I:19:VAL:H	1.57	0.70
26:3:13:ARG:NE	26:3:25:PHE:H	1.89	0.70
5:E:33:LEU:HD21	5:E:136:ILE:HB	1.73	0.70
27:X:113:C:HO2'	27:X:125:A:HO2'	1.40	0.69
1:A:96:HIS:NE2	27:X:1517:C:O2'	2.21	0.69
27:X:538:A:HO2'	27:X:539:A:P	2.15	0.69
27:X:661:C:H2'	27:X:662:G:C8	2.27	0.69
5:E:124:ALA:HB3	5:E:132:ASP:HB3	1.73	0.69
10:K:24:GLN:HB3	10:K:44:LEU:HD22	1.74	0.69
27:X:2241:U:H2'	27:X:2242:C:H6	1.56	0.69
27:X:27:G:H22	27:X:522:G:H1'	1.58	0.69
1:A:231:HIS:CD2	1:A:232:PRO:HD2	2.26	0.69
1:A:249:PRO:HD3	27:X:2218:G:H5'	1.73	0.69
27:X:793:G:H21	27:X:796:A:H62	1.38	0.69
27:X:2237:C:O2'	27:X:2406:C:OP2	2.11	0.69
12:M:31:ASP:HB2	12:M:94:VAL:HB	1.75	0.69
27:X:953:G:O2'	27:X:1203:A:N3	2.24	0.69
14:O:23:GLU:HB2	14:O:91:THR:HG21	1.75	0.69
6:G:106:TYR:CD2	6:G:108:GLY:HA2	2.28	0.68
27:X:1030:U:O2	27:X:1155:G:N2	2.26	0.68
27:X:1082:G:O6	27:X:1103:C:N4	2.26	0.68
27:X:2617:G:H1	27:X:2755:A:H2'	1.58	0.68
27:X:224:G:OP2	27:X:226:C:N4	2.26	0.68
27:X:105:G:H21	27:X:357:A:H61	1.42	0.68
11:L:28:ARG:NH1	11:L:90:ASP:OD1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1342:U:H5''	27:X:1343:C:H5	1.57	0.68
4:D:66:ILE:HD11	28:Y:43:G:H3'	1.75	0.68
19:T:41:ARG:HH12	27:X:2366:U:H1'	1.59	0.68
21:V:48:ARG:NH2	27:X:76:C:OP1	2.27	0.68
6:G:50:PRO:HG2	6:G:53:ARG:HB2	1.76	0.68
1:A:55:GLY:N	1:A:217:ARG:HB2	2.07	0.68
25:2:33:ARG:NE	27:X:478:G:OP1	2.25	0.68
8:I:51:GLY:HA3	26:3:59:LYS:HE3	1.74	0.68
11:L:39:TYR:OH	28:Y:118:G:N3	2.27	0.68
9:J:61:ARG:HH11	18:S:175:ARG:HB2	1.58	0.68
27:X:2200:G:H2'	27:X:2201:G:C8	2.29	0.67
27:X:226:C:OP2	27:X:2373:C:O2'	2.12	0.67
26:3:19:THR:OG1	27:X:661:C:OP1	2.12	0.67
2:B:78:LEU:O	2:B:79:ARG:NE	2.27	0.67
3:C:48:ARG:NH1	3:C:51:VAL:HG13	2.09	0.67
9:J:81:GLU:HG2	9:J:82:THR:HG23	1.76	0.67
27:X:1573:G:O6	27:X:1574:A:N6	2.27	0.67
3:C:111:ARG:NH1	3:C:180:ILE:O	2.27	0.67
10:K:12:ARG:HD3	10:K:16:ALA:HB1	1.77	0.67
2:B:26:VAL:HB	2:B:182:ILE:HG23	1.77	0.67
8:I:56:LEU:HB3	26:3:52:LYS:HZ1	1.60	0.67
15:P:28:ALA:HB2	15:P:71:VAL:HG21	1.76	0.67
27:X:1202:U:H2'	27:X:1203:A:H8	1.60	0.67
27:X:2672:U:H2'	27:X:2673:G:H8	1.60	0.67
27:X:760:U:O2'	27:X:761:G:OP2	2.12	0.67
4:D:115:ARG:HH22	4:D:178:ARG:HH12	1.43	0.67
7:H:40:GLY:HA3	27:X:2545:A:N6	2.08	0.67
27:X:2040:A:H2'	27:X:2041:A:C8	2.29	0.67
27:X:203:G:O2'	27:X:205:A:N1	2.23	0.67
23:Z:36:CYS:SG	23:Z:49:CYS:N	2.67	0.67
3:C:59:TYR:OH	3:C:67:ALA:HB1	1.93	0.67
15:P:99:ALA:HB1	27:X:25:U:H5'	1.76	0.67
4:D:62:LEU:O	4:D:95:ARG:NH1	2.28	0.66
10:K:28:LEU:HD21	10:K:115:LEU:HG	1.78	0.66
14:O:10:LYS:HG3	14:O:13:ARG:HH22	1.60	0.66
18:S:47:SER:OG	18:S:48:THR:N	2.18	0.66
27:X:1287:A:N1	27:X:1661:C:O2'	2.26	0.66
9:J:38:MET:HB2	9:J:129:GLN:HB2	1.76	0.66
27:X:1278:A:N6	27:X:1996:A:H5''	2.10	0.66
25:2:16:HIS:HB3	25:2:43:THR:HG21	1.77	0.66
27:X:1173:G:H2'	27:X:1174:G:C8	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:18:U:O2'	27:X:563:U:OP1	2.14	0.66
27:X:571:U:O2'	27:X:581:A:H8	1.77	0.66
27:X:617:U:H5	27:X:632:A:C2	2.12	0.66
23:Z:31:THR:OG1	27:X:2861:A:O2'	2.12	0.66
27:X:1850:G:O2'	27:X:1867:A:N6	2.29	0.66
27:X:854:G:H1	27:X:948:C:N4	1.86	0.66
3:C:46:ARG:HB3	3:C:51:VAL:HB	1.77	0.66
12:M:101:ARG:NH2	27:X:1745:C:OP1	2.29	0.66
17:R:61:SER:HA	17:R:65:PRO:HG3	1.77	0.66
27:X:2298:U:O2	27:X:2299:A:N6	2.28	0.66
2:B:77:ILE:HD13	2:B:195:LEU:HD22	1.77	0.66
27:X:1089:C:O2'	27:X:1099:A:OP1	2.10	0.66
27:X:2324:G:N3	27:X:2360:C:H2'	2.10	0.66
6:G:122:HIS:HB3	6:G:125:ARG:HB2	1.78	0.66
27:X:2284:U:H5'	27:X:2286:G:H1	1.59	0.66
7:H:13:ASN:HD21	7:H:109:ARG:HG2	1.61	0.65
17:R:84:VAL:HG11	17:R:90:LYS:H	1.59	0.65
27:X:1283:C:H5''	27:X:1284:G:H5'	1.78	0.65
3:C:83:ALA:HB3	27:X:595:A:H5'	1.77	0.65
28:Y:46:G:N3	28:Y:49:C:N4	2.44	0.65
6:G:103:TYR:CG	6:G:111:LYS:HB2	2.31	0.65
9:J:36:ILE:HG12	9:J:103:VAL:HA	1.78	0.65
27:X:1329:U:H2'	27:X:1330:G:C8	2.30	0.65
1:A:183:ARG:NH1	27:X:1790:G:O2'	2.29	0.65
7:H:13:ASN:ND2	7:H:109:ARG:HG2	2.11	0.65
19:T:74:LYS:HA	19:T:77:ARG:HG3	1.77	0.65
6:G:130:ALA:O	27:X:1148:G:O2'	2.14	0.65
1:A:52:ARG:HD3	27:X:1816:G:OP1	1.96	0.65
6:G:61:ARG:HH12	6:G:66:HIS:H	1.45	0.65
13:N:93:LYS:HE2	14:O:10:LYS:HD3	1.76	0.65
27:X:1109:A:H3'	27:X:1110:G:H8	1.62	0.65
27:X:1466:C:H42	27:X:1476:G:H1	1.45	0.65
27:X:2015:G:OP2	27:X:2433:G:O2'	2.09	0.65
27:X:1562:G:H5'	27:X:1563:U:H5'	1.78	0.65
27:X:578:U:O2'	27:X:994:A:N1	2.26	0.65
2:B:140:SER:HB3	27:X:2554:C:O2'	1.96	0.65
27:X:1082:G:O2'	27:X:1100:G:OP2	2.14	0.65
7:H:1:MET:HE2	27:X:1682:A:H1'	1.78	0.65
27:X:840:U:H4'	27:X:841:G:C2	2.32	0.65
23:Z:6:VAL:HG22	23:Z:7:PRO:HD2	1.79	0.65
27:X:219:G:HO2'	27:X:231:G:H1	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:ARG:NH2	27:X:2804:G:O3'	2.30	0.65
17:R:56:LYS:HD2	27:X:494:A:C8	2.31	0.65
27:X:87:G:H2'	27:X:88:G:H5''	1.77	0.65
3:C:163:ASN:ND2	3:C:167:VAL:H	1.95	0.65
15:P:105:ARG:O	15:P:105:ARG:NE	2.29	0.65
27:X:1067:G:H5''	27:X:1068:A:H5'	1.77	0.65
27:X:545:C:H2'	27:X:546:A:C8	2.32	0.65
27:X:812:G:H3'	27:X:813:A:H2'	1.79	0.65
27:X:308:C:O2	27:X:352:G:N2	2.23	0.65
27:X:403:A:H4'	27:X:404:A:H5'	1.79	0.65
3:C:9:GLN:HG2	3:C:120:VAL:HG21	1.79	0.64
6:G:132:PHE:CZ	6:G:145:HIS:HB2	2.32	0.64
27:X:1225:G:O2'	27:X:1250:A:N6	2.30	0.64
27:X:1742:G:HO2'	27:X:2836:U:HO2'	1.43	0.64
8:I:40:ARG:NH1	27:X:576:A:O3'	2.30	0.64
10:K:87:TYR:HE1	10:K:94:TYR:HD1	1.46	0.64
11:L:38:ILE:HD11	11:L:40:ALA:HB2	1.77	0.64
19:T:40:GLN:NE2	19:T:42:GLY:O	2.30	0.64
27:X:1373:G:H22	27:X:2192:U:H3	1.45	0.64
27:X:2432:A:H61	27:X:2479:U:H3	1.45	0.64
27:X:304:A:N6	27:X:356:A:N7	2.44	0.64
2:B:16:LYS:HD3	2:B:173:VAL:HG12	1.80	0.64
5:E:94:PHE:HB3	5:E:107:ILE:HG22	1.80	0.64
20:U:47:HIS:ND1	27:X:410:A:OP1	2.30	0.64
27:X:759:C:H5''	27:X:761:G:H1'	1.79	0.64
27:X:800:U:H5''	27:X:801:A:H5'	1.79	0.64
2:B:5:LEU:HD11	2:B:79:ARG:HB2	1.79	0.64
27:X:1225:G:H2'	27:X:1249:G:N2	2.12	0.64
7:H:104:GLU:OE2	7:H:125:LYS:NZ	2.31	0.64
10:K:102:THR:HA	10:K:109:THR:HA	1.80	0.64
27:X:1017:C:H2'	27:X:1018:C:H6	1.60	0.64
10:K:68:GLN:NE2	27:X:2686:C:O3'	2.28	0.64
27:X:542:A:OP1	27:X:570:G:N2	2.29	0.64
4:D:92:ARG:CZ	28:Y:47:A:H1'	2.27	0.64
17:R:90:LYS:HG3	17:R:108:VAL:HG21	1.79	0.64
27:X:1504:G:N2	27:X:1517:C:O2	2.31	0.64
9:J:84:MET:HG2	27:X:2229:G:H5'	1.80	0.64
9:J:15:ARG:HD3	9:J:74:PRO:HD2	1.79	0.64
12:M:103:LYS:HG2	27:X:2698:G:H4'	1.79	0.64
27:X:1882:G:H21	27:X:1885:C:H41	1.45	0.64
3:C:2:ALA:HA	3:C:13:ARG:HA	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2811:G:H2'	27:X:2812:A:H8	1.58	0.64
27:X:5:A:H2'	27:X:6:A:C8	2.33	0.64
5:E:8:PRO:HD2	5:E:69:ARG:HH11	1.62	0.63
2:B:14:ILE:HG12	12:M:20:HIS:CD2	2.29	0.63
6:G:70:PHE:HB3	13:N:64:ARG:HG2	1.78	0.63
2:B:92:ASN:HA	2:B:95:ILE:HB	1.78	0.63
5:E:90:ARG:HH21	5:E:163:ARG:HD2	1.64	0.63
16:Q:48:VAL:HG21	16:Q:82:LEU:HD13	1.79	0.63
27:X:619:A:N6	27:X:630:G:O2'	2.31	0.63
27:X:874:A:H2'	27:X:875:G:O4'	1.99	0.63
14:O:5:ILE:HG23	14:O:13:ARG:NH1	2.13	0.63
16:Q:88:ILE:HG13	16:Q:92:ALA:HB2	1.80	0.63
3:C:58:MET:HG2	3:C:59:TYR:CD1	2.33	0.63
1:A:159:ALA:HB3	27:X:1812:U:H3'	1.80	0.63
1:A:254:THR:OG1	27:X:1835:C:O2'	2.15	0.63
27:X:1827:G:H1	27:X:1888:C:H42	1.45	0.63
26:3:17:THR:HG22	26:3:21:LYS:H	1.62	0.63
7:H:123:PHE:HB3	7:H:126:ILE:HG13	1.80	0.63
27:X:1422:C:H2'	27:X:1423:A:H8	1.63	0.63
27:X:584:A:OP2	27:X:2038:C:N4	2.31	0.63
27:X:826:U:H2'	27:X:827:C:C6	2.33	0.63
27:X:1030:U:H2'	27:X:1032:A:H2	1.63	0.63
27:X:2039:G:C2	27:X:2040:A:C8	2.87	0.63
27:X:646:C:O2'	27:X:650:U:OP1	2.17	0.63
27:X:748:A:H5'	27:X:749:C:OP2	1.99	0.63
14:O:21:ARG:HH22	27:X:1005:U:H1'	1.64	0.62
19:T:51:VAL:HG21	19:T:79:ILE:HG22	1.80	0.62
27:X:1502:G:H22	27:X:1518:C:H42	1.46	0.62
27:X:1554:G:H2'	27:X:1555:A:H8	1.64	0.62
27:X:160:C:O2'	27:X:445:A:N3	2.28	0.62
28:Y:27:A:O2'	28:Y:28:A:O5'	2.17	0.62
8:I:61:PRO:HB2	26:3:30:ARG:HD3	1.80	0.62
4:D:16:LEU:O	4:D:20:PHE:N	2.27	0.62
6:G:119:LEU:HD12	6:G:122:HIS:HB2	1.80	0.62
15:P:70:LYS:NZ	27:X:500:G:O6	2.31	0.62
18:S:91:PRO:HD3	18:S:127:PRO:HD3	1.80	0.62
27:X:661:C:H2'	27:X:662:G:H8	1.62	0.62
28:Y:42:U:O2'	28:Y:47:A:N6	2.32	0.62
1:A:46:ARG:NE	27:X:1383:C:OP1	2.32	0.62
2:B:51:TYR:CE2	12:M:3:THR:HG21	2.33	0.62
27:X:2200:G:H2'	27:X:2201:G:H8	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:59:ARG:HB2	27:X:2371:A:H8	1.63	0.62
27:X:725:C:O2	27:X:732:G:N2	2.26	0.62
15:P:57:LEU:HD13	15:P:69:ALA:HA	1.82	0.62
8:I:59:ARG:HB2	27:X:2371:A:C8	2.34	0.62
27:X:2679:G:H1	27:X:2686:C:H42	1.48	0.62
27:X:772:G:H2'	27:X:773:G:H8	1.65	0.62
4:D:39:GLY:O	4:D:150:ARG:NH2	2.33	0.62
6:G:157:PRO:O	6:G:161:GLN:NE2	2.32	0.62
7:H:25:LEU:HD21	7:H:52:VAL:HG23	1.81	0.62
27:X:1919:A:N6	27:X:1946:U:H3	1.97	0.62
27:X:313:U:H2'	27:X:314:G:C8	2.35	0.62
5:E:45:GLN:NE2	5:E:48:ASP:O	2.32	0.62
27:X:588:G:O2'	27:X:2002:A:OP1	2.14	0.62
2:B:115:GLY:HA2	2:B:136:ARG:HD2	1.81	0.62
17:R:22:VAL:HG22	17:R:82:ALA:HA	1.81	0.62
27:X:1361:G:H1	27:X:1614:C:N4	1.97	0.62
8:I:102:LYS:O	8:I:104:ARG:N	2.32	0.62
20:U:53:GLU:HB3	20:U:58:LYS:H	1.65	0.62
23:Z:51:TYR:CE1	23:Z:55:ARG:HB2	2.35	0.62
19:T:41:ARG:NH2	27:X:2366:U:O2'	2.25	0.61
27:X:2617:G:N1	27:X:2755:A:H2'	2.15	0.61
4:D:4:LEU:HG	4:D:5:LYS:H	1.66	0.61
10:K:6:ALA:HB1	27:X:2848:A:H2	1.63	0.61
13:N:66:ASN:ND2	27:X:1021:A:OP1	2.33	0.61
27:X:2417:U:O2'	27:X:2419:C:OP1	2.16	0.61
1:A:252:LYS:NZ	1:A:252:LYS:H	1.97	0.61
4:D:106:ILE:HG21	4:D:139:PRO:HB3	1.81	0.61
5:E:86:ASN:HB2	5:E:165:VAL:HG13	1.82	0.61
15:P:25:PHE:HD1	15:P:130:ILE:HD11	1.66	0.61
27:X:1140:A:O2'	27:X:2494:C:O2'	2.15	0.61
27:X:605:G:H2'	27:X:606:A:H8	1.66	0.61
28:Y:78:A:H2'	28:Y:79:U:O4'	2.01	0.61
7:H:13:ASN:OD1	7:H:108:THR:N	2.32	0.61
12:M:18:GLN:HA	12:M:21:THR:HB	1.82	0.61
13:N:50:ARG:HA	13:N:53:LYS:HE2	1.83	0.61
27:X:1440:G:H5''	27:X:1441:A:H2'	1.83	0.61
27:X:2191:A:OP1	27:X:2193:C:N4	2.32	0.61
2:B:189:PRO:HA	27:X:2659:C:H5'	1.82	0.61
12:M:17:GLU:HG3	12:M:62:SER:H	1.65	0.61
14:O:36:LYS:HB2	14:O:51:ALA:HB1	1.82	0.61
27:X:165:G:H1	27:X:185:C:H42	1.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:ARG:HB3	27:X:1673:C:H5''	1.81	0.61
12:M:66:PHE:HB3	12:M:83:PHE:HE1	1.66	0.61
22:W:4:LYS:HG3	22:W:52:GLU:HB3	1.83	0.61
27:X:1070:G:H5''	27:X:1071:U:H2'	1.82	0.61
25:2:7:PRO:HB2	27:X:1322:G:H4'	1.81	0.61
1:A:246:PRO:HD3	1:A:252:LYS:HE3	1.82	0.61
6:G:35:LYS:N	6:G:69:ASP:OD2	2.34	0.61
13:N:5:LYS:HG2	13:N:7:GLY:H	1.64	0.61
20:U:51:ILE:HG23	20:U:59:THR:HA	1.82	0.61
21:V:15:ALA:HA	21:V:18:ILE:HD12	1.83	0.61
27:X:1514:C:H4'	27:X:1592:U:O2'	2.01	0.61
27:X:540:G:HO2'	27:X:542:A:H2	1.48	0.61
27:X:635:C:O2'	27:X:670:U:OP1	2.17	0.61
2:B:174:GLU:HB3	2:B:183:LEU:HD12	1.82	0.61
17:R:42:ARG:NH2	27:X:86:U:OP2	2.33	0.61
27:X:810:U:H2'	27:X:811:G:O4'	2.01	0.61
7:H:99:ILE:HD12	7:H:103:GLY:HA2	1.83	0.60
11:L:28:ARG:NH2	28:Y:10:U:O3'	2.34	0.60
20:U:49:LYS:HD3	20:U:61:TRP:CE2	2.36	0.60
27:X:2820:C:H2'	27:X:2821:G:C8	2.36	0.60
3:C:15:ILE:HD11	3:C:195:ILE:H	1.66	0.60
27:X:2591:C:H2'	27:X:2592:U:H5	1.65	0.60
7:H:47:VAL:HG23	7:H:77:THR:HG23	1.83	0.60
8:I:81:GLN:HB3	8:I:114:ILE:HG23	1.84	0.60
20:U:52:ARG:HD2	20:U:79:GLU:HA	1.82	0.60
27:X:1073:G:H22	27:X:1087:C:H42	1.48	0.60
27:X:1301:U:O2'	27:X:1664:G:N2	2.34	0.60
27:X:2191:A:H5''	27:X:2192:U:H5	1.66	0.60
11:L:50:THR:N	28:Y:116:C:O2'	2.33	0.60
8:I:62:LYS:HB3	26:3:12:ARG:HA	1.83	0.60
18:S:117:VAL:HB	18:S:168:VAL:HG22	1.82	0.60
27:X:2591:C:H2'	27:X:2592:U:C5	2.35	0.60
1:A:252:LYS:N	1:A:252:LYS:HZ2	1.99	0.60
4:D:45:GLU:OE1	4:D:78:LYS:NZ	2.30	0.60
5:E:103:LEU:HD23	5:E:115:ILE:HD12	1.83	0.60
13:N:13:ARG:NH1	27:X:1264:C:H5''	2.17	0.60
27:X:482:A:H2'	27:X:483:A:O4'	2.02	0.60
27:X:623:G:C2	27:X:624:A:H1'	2.37	0.60
2:B:169:ASN:HD21	2:B:204:ALA:HB2	1.66	0.60
16:Q:13:SER:OG	16:Q:14:GLU:N	2.32	0.60
18:S:28:ASN:OD1	18:S:28:ASN:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1430:G:H1	27:X:1598:C:H42	1.50	0.60
15:P:118:ASN:HA	27:X:1996:A:O2'	2.01	0.60
28:Y:3:A:N6	28:Y:121:G:O6	2.34	0.60
1:A:68:LYS:H	1:A:68:LYS:HD3	1.67	0.60
2:B:52:ALA:O	2:B:76:ARG:N	2.25	0.60
3:C:71:ASP:OD1	3:C:72:ARG:N	2.34	0.60
7:H:11:ALA:O	7:H:111:PHE:N	2.30	0.60
9:J:6:LYS:HB3	9:J:45:SER:HB2	1.84	0.60
18:S:26:LYS:HG3	18:S:27:GLU:HG3	1.83	0.60
27:X:663:G:H3'	27:X:664:C:H5''	1.84	0.60
3:C:48:ARG:HB2	3:C:50:GLN:HB3	1.82	0.60
7:H:9:ASP:O	7:H:96:ALA:N	2.34	0.60
27:X:1451:C:H2'	27:X:1452:U:H6	1.67	0.60
27:X:615:C:O2	27:X:670:U:O2'	2.17	0.60
26:3:17:THR:HG23	26:3:19:THR:H	1.67	0.60
2:B:105:THR:HB	2:B:166:THR:HG23	1.84	0.60
3:C:158:ARG:HB3	3:C:169:VAL:HG11	1.83	0.60
6:G:62:ILE:O	6:G:77:GLY:HA3	2.02	0.60
4:D:133:LYS:HE2	27:X:2284:U:H4'	1.83	0.60
27:X:2707:G:H2'	27:X:2708:U:C6	2.36	0.60
1:A:63:ARG:HE	1:A:85:ASP:HB3	1.67	0.60
12:M:3:THR:HG22	12:M:5:ILE:HG13	1.84	0.60
12:M:27:PHE:HA	12:M:96:ARG:NH2	2.16	0.60
27:X:1350:G:H2'	27:X:1351:G:H8	1.66	0.60
27:X:13:A:O2'	27:X:15:G:N7	2.35	0.60
27:X:2767:C:HO2'	27:X:2785:A:HO2'	1.49	0.60
10:K:10:LEU:HD11	10:K:17:ARG:HE	1.66	0.59
18:S:71:MET:HA	18:S:78:PRO:HA	1.84	0.59
27:X:1777:A:H1'	27:X:1921:A:N6	2.17	0.59
27:X:2330:G:H21	27:X:2345:A:H62	1.50	0.59
4:D:171:GLN:HE21	4:D:177:PHE:HE1	1.49	0.59
27:X:1997:A:H2'	27:X:1998:A:C8	2.37	0.59
27:X:2279:G:N2	27:X:2295:C:O2	2.33	0.59
27:X:242:A:N6	27:X:441:A:N7	2.50	0.59
4:D:112:ARG:NH2	4:D:134:GLU:OE2	2.35	0.59
4:D:70:ALA:HB3	4:D:82:GLY:HA2	1.83	0.59
13:N:93:LYS:HE3	14:O:6:GLN:HG3	1.84	0.59
14:O:85:GLY:O	27:X:1237:G:H4'	2.02	0.59
28:Y:7:C:O2'	28:Y:29:C:O2	2.14	0.59
1:A:163:VAL:HG22	1:A:177:LEU:HA	1.84	0.59
2:B:136:ARG:HD3	27:X:1673:C:H5'	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:20:ARG:HD2	13:N:39:LEU:HD13	1.84	0.59
27:X:2174:G:H2'	27:X:2175:A:H8	1.68	0.59
8:I:26:THR:OG1	27:X:676:G:OP1	2.15	0.59
25:2:3:ARG:O	25:2:6:GLN:NE2	2.30	0.59
2:B:56:GLU:HG2	2:B:74:PRO:HG3	1.83	0.59
27:X:721:C:H42	27:X:736:G:H1	1.51	0.59
8:I:30:ALA:CA	27:X:824:U:H2'	2.33	0.59
1:A:168:LYS:HD3	1:A:173:VAL:HG22	1.83	0.59
2:B:60:ASN:HB3	2:B:62:PRO:HD2	1.85	0.59
5:E:22:GLY:HA3	5:E:39:THR:HG22	1.85	0.59
7:H:2:ILE:HD12	7:H:8:LEU:HD21	1.85	0.59
14:O:70:TYR:OH	27:X:1236:G:O6	2.21	0.59
27:X:1563:U:H2'	27:X:1564:U:C6	2.38	0.59
27:X:2837:G:H2'	27:X:2838:U:H6	1.67	0.59
5:E:107:ILE:HD11	5:E:151:VAL:HG12	1.85	0.59
17:R:107:ALA:HB2	17:R:111:GLY:HA2	1.83	0.59
27:X:2283:G:H1	27:X:2291:U:H3	1.51	0.59
27:X:711:C:O2'	27:X:747:A:N6	2.36	0.59
27:X:1141:U:O5'	27:X:1141:U:H6	1.86	0.59
27:X:1479:G:H2'	27:X:1480:G:C8	2.38	0.59
24:1:14:SER:HB2	24:1:23:THR:H	1.68	0.59
16:Q:26:SER:HB3	16:Q:79:ILE:HG12	1.85	0.59
27:X:1937:G:O2'	27:X:1939:U:O4	2.14	0.59
2:B:128:SER:OG	27:X:1976:U:O3'	2.21	0.59
27:X:2849:C:H2'	27:X:2850:U:H6	1.68	0.59
1:A:172:TYR:HA	1:A:186:HIS:HA	1.84	0.59
2:B:121:ASN:O	2:B:122:PHE:HB2	2.03	0.59
13:N:49:ASP:HA	13:N:52:ASN:HB2	1.85	0.59
3:C:48:ARG:NE	3:C:51:VAL:HG22	2.18	0.58
3:C:68:ARG:NH1	27:X:687:G:H1'	2.18	0.58
10:K:79:VAL:HA	10:K:83:VAL:HB	1.85	0.58
15:P:30:TYR:O	15:P:123:ARG:NE	2.27	0.58
27:X:2201:G:H2'	27:X:2202:G:H8	1.68	0.58
2:B:5:LEU:HD22	2:B:195:LEU:HD11	1.85	0.58
27:X:139:A:H2'	27:X:140:G:H8	1.68	0.58
27:X:1854:G:H2'	27:X:1855:G:H8	1.69	0.58
27:X:2522:G:H2'	27:X:2523:G:C8	2.38	0.58
2:B:133:LYS:HG3	2:B:137:ARG:HB3	1.85	0.58
2:B:76:ARG:HH22	27:X:2805:G:P	2.25	0.58
10:K:10:LEU:HD23	10:K:13:ASN:O	2.03	0.58
17:R:26:SER:OG	17:R:27:GLY:N	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:SER:CB	27:X:1976:U:H4'	2.34	0.58
13:N:24:PHE:CE1	27:X:543:G:H5'	2.38	0.58
1:A:245:VAL:HB	1:A:249:PRO:HA	1.85	0.58
20:U:51:ILE:HG12	20:U:59:THR:HB	1.84	0.58
27:X:154:U:H3'	27:X:155:G:H8	1.68	0.58
27:X:1785:A:H2'	27:X:1786:C:H6	1.66	0.58
4:D:122:PHE:HA	27:X:2282:G:H4'	1.85	0.58
1:A:16:MET:SD	1:A:17:THR:N	2.74	0.58
17:R:84:VAL:HG21	17:R:89:GLY:HA2	1.85	0.58
27:X:1210:C:H2'	27:X:1211:G:H8	1.68	0.58
27:X:1468:A:H8	27:X:1468:A:O5'	1.87	0.58
27:X:500:G:C2	27:X:501:G:H1'	2.39	0.58
1:A:76:ASN:ND2	1:A:118:ASN:OD1	2.37	0.58
6:G:61:ARG:NH1	6:G:65:LYS:HB3	2.19	0.58
7:H:75:VAL:HG22	7:H:96:ALA:HA	1.84	0.58
9:J:61:ARG:HB3	18:S:175:ARG:H	1.69	0.58
27:X:1554:G:H2'	27:X:1555:A:C8	2.38	0.58
27:X:2245:A:H4'	27:X:2246:A:N3	2.18	0.58
10:K:68:GLN:HG2	27:X:2686:C:O2'	2.04	0.58
27:X:312:G:HO2'	27:X:313:U:H6	1.52	0.58
1:A:252:LYS:HZ2	1:A:253:PRO:HD2	1.67	0.58
27:X:1019:U:O2'	27:X:1020:A:O5'	2.19	0.58
27:X:1501:C:H42	27:X:1519:G:H1	1.50	0.58
27:X:1140:A:HO2'	27:X:2494:C:HO2'	1.42	0.58
4:D:64:LYS:O	28:Y:44:C:O2'	2.20	0.58
27:X:1919:A:H2	27:X:1926:U:H3	1.52	0.58
2:B:176:ARG:HH21	12:M:16:ILE:CG2	2.17	0.58
6:G:103:TYR:CD2	6:G:111:LYS:HB2	2.39	0.58
6:G:84:ASN:O	6:G:152:ALA:HA	2.03	0.58
13:N:37:GLN:HB3	27:X:1265:G:H1	1.69	0.58
27:X:712:A:H2'	27:X:713:G:O4'	2.04	0.58
12:M:7:ILE:HD12	12:M:8:ASN:H	1.68	0.58
27:X:163:A:H2'	27:X:164:G:C8	2.39	0.58
27:X:2006:G:H5'	27:X:2596:C:H4'	1.85	0.58
27:X:670:U:H2'	27:X:671:A:C8	2.38	0.58
27:X:70:A:H4'	27:X:71:A:H5"	1.85	0.58
19:T:72:LYS:HD3	28:Y:14:C:H5"	1.85	0.57
19:T:68:VAL:HB	19:T:80:SER:HB2	1.86	0.57
27:X:1699:A:H61	27:X:1723:U:H3	1.52	0.57
27:X:2492:G:C2	27:X:2493:U:C2	2.92	0.57
27:X:222:G:O2'	27:X:397:U:O2	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:15:LYS:O	26:3:23:MET:N	2.35	0.57
3:C:176:ASN:HB3	3:C:179:ASP:H	1.68	0.57
8:I:73:GLU:HG3	8:I:101:ARG:HG3	1.84	0.57
15:P:95:ALA:HB2	15:P:129:ILE:HG23	1.86	0.57
27:X:1443:G:H2'	27:X:1444:C:C6	2.39	0.57
27:X:1454:U:H2'	27:X:1455:C:C6	2.40	0.57
6:G:69:ASP:H	6:G:76:GLN:HE22	1.51	0.57
9:J:15:ARG:HH21	9:J:73:LYS:HZ2	1.51	0.57
2:B:143:GLN:O	27:X:2035:G:H4'	2.03	0.57
27:X:2594:U:H2'	27:X:2595:C:H6	1.69	0.57
4:D:60:ILE:HG13	4:D:61:THR:HG23	1.86	0.57
5:E:6:LYS:HB2	5:E:69:ARG:HG3	1.85	0.57
11:L:32:TYR:CZ	11:L:34:SER:HB3	2.39	0.57
18:S:3:LEU:HD23	18:S:56:VAL:HG13	1.86	0.57
3:C:69:HIS:HE2	27:X:1270:C:P	2.27	0.57
27:X:346:C:H2'	27:X:347:C:C6	2.40	0.57
28:Y:17:A:H1'	28:Y:112:A:C8	2.39	0.57
1:A:158:SER:OG	1:A:159:ALA:N	2.35	0.57
19:T:74:LYS:C	19:T:76:ALA:H	2.07	0.57
27:X:1310:C:H2'	27:X:1311:C:C6	2.39	0.57
27:X:1342:U:H5''	27:X:1343:C:C5	2.37	0.57
27:X:303:C:H3'	27:X:304:A:H5''	1.86	0.57
13:N:105:ALA:HB2	14:O:45:THR:HG21	1.86	0.57
13:N:78:THR:HG23	13:N:117:ARG:CZ	2.34	0.57
27:X:1422:C:H2'	27:X:1423:A:C8	2.38	0.57
27:X:2528:G:H2'	27:X:2529:G:H8	1.69	0.57
27:X:2570:C:H2'	27:X:2571:G:C8	2.40	0.57
17:R:92:THR:O	17:R:92:THR:OG1	2.21	0.57
27:X:1185:C:H2'	27:X:1186:G:H2'	1.85	0.57
27:X:1373:G:N2	27:X:2192:U:H3	2.03	0.57
27:X:2493:U:H2'	27:X:2494:C:C6	2.40	0.57
27:X:554:U:H5''	27:X:556:A:C2	2.39	0.57
27:X:751:G:H2'	27:X:752:G:C8	2.40	0.57
24:I:16:ALA:HB2	24:I:50:PHE:CZ	2.40	0.57
6:G:132:PHE:HZ	6:G:142:ARG:HA	1.70	0.57
10:K:32:GLY:HA2	10:K:115:LEU:HD12	1.86	0.57
22:W:3:ILE:HD11	22:W:44:VAL:HG11	1.86	0.57
27:X:1645:U:H2'	27:X:1646:G:C8	2.40	0.57
9:J:81:GLU:HB2	27:X:2473:G:O2'	2.05	0.57
27:X:2590:U:H1'	30:X:2902:ERY:H361	1.85	0.57
27:X:772:G:H2'	27:X:773:G:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:859:U:H3	27:X:944:A:N6	2.03	0.57
27:X:992:A:N1	27:X:2010:G:O2'	2.32	0.57
1:A:223:GLY:HA2	1:A:226:MET:HG3	1.87	0.57
1:A:252:LYS:O	27:X:1787:U:O2'	2.22	0.57
2:B:136:ARG:HB3	27:X:1673:C:C5'	2.34	0.57
10:K:76:VAL:HA	10:K:79:VAL:HG12	1.87	0.57
10:K:87:TYR:CE1	10:K:94:TYR:HD1	2.23	0.57
18:S:64:ALA:HB2	18:S:85:MET:HG2	1.86	0.57
27:X:82:G:H1	27:X:100:G:HO2'	1.52	0.57
27:X:436:A:H5''	27:X:437:G:H5''	1.85	0.57
27:X:638:A:H4'	27:X:639:G:H5'	1.86	0.57
1:A:89:SER:C	1:A:198:ASN:HD21	2.08	0.56
27:X:1333:G:N7	27:X:1342:U:H5'	2.20	0.56
27:X:1455:C:H2'	27:X:1456:C:H6	1.70	0.56
27:X:1774:A:H5'	27:X:2587:G:H4'	1.87	0.56
27:X:1982:C:H5''	27:X:2703:C:O2'	2.05	0.56
8:I:30:ALA:HA	27:X:824:U:H2'	1.87	0.56
9:J:26:ASP:OD1	9:J:27:TYR:N	2.38	0.56
12:M:17:GLU:OE2	12:M:63:ARG:NH2	2.31	0.56
13:N:13:ARG:HH12	27:X:1264:C:H5''	1.70	0.56
27:X:1033:G:H22	27:X:1153:A:H2	1.53	0.56
27:X:2025:A:H5''	27:X:2026:C:OP2	2.05	0.56
27:X:2085:G:H22	27:X:2171:U:H1'	1.69	0.56
27:X:2222:U:H2'	27:X:2223:U:C6	2.39	0.56
27:X:2336:G:N2	27:X:2339:A:OP2	2.38	0.56
27:X:2708:U:H2'	27:X:2709:C:H6	1.70	0.56
27:X:2736:U:H1'	27:X:2737:A:H5''	1.87	0.56
27:X:2763:U:H2'	27:X:2764:U:H6	1.70	0.56
9:J:86:LYS:O	9:J:88:LYS:HE3	2.05	0.56
27:X:1017:C:H2'	27:X:1018:C:C6	2.40	0.56
27:X:1830:C:N4	27:X:1882:G:OP2	2.39	0.56
27:X:540:G:C6	27:X:2005:U:H5''	2.40	0.56
27:X:726:G:H21	27:X:731:A:H2	1.53	0.56
4:D:13:ARG:HG3	4:D:28:VAL:HG11	1.87	0.56
9:J:26:ASP:H	9:J:103:VAL:HG12	1.70	0.56
12:M:22:ARG:HB2	12:M:84:ALA:HB2	1.87	0.56
19:T:21:LEU:HD11	19:T:41:ARG:HG2	1.87	0.56
20:U:63:SER:O	20:U:67:LEU:N	2.38	0.56
27:X:1327:C:N4	27:X:1351:G:H1	2.02	0.56
1:A:43:ARG:NH1	27:X:704:G:O2'	2.39	0.56
2:B:87:ASP:OD2	2:B:87:ASP:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:22:ARG:NH1	12:M:83:PHE:O	2.39	0.56
27:X:705:C:O2'	27:X:1367:A:O2'	2.21	0.56
27:X:1674:C:H2'	27:X:1675:C:C6	2.41	0.56
27:X:2431:C:H2'	27:X:2432:A:C8	2.40	0.56
27:X:2871:U:H2'	27:X:2872:U:C6	2.40	0.56
15:P:117:ALA:HB3	27:X:1997:A:H5''	1.87	0.56
15:P:117:ALA:O	15:P:118:ASN:ND2	2.38	0.56
27:X:2174:G:H2'	27:X:2175:A:C8	2.41	0.56
2:B:176:ARG:NH2	12:M:16:ILE:HG23	2.18	0.56
3:C:54:THR:HG21	3:C:72:ARG:HB2	1.88	0.56
13:N:104:GLU:OE2	13:N:104:GLU:N	2.37	0.56
10:K:7:GLY:N	27:X:2848:A:N3	2.52	0.56
17:R:54:ILE:HG12	17:R:71:GLN:HG3	1.86	0.56
27:X:1467:U:C6	27:X:1468:A:H5'	2.41	0.56
27:X:2492:G:H2'	27:X:2493:U:C6	2.40	0.56
27:X:597:U:H2'	27:X:598:U:C6	2.41	0.56
12:M:28:ARG:HB2	12:M:29:PRO:HD3	1.87	0.56
27:X:1174:G:H2'	27:X:1175:A:H8	1.71	0.56
27:X:75:C:H2'	27:X:76:C:C6	2.41	0.56
24:1:12:MET:HB2	24:1:27:ASN:ND2	2.21	0.56
24:1:9:ILE:HA	24:1:28:ARG:HA	1.87	0.56
15:P:44:VAL:HG11	23:Z:27:ALA:HB2	1.86	0.56
27:X:1501:C:H2'	27:X:1502:G:O4'	2.06	0.56
27:X:388:G:H2'	27:X:389:G:C8	2.41	0.56
28:Y:51:G:H2'	28:Y:52:G:C8	2.38	0.56
1:A:43:ARG:HH21	1:A:55:GLY:HA2	1.71	0.55
7:H:117:GLU:O	7:H:120:ASP:HB2	2.05	0.55
21:V:23:LYS:O	21:V:27:GLU:HG2	2.06	0.55
2:B:143:GLN:NE2	2:B:151:TYR:OH	2.39	0.55
3:C:152:THR:OG1	3:C:153:ASP:O	2.22	0.55
3:C:144:GLY:HA3	3:C:166:TRP:CD1	2.42	0.55
13:N:58:ARG:O	13:N:62:ILE:HG13	2.07	0.55
27:X:1795:C:H2'	27:X:1796:A:H8	1.71	0.55
25:2:39:ARG:O	27:X:469:G:H3'	2.07	0.55
6:G:132:PHE:CZ	6:G:142:ARG:HA	2.41	0.55
23:Z:42:SER:O	23:Z:44:HIS:HD2	1.88	0.55
25:2:1:MET:HB3	25:2:3:ARG:HH12	1.71	0.55
17:R:16:PHE:CZ	17:R:46:VAL:HG22	2.42	0.55
27:X:1918:G:H1'	27:X:1947:G:N2	2.22	0.55
27:X:388:G:H2'	27:X:389:G:H8	1.72	0.55
27:X:533:C:O2	27:X:563:U:O2'	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:30:ASN:ND2	27:X:2264:C:OP2	2.40	0.55
6:G:151:TYR:CE1	6:G:160:ALA:HB3	2.41	0.55
17:R:83:LEU:HD13	17:R:113:THR:HB	1.87	0.55
18:S:3:LEU:HB3	18:S:56:VAL:HA	1.88	0.55
27:X:1336:G:H2'	27:X:1337:G:H5'	1.88	0.55
27:X:1348:C:H2'	27:X:1349:A:C8	2.41	0.55
1:A:28:ARG:HD2	27:X:1583:A:N6	2.22	0.55
2:B:4:ILE:HD13	2:B:28:ALA:HB1	1.88	0.55
15:P:90:LEU:HD22	15:P:131:VAL:HG12	1.88	0.55
17:R:11:ASN:ND2	17:R:11:ASN:O	2.36	0.55
27:X:1825:C:O2'	27:X:1952:A:N1	2.33	0.55
27:X:542:A:O2'	27:X:543:G:OP1	2.25	0.55
1:A:48:ARG:H	1:A:48:ARG:HD2	1.72	0.55
2:B:146:THR:OG1	27:X:2550:C:O2'	2.00	0.55
27:X:2828:C:H2'	27:X:2829:A:H8	1.71	0.55
15:P:27:VAL:HG13	27:X:504:G:H4'	1.88	0.55
28:Y:39:C:N4	28:Y:51:G:O4'	2.40	0.55
3:C:48:ARG:HB2	3:C:50:GLN:H	1.72	0.55
4:D:123:ASP:HB3	4:D:127:ASN:H	1.71	0.55
10:K:96:ARG:NE	27:X:2857:C:OP1	2.39	0.55
15:P:47:GLY:H	15:P:92:VAL:HG23	1.71	0.55
27:X:1480:G:C2	27:X:1481:U:O2	2.59	0.55
13:N:54:LYS:NZ	27:X:1006:C:OP2	2.40	0.55
14:O:12:TYR:HD2	14:O:40:VAL:HB	1.72	0.55
18:S:168:VAL:HG12	18:S:169:VAL:HG23	1.89	0.55
27:X:2594:U:H2'	27:X:2595:C:C6	2.42	0.55
27:X:2856:U:H2'	27:X:2857:C:C6	2.41	0.55
1:A:60:ARG:HD3	1:A:86:PRO:HB2	1.89	0.54
11:L:8:ARG:HG3	11:L:9:ARG:H	1.71	0.54
19:T:40:GLN:HE22	19:T:43:THR:HA	1.71	0.54
14:O:83:ARG:NH2	27:X:1239:A:OP1	2.40	0.54
27:X:2235:G:N2	27:X:2254:C:C4	2.75	0.54
27:X:2860:C:H2'	27:X:2861:A:O4'	2.07	0.54
2:B:118:LYS:HG2	2:B:160:MET:SD	2.48	0.54
2:B:104:ALA:HB3	2:B:170:LEU:HD12	1.88	0.54
3:C:66:ASN:HA	27:X:1268:U:H2'	1.89	0.54
4:D:130:LEU:HD13	4:D:131:GLY:H	1.71	0.54
4:D:74:ILE:HA	4:D:79:LEU:HB3	1.89	0.54
27:X:1412:C:O2'	27:X:1413:U:O5'	2.25	0.54
27:X:1454:U:H3	27:X:1567:A:H61	1.53	0.54
27:X:188:G:H2'	27:X:189:A:C8	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:228:A:C5	27:X:229:G:H1'	2.42	0.54
28:Y:58:G:H4'	28:Y:59:A:O5'	2.07	0.54
1:A:44:ASN:HB3	1:A:49:ILE:HA	1.89	0.54
5:E:86:ASN:HB3	5:E:130:ARG:HH21	1.72	0.54
13:N:93:LYS:HB3	27:X:1007:A:H4'	1.89	0.54
27:X:1919:A:H2	27:X:1926:U:N3	2.04	0.54
27:X:1279:G:O2'	27:X:1995:G:O6	2.11	0.54
27:X:540:G:N1	27:X:2005:U:OP1	2.40	0.54
27:X:946:U:H2'	27:X:947:C:H6	1.72	0.54
1:A:146:GLU:HB2	1:A:189:CYS:HB3	1.88	0.54
1:A:93:ALA:HB2	1:A:107:ALA:HB2	1.88	0.54
3:C:129:LYS:C	3:C:131:LYS:H	2.11	0.54
3:C:65:GLY:HA3	27:X:2042:A:H5''	1.90	0.54
27:X:2384:G:N2	27:X:2390:A:N7	2.56	0.54
23:Z:51:TYR:CE1	23:Z:55:ARG:HD3	2.43	0.54
1:A:27:LYS:HZ3	1:A:29:PRO:HB3	1.72	0.54
12:M:29:PRO:HB3	12:M:99:VAL:HG12	1.90	0.54
15:P:13:GLN:O	15:P:17:GLN:HG2	2.07	0.54
27:X:1673:C:H2'	27:X:1674:C:C6	2.38	0.54
27:X:1785:A:H2'	27:X:1786:C:C6	2.42	0.54
27:X:219:G:N2	27:X:231:G:H2'	2.23	0.54
27:X:627:A:H2'	27:X:628:A:C8	2.43	0.54
27:X:825:C:H5''	27:X:1263:G:O2'	2.07	0.54
28:Y:27:A:N6	28:Y:56:G:OP2	2.41	0.54
11:L:32:TYR:CE2	28:Y:9:G:H5'	2.43	0.54
15:P:116:SER:OG	15:P:117:ALA:N	2.40	0.54
27:X:317:U:O2'	27:X:1224:A:N7	2.40	0.54
27:X:1787:U:H2'	27:X:1788:C:C6	2.43	0.54
27:X:1827:G:H1'	27:X:1914:U:C2	2.43	0.54
27:X:1991:C:H2'	27:X:1992:G:H8	1.72	0.54
27:X:1141:U:O2	27:X:2008:C:H5''	2.08	0.54
27:X:963:G:H1	27:X:976:C:H42	1.56	0.54
25:2:12:ARG:NH2	25:2:46:ASP:O	2.36	0.54
2:B:62:PRO:O	27:X:2766:U:O2'	2.22	0.54
4:D:17:MET:HA	4:D:21:GLY:H	1.72	0.54
27:X:1790:G:H5'	27:X:1811:A:N6	2.23	0.54
27:X:2054:A:H2'	27:X:2055:G:H8	1.71	0.54
27:X:838:A:H4'	27:X:2407:G:C5	2.42	0.54
27:X:490:A:H1'	27:X:491:A:H5'	1.89	0.54
27:X:653:G:H2'	27:X:654:A:H5''	1.89	0.54
25:2:26:SER:O	25:2:30:ILE:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:48:ARG:HD2	3:C:50:GLN:HB3	1.90	0.54
14:O:5:ILE:HG23	14:O:13:ARG:HH12	1.73	0.54
27:X:2705:A:H1'	27:X:2706:U:H2'	1.89	0.54
27:X:343:A:H1'	27:X:346:C:H41	1.73	0.54
15:P:19:LYS:NZ	27:X:507:A:OP2	2.23	0.54
27:X:684:C:H2'	27:X:685:U:C6	2.42	0.54
5:E:44:ARG:HH22	5:E:51:LEU:HB3	1.72	0.54
15:P:97:VAL:HG22	15:P:127:ILE:HA	1.90	0.54
27:X:1484:G:H2'	27:X:1485:U:C6	2.43	0.54
27:X:2791:C:O2'	27:X:2792:C:H5'	2.08	0.54
24:1:33:ALA:O	24:1:34:LYS:HD2	2.08	0.54
1:A:61:LEU:HG	27:X:1584:G:H5''	1.90	0.54
3:C:74:VAL:HG23	3:C:76:THR:H	1.72	0.54
27:X:1296:G:H22	27:X:1299:A:H5'	1.73	0.54
27:X:1974:U:H2'	27:X:1975:G:H5''	1.90	0.54
27:X:805:G:O2'	27:X:2419:C:N3	2.35	0.54
27:X:2707:G:H2'	27:X:2708:U:H6	1.72	0.54
27:X:774:A:H8	27:X:774:A:O5'	1.90	0.54
27:X:946:U:H2'	27:X:947:C:C6	2.43	0.54
3:C:48:ARG:O	3:C:51:VAL:HG23	2.07	0.53
8:I:62:LYS:H	26:3:12:ARG:HG3	1.72	0.53
3:C:67:ALA:HB2	15:P:112:ARG:HH22	1.73	0.53
17:R:56:LYS:HD3	17:R:69:GLN:HE21	1.73	0.53
13:N:93:LYS:HB3	27:X:1007:A:O3'	2.08	0.53
27:X:171:G:H2'	27:X:172:A:O4'	2.08	0.53
27:X:2378:G:H1	27:X:2396:C:H42	1.56	0.53
27:X:2555:G:N2	27:X:2555:G:OP2	2.41	0.53
27:X:455:A:H2	27:X:1258:G:N3	2.06	0.53
5:E:160:LYS:HZ1	27:X:2637:C:H5'	1.72	0.53
20:U:21:ARG:HH12	27:X:400:U:H2'	1.74	0.53
3:C:50:GLN:HE22	3:C:56:ARG:HH12	1.56	0.53
25:2:19:ARG:HG2	27:X:123:A:C5'	2.36	0.53
27:X:1374:G:N2	27:X:1384:G:H1'	2.23	0.53
27:X:2241:U:H2'	27:X:2242:C:C6	2.38	0.53
2:B:118:LYS:NZ	27:X:2704:U:OP1	2.24	0.53
4:D:75:SER:H	4:D:79:LEU:HD12	1.73	0.53
10:K:40:LYS:NZ	27:X:1290:A:OP1	2.42	0.53
27:X:1854:G:H2'	27:X:1855:G:C8	2.44	0.53
27:X:2374:C:H42	27:X:2400:G:H1	1.56	0.53
27:X:2572:U:H3	27:X:2579:A:H61	1.57	0.53
10:K:14:SER:HB3	27:X:2693:U:OP1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:41:GLN:NE2	27:X:470:U:OP1	2.36	0.53
27:X:75:C:H2'	27:X:76:C:H6	1.73	0.53
8:I:89:ASP:HB2	8:I:120:VAL:HG13	1.90	0.53
17:R:52:ASN:HA	17:R:74:LEU:H	1.72	0.53
18:S:68:ALA:HB3	18:S:82:ASP:HB2	1.91	0.53
27:X:1714:A:OP2	27:X:1715:A:O2'	2.26	0.53
27:X:605:G:H2'	27:X:606:A:C8	2.44	0.53
27:X:978:U:H2'	27:X:979:A:C8	2.43	0.53
26:3:15:LYS:HZ3	26:3:60:LEU:HD11	1.73	0.53
3:C:106:MET:O	3:C:110:SER:OG	2.19	0.53
3:C:148:VAL:HB	3:C:167:VAL:HG12	1.91	0.53
5:E:155:ASP:N	5:E:155:ASP:OD1	2.36	0.53
10:K:81:ASP:O	10:K:85:PRO:HG2	2.09	0.53
13:N:84:LYS:HB2	13:N:92:ARG:HH12	1.74	0.53
18:S:6:LYS:HD3	18:S:32:PHE:HD2	1.73	0.53
1:A:50:THR:HG21	27:X:1805:G:N3	2.24	0.53
17:R:26:SER:HB2	27:X:321:A:H5''	1.90	0.53
27:X:538:A:H62	27:X:2026:C:C5'	2.16	0.53
28:Y:16:U:H1'	28:Y:109:G:H21	1.74	0.53
6:G:132:PHE:CE2	6:G:145:HIS:HB2	2.44	0.53
15:P:122:LYS:HB3	15:P:124:THR:HG23	1.90	0.53
27:X:1184:G:H1	27:X:1190:C:H42	1.57	0.53
27:X:542:A:H62	27:X:2002:A:H2	1.55	0.53
27:X:746:G:OP2	27:X:774:A:N6	2.32	0.53
1:A:25:THR:HG22	1:A:26:LYS:H	1.74	0.53
1:A:28:ARG:HD3	1:A:84:TYR:HB3	1.90	0.53
3:C:112:GLN:HE22	3:C:116:LYS:HG3	1.73	0.53
9:J:44:LYS:HA	9:J:95:VAL:HG12	1.91	0.53
11:L:91:ARG:HG2	11:L:92:GLY:O	2.08	0.53
12:M:63:ARG:HD3	27:X:2661:G:H4'	1.90	0.53
27:X:2870:C:H2'	27:X:2871:U:C6	2.44	0.53
27:X:746:G:N7	27:X:774:A:C5	2.76	0.53
1:A:186:HIS:HB2	1:A:188:GLU:HG2	1.91	0.53
27:X:2083:G:H1	27:X:2172:U:H3	1.56	0.53
27:X:2633:A:N1	27:X:2644:A:H5''	2.23	0.53
27:X:5:A:H2'	27:X:6:A:H8	1.71	0.53
28:Y:7:C:H2'	28:Y:8:C:H6	1.74	0.53
1:A:108:PRO:HB3	1:A:143:HIS:CE1	2.45	0.52
1:A:254:THR:HG1	27:X:1835:C:HO2'	1.56	0.52
5:E:7:GLN:N	5:E:7:GLN:OE1	2.42	0.52
6:G:100:TYR:HB2	6:G:116:ARG:HH11	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:24:GLY:O	15:P:130:ILE:HA	2.09	0.52
27:X:1348:C:H2'	27:X:1349:A:H8	1.73	0.52
27:X:754:G:H2'	27:X:755:C:H6	1.74	0.52
13:N:39:LEU:HA	13:N:42:ALA:HB3	1.92	0.52
27:X:2245:A:H4'	27:X:2246:A:C2	2.44	0.52
24:1:7:ARG:NH2	27:X:2262:C:OP1	2.42	0.52
27:X:88:G:H3'	27:X:89:A:H5''	1.91	0.52
26:3:6:THR:OG1	26:3:7:HIS:N	2.42	0.52
1:A:91:ARG:NH1	1:A:109:GLU:OE1	2.43	0.52
9:J:83:ARG:HH22	27:X:971:A:N6	1.99	0.52
21:V:28:LEU:HD21	21:V:42:ARG:HG2	1.91	0.52
21:V:7:ARG:HB2	21:V:60:LEU:HD11	1.91	0.52
27:X:1250:A:H5'	27:X:1250:A:H8	1.73	0.52
27:X:1744:G:N2	27:X:1746:A:H3'	2.25	0.52
27:X:2837:G:H2'	27:X:2838:U:C6	2.45	0.52
27:X:2856:U:H2'	27:X:2857:C:H6	1.74	0.52
27:X:732:G:H2'	27:X:733:G:H8	1.74	0.52
27:X:872:G:OP2	27:X:872:G:H8	1.91	0.52
27:X:90:G:H3'	27:X:91:A:C8	2.45	0.52
1:A:108:PRO:HB3	1:A:143:HIS:HE1	1.75	0.52
15:P:104:LYS:HE2	15:P:119:ILE:HD12	1.90	0.52
18:S:74:ARG:HH22	28:Y:94:G:H5''	1.75	0.52
27:X:1333:G:N2	27:X:1344:C:H41	2.08	0.52
27:X:1556:A:H2'	27:X:1557:G:H8	1.74	0.52
27:X:2014:A:C6	27:X:2477:C:H1'	2.44	0.52
1:A:212:SER:O	1:A:215:LEU:HD12	2.10	0.52
11:L:89:PHE:O	11:L:91:ARG:NH2	2.43	0.52
17:R:51:VAL:HG12	17:R:74:LEU:HD21	1.91	0.52
19:T:23:VAL:HB	19:T:26:PHE:HE2	1.74	0.52
19:T:64:ASP:N	19:T:64:ASP:OD1	2.41	0.52
27:X:2062:U:H2'	27:X:2063:A:C8	2.45	0.52
1:A:227:ASN:ND2	27:X:797:A:H5''	2.24	0.52
28:Y:64:C:H2'	28:Y:65:A:H8	1.75	0.52
2:B:120:TRP:CD2	2:B:155:ARG:HD2	2.44	0.52
5:E:76:VAL:HA	5:E:79:VAL:HG22	1.91	0.52
10:K:45:ARG:HD3	10:K:95:THR:HG22	1.91	0.52
16:Q:71:GLN:NE2	27:X:64:C:OP1	2.42	0.52
28:Y:36:A:H61	28:Y:46:G:H2'	1.74	0.52
1:A:48:ARG:HB2	27:X:792:U:P	2.49	0.52
2:B:55:ALA:HB3	2:B:58:LYS:HD2	1.92	0.52
9:J:15:ARG:NH2	9:J:73:LYS:HZ2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:5:ILE:HD12	12:M:5:ILE:H	1.75	0.52
15:P:31:VAL:N	15:P:125:SER:OG	2.43	0.52
27:X:1350:G:H2'	27:X:1351:G:C8	2.45	0.52
20:U:48:LYS:HE3	27:X:2074:U:H1'	1.92	0.52
27:X:2306:A:O2'	27:X:2307:A:O4'	2.26	0.52
27:X:447:U:O2'	27:X:449:C:N4	2.42	0.52
16:Q:29:VAL:HG21	16:Q:38:ILE:HD11	1.91	0.52
27:X:1441:A:H4'	27:X:1442:C:O5'	2.10	0.52
27:X:1762:C:H2'	27:X:1763:G:C8	2.45	0.52
7:H:44:TYR:OH	27:X:1978:U:O2	2.28	0.52
27:X:2335:U:H2'	27:X:2336:G:C8	2.45	0.52
1:A:49:ILE:HD11	1:A:52:ARG:HA	1.92	0.52
1:A:94:LEU:HD12	1:A:95:LEU:H	1.75	0.52
5:E:67:LEU:HD21	27:X:2738:A:C4	2.45	0.52
8:I:55:ARG:HH21	27:X:846:A:H4'	1.74	0.52
9:J:15:ARG:HH21	9:J:73:LYS:NZ	2.07	0.52
12:M:29:PRO:HG2	12:M:97:GLY:H	1.75	0.52
14:O:36:LYS:HE2	14:O:56:VAL:HB	1.92	0.52
20:U:39:LYS:HA	27:X:2063:A:H4'	1.92	0.52
27:X:2309:G:H2'	27:X:2310:G:O4'	2.10	0.52
27:X:1655:C:H5''	27:X:2689:C:O2'	2.10	0.52
3:C:187:VAL:HG12	3:C:189:ASP:HB2	1.92	0.52
7:H:116:ARG:NH2	12:M:41:GLU:OE2	2.35	0.52
16:Q:17:TYR:HA	16:Q:20:MET:HB2	1.92	0.52
27:X:1316:G:H5'	27:X:1659:G:H21	1.75	0.52
1:A:43:ARG:O	27:X:1805:G:O2'	2.28	0.52
27:X:188:G:H2'	27:X:189:A:H8	1.73	0.52
27:X:2299:A:H4'	27:X:2300:G:O5'	2.09	0.52
25:2:34:ARG:HD3	25:2:37:LYS:HD2	1.92	0.51
2:B:52:ALA:HB3	2:B:76:ARG:HB2	1.91	0.51
3:C:34:GLN:O	3:C:37:SER:OG	2.19	0.51
6:G:43:VAL:HG21	6:G:158:HIS:HE1	1.75	0.51
14:O:36:LYS:NZ	14:O:54:TYR:HB3	2.25	0.51
27:X:1573:G:O5'	27:X:1574:A:H5''	2.10	0.51
27:X:1662:G:H5''	27:X:1663:C:H5'	1.92	0.51
27:X:2234:G:H2'	27:X:2235:G:O4'	2.10	0.51
7:H:42:LYS:HA	27:X:2653:A:O3'	2.10	0.51
8:I:35:LYS:NZ	27:X:575:U:H5''	2.25	0.51
26:3:20:GLY:O	26:3:57:ARG:NH1	2.43	0.51
12:M:55:ILE:O	12:M:103:LYS:O	2.28	0.51
15:P:103:LEU:HB2	15:P:121:LYS:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:50:VAL:HG23	15:P:91:PHE:HA	1.92	0.51
16:Q:62:ARG:O	16:Q:70:GLY:HA2	2.09	0.51
27:X:1296:G:N2	27:X:1299:A:H5'	2.25	0.51
27:X:185:C:H2'	27:X:186:C:H6	1.74	0.51
11:L:91:ARG:NH2	27:X:2355:A:H61	2.08	0.51
28:Y:96:C:H2'	28:Y:97:C:H6	1.76	0.51
26:3:62:LEU:HD13	27:X:603:C:H5''	1.91	0.51
7:H:129:LEU:O	7:H:131:PRO:HD3	2.11	0.51
9:J:15:ARG:HE	9:J:73:LYS:HZ2	1.58	0.51
20:U:61:TRP:O	20:U:62:LEU:HD12	2.10	0.51
27:X:2007:G:C2	27:X:2023:C:C2	2.98	0.51
27:X:2451:G:O2'	27:X:2457:A:N6	2.42	0.51
27:X:939:C:OP2	27:X:940:G:H8	1.94	0.51
4:D:102:LYS:NZ	4:D:140:GLU:OE2	2.33	0.51
18:S:17:SER:HB2	18:S:36:ARG:HB3	1.93	0.51
27:X:2171:U:H2'	27:X:2172:U:C5	2.46	0.51
27:X:2826:C:H2'	27:X:2827:G:O4'	2.11	0.51
27:X:503:G:H2'	27:X:504:G:O4'	2.10	0.51
5:E:24:PHE:HB2	5:E:37:TYR:CD1	2.45	0.51
6:G:58:ILE:HG12	6:G:80:VAL:HG11	1.93	0.51
15:P:36:ARG:HD3	27:X:1279:G:N7	2.26	0.51
27:X:2824:C:H4'	27:X:2825:A:O5'	2.10	0.51
27:X:2:G:O2'	27:X:3:U:H5'	2.10	0.51
27:X:636:G:O2'	27:X:669:G:H4'	2.10	0.51
27:X:746:G:C8	27:X:774:A:C6	2.98	0.51
2:B:54:LYS:HD3	2:B:59:VAL:HG22	1.92	0.51
4:D:46:ASP:HB2	4:D:49:ALA:H	1.75	0.51
6:G:61:ARG:HH22	6:G:65:LYS:H	1.59	0.51
14:O:12:TYR:CD2	14:O:40:VAL:HB	2.46	0.51
17:R:100:ASP:HB3	17:R:103:LYS:HB2	1.93	0.51
27:X:3:U:O2'	27:X:4:C:O5'	2.26	0.51
23:Z:4:HIS:HB2	23:Z:5:PRO:HD3	1.93	0.51
7:H:27:SER:HB2	7:H:50:ILE:HB	1.93	0.51
12:M:50:PHE:HE2	12:M:70:LYS:HB2	1.76	0.51
27:X:1316:G:N2	27:X:1317:G:H1'	2.26	0.51
27:X:1599:G:C2	27:X:1600:U:H1'	2.46	0.51
27:X:2250:G:H2'	27:X:2251:U:C6	2.45	0.51
9:J:86:LYS:NZ	27:X:2256:G:OP2	2.29	0.51
27:X:474:G:N2	27:X:477:A:OP2	2.38	0.51
3:C:39:ARG:HG3	27:X:455:A:C8	2.46	0.51
19:T:26:PHE:HD1	27:X:934:G:H1'	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:40:PRO:HD2	27:X:94:C:H1'	1.92	0.51
27:X:1692:C:N4	27:X:1976:U:O4'	2.44	0.51
27:X:2167:A:H2	27:X:2168:A:H62	1.59	0.51
27:X:959:C:H42	27:X:980:G:H1	1.59	0.51
23:Z:35:GLN:HG3	23:Z:51:TYR:HB3	1.91	0.51
3:C:48:ARG:CZ	3:C:51:VAL:HG13	2.41	0.51
5:E:154:PRO:HA	5:E:160:LYS:O	2.10	0.51
6:G:67:ARG:CG	6:G:70:PHE:HA	2.41	0.51
3:C:67:ALA:HB2	15:P:112:ARG:HH12	1.76	0.51
5:E:109:TYR:HD2	27:X:2646:C:H1'	1.75	0.51
27:X:577:U:O5'	27:X:956:A:N6	2.44	0.51
27:X:796:A:C8	27:X:797:A:H4'	2.45	0.51
3:C:25:GLY:HA3	8:I:18:ARG:NH1	2.26	0.51
3:C:58:MET:HG2	3:C:59:TYR:HD1	1.76	0.51
20:U:20:ARG:HB2	20:U:43:ARG:HD2	1.92	0.51
15:P:36:ARG:NH2	27:X:1279:G:O5'	2.44	0.51
27:X:1443:G:H2'	27:X:1444:C:H6	1.75	0.51
3:C:162:ARG:HH21	27:X:333:A:H2'	1.76	0.50
15:P:119:ILE:HG13	15:P:120:ILE:H	1.76	0.50
18:S:25:ASN:HD22	18:S:85:MET:HB2	1.75	0.50
11:L:15:ARG:HH21	27:X:2272:A:P	2.34	0.50
27:X:541:C:H4'	27:X:542:A:H5''	1.92	0.50
25:2:17:GLY:O	25:2:21:ARG:HG2	2.11	0.50
2:B:117:MET:HA	2:B:121:ASN:O	2.11	0.50
3:C:149:LEU:HD23	3:C:180:ILE:HG22	1.92	0.50
5:E:136:ILE:HD12	5:E:137:ASP:H	1.76	0.50
6:G:101:THR:HG23	6:G:103:TYR:CE1	2.46	0.50
16:Q:56:MET:HG2	27:X:1354:A:H4'	1.93	0.50
17:R:15:HIS:CE1	17:R:80:LYS:HE2	2.45	0.50
18:S:13:LYS:HA	18:S:18:MET:HB2	1.93	0.50
27:X:1539:U:H2'	27:X:1540:C:C6	2.45	0.50
27:X:493:A:H5''	27:X:494:A:OP1	2.10	0.50
27:X:943:U:H2'	27:X:944:A:C8	2.46	0.50
26:3:6:THR:N	26:3:9:MET:HG2	2.26	0.50
8:I:90:ARG:HG2	8:I:121:HIS:CE1	2.47	0.50
11:L:30:SER:HB2	11:L:43:ILE:HD11	1.93	0.50
15:P:35:PRO:HD3	15:P:124:THR:CB	2.41	0.50
6:G:53:ARG:NH2	27:X:1150:C:O3'	2.43	0.50
27:X:116:A:N3	27:X:155:G:H1'	2.26	0.50
27:X:1843:U:H3	27:X:1874:G:H1	1.58	0.50
27:X:1870:U:H3'	27:X:1871:G:H21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2020:G:H2'	27:X:2021:G:H8	1.76	0.50
19:T:39:ARG:NH2	27:X:2334:C:O2	2.44	0.50
27:X:2380:U:H3	27:X:2394:G:H1	1.58	0.50
27:X:2664:G:H2'	27:X:2665:G:H8	1.74	0.50
2:B:11:MET:HG2	2:B:24:THR:OG1	2.10	0.50
6:G:84:ASN:HD21	6:G:154:GLU:HG2	1.74	0.50
7:H:10:VAL:HA	7:H:96:ALA:O	2.11	0.50
9:J:68:ARG:CZ	9:J:103:VAL:HG11	2.42	0.50
15:P:134:LYS:HG3	15:P:136:ASN:H	1.75	0.50
19:T:23:VAL:HG13	19:T:38:VAL:HG22	1.92	0.50
8:I:35:LYS:HZ2	27:X:575:U:H5''	1.75	0.50
27:X:633:G:H2'	27:X:634:G:H8	1.77	0.50
1:A:63:ARG:O	1:A:65:ILE:HG22	2.12	0.50
10:K:35:GLN:HB3	10:K:112:LEU:HD23	1.94	0.50
27:X:1332:G:O2'	27:X:1333:G:H5'	2.11	0.50
27:X:163:A:H2'	27:X:164:G:H8	1.76	0.50
27:X:1770:U:H5	27:X:1775:A:N7	2.10	0.50
27:X:1867:A:O2'	27:X:1868:A:H8	1.95	0.50
27:X:2067:U:H2'	27:X:2068:C:C6	2.47	0.50
27:X:2674:C:H2'	27:X:2675:U:C6	2.46	0.50
27:X:461:A:C4	27:X:462:G:C8	2.99	0.50
27:X:700:C:H2'	27:X:701:U:O4'	2.11	0.50
26:3:30:ARG:HE	26:3:31:HIS:HE1	1.57	0.50
6:G:106:TYR:CE2	6:G:108:GLY:HA2	2.47	0.50
9:J:44:LYS:HB2	9:J:47:GLN:NE2	2.26	0.50
15:P:28:ALA:HB2	15:P:71:VAL:CG2	2.42	0.50
21:V:42:ARG:O	21:V:46:LEU:HG	2.11	0.50
22:W:20:VAL:HG23	22:W:47:VAL:HG11	1.94	0.50
27:X:2270:U:O2'	27:X:2353:G:N3	2.43	0.50
4:D:170:LEU:HB2	4:D:175:LEU:HD22	1.92	0.50
14:O:64:GLY:HA3	14:O:90:PHE:CZ	2.46	0.50
1:A:244:ARG:HD2	27:X:1884:A:O2'	2.11	0.50
27:X:358:C:H2'	27:X:359:G:O4'	2.11	0.50
27:X:857:U:H2'	27:X:858:G:O4'	2.11	0.50
3:C:163:ASN:HD21	3:C:167:VAL:N	2.03	0.50
6:G:125:ARG:HD2	6:G:129:HIS:CE1	2.45	0.50
8:I:38:LYS:HE3	8:I:41:SER:OG	2.12	0.50
11:L:32:TYR:CE1	11:L:34:SER:HB3	2.46	0.50
12:M:85:SER:O	12:M:88:VAL:N	2.42	0.50
15:P:66:GLU:HB3	15:P:67:PRO:HD3	1.93	0.50
21:V:5:GLU:HA	21:V:7:ARG:HH21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1001:A:H1'	27:X:1167:A:N3	2.26	0.50
27:X:1399:C:H2'	27:X:1400:A:H8	1.77	0.50
27:X:2482:A:H4'	27:X:2483:U:OP1	2.10	0.50
27:X:2828:C:H2'	27:X:2829:A:C8	2.47	0.50
27:X:806:A:OP2	27:X:806:A:H8	1.94	0.50
26:3:11:LYS:HD2	26:3:11:LYS:H	1.77	0.50
1:A:161:THR:H	1:A:196:VAL:HG23	1.76	0.50
2:B:115:GLY:CA	2:B:136:ARG:HD2	2.42	0.50
3:C:146:GLU:OE2	3:C:185:ARG:NH2	2.45	0.50
15:P:21:ARG:HG3	15:P:22:LYS:H	1.77	0.50
20:U:51:ILE:O	20:U:52:ARG:HD3	2.11	0.50
27:X:1059:A:O2'	27:X:1060:C:OP1	2.26	0.50
27:X:1098:G:N2	27:X:1114:A:H1'	2.27	0.50
27:X:1148:G:H5''	27:X:1149:G:OP2	2.11	0.50
27:X:121:G:H2'	27:X:122:G:O4'	2.12	0.50
27:X:1481:U:O2'	27:X:1562:G:O2'	2.18	0.50
27:X:2557:G:H2'	27:X:2558:C:H6	1.77	0.50
27:X:2628:C:H2'	27:X:2629:U:H6	1.77	0.50
27:X:958:G:H2'	27:X:959:C:H6	1.77	0.50
28:Y:43:G:H5'	28:Y:44:C:H5''	1.94	0.50
1:A:169:GLU:N	1:A:172:TYR:O	2.36	0.49
10:K:39:THR:O	10:K:42:LYS:N	2.45	0.49
17:R:105:ARG:NH2	17:R:111:GLY:O	2.43	0.49
27:X:1060:C:O2	27:X:1124:U:H4'	2.12	0.49
27:X:1383:C:H3'	27:X:1384:G:H8	1.76	0.49
27:X:2528:G:H2'	27:X:2529:G:C8	2.47	0.49
27:X:820:U:H2'	27:X:821:A:H8	1.76	0.49
1:A:132:PRO:HD3	1:A:190:TYR:CE2	2.47	0.49
1:A:244:ARG:HD3	27:X:1885:C:O4'	2.12	0.49
3:C:14:THR:HG22	3:C:15:ILE:H	1.77	0.49
6:G:103:TYR:HD2	27:X:1142:G:O4'	1.94	0.49
15:P:102:THR:HA	15:P:123:ARG:H	1.76	0.49
1:A:160:GLY:HA3	27:X:1812:U:C4	2.47	0.49
27:X:1665:C:H42	27:X:1992:G:H1	1.59	0.49
1:A:145:LEU:HD21	1:A:185:VAL:HG11	1.93	0.49
1:A:169:GLU:HB3	1:A:172:TYR:HB2	1.94	0.49
4:D:111:ILE:HG23	4:D:137:ILE:HG21	1.94	0.49
16:Q:63:LYS:HD3	16:Q:69:ILE:H	1.78	0.49
22:W:2:LYS:HZ1	22:W:31:SER:HB2	1.76	0.49
27:X:116:A:OP2	27:X:117:A:H2'	2.12	0.49
27:X:1310:C:H2'	27:X:1311:C:H6	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1938:U:H5	27:X:2536:G:N2	2.10	0.49
27:X:50:G:O2'	27:X:51:A:OP2	2.30	0.49
27:X:520:C:H2'	27:X:521:U:O4'	2.13	0.49
27:X:705:C:HO2'	27:X:1367:A:HO2'	1.52	0.49
28:Y:6:C:H2'	28:Y:7:C:C6	2.47	0.49
24:1:8:ILE:HG12	24:1:9:ILE:HG23	1.93	0.49
3:C:56:ARG:NE	27:X:814:G:OP2	2.45	0.49
6:G:103:TYR:O	6:G:107:GLN:NE2	2.46	0.49
9:J:21:ASP:C	9:J:99:LYS:HG2	2.33	0.49
15:P:41:VAL:HG21	15:P:64:ALA:HB3	1.94	0.49
16:Q:15:LYS:HG2	27:X:1404:C:O2	2.13	0.49
16:Q:73:ASN:OD1	16:Q:73:ASN:N	2.44	0.49
27:X:1035:G:C6	27:X:1036:G:C6	3.00	0.49
27:X:1277:G:H2'	27:X:1997:A:N6	2.28	0.49
27:X:1313:U:H4'	27:X:1314:A:H5'	1.93	0.49
27:X:1482:U:HO2'	27:X:1483:G:H8	1.60	0.49
27:X:1703:C:H2'	27:X:1704:G:O4'	2.12	0.49
27:X:2324:G:O2'	27:X:2360:C:O2'	2.13	0.49
27:X:2484:G:N2	30:X:2902:ERY:H191	2.26	0.49
27:X:562:G:H2'	27:X:563:U:O4'	2.12	0.49
1:A:226:MET:HB3	1:A:230:ASP:HB2	1.93	0.49
2:B:50:GLY:HA3	2:B:75:THR:HG21	1.93	0.49
3:C:3:GLN:N	3:C:12:GLY:O	2.30	0.49
10:K:6:ALA:HB1	27:X:2848:A:C2	2.47	0.49
14:O:10:LYS:HE3	14:O:13:ARG:HH22	1.77	0.49
13:N:20:ARG:NH1	14:O:83:ARG:HH11	2.11	0.49
17:R:45:LYS:HA	17:R:76:LEU:O	2.12	0.49
27:X:1255:A:H2'	27:X:1256:C:C6	2.48	0.49
27:X:1640:C:H2'	27:X:1641:C:H6	1.78	0.49
27:X:1790:G:H5'	27:X:1811:A:H62	1.77	0.49
27:X:2189:A:H3'	27:X:2190:A:H5''	1.93	0.49
4:D:37:ASN:ND2	27:X:2291:U:O2'	2.39	0.49
27:X:2457:A:C8	27:X:2508:G:C5	3.01	0.49
27:X:2557:G:H2'	27:X:2558:C:C6	2.47	0.49
27:X:1922:U:H1'	27:X:2571:G:O4'	2.12	0.49
27:X:2520:A:H2	27:X:2745:A:H61	1.58	0.49
27:X:2839:G:H2'	27:X:2840:U:C6	2.48	0.49
28:Y:58:G:O2'	28:Y:59:A:H5''	2.13	0.49
23:Z:44:HIS:CD2	23:Z:44:HIS:N	2.80	0.49
1:A:48:ARG:HD3	27:X:1797:C:H4'	1.94	0.49
8:I:72:TYR:CE2	8:I:105:PRO:HG2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:27:PHE:HA	12:M:96:ARG:HH22	1.78	0.49
17:R:37:LEU:HD11	17:R:49:GLU:HG2	1.95	0.49
27:X:1787:U:H2'	27:X:1788:C:H6	1.75	0.49
27:X:1979:C:H4'	27:X:1980:A:OP1	2.13	0.49
27:X:2053:G:H2'	27:X:2054:A:C8	2.48	0.49
27:X:32:C:O2'	27:X:33:C:H5'	2.13	0.49
27:X:828:C:H2'	27:X:829:C:C6	2.47	0.49
28:Y:73:C:H2'	28:Y:74:A:O4'	2.13	0.49
24:1:38:LYS:HE2	24:1:40:TYR:HE1	1.78	0.49
24:1:9:ILE:HB	24:1:27:ASN:O	2.13	0.49
1:A:252:LYS:H	1:A:252:LYS:CE	2.26	0.49
1:A:38:PRO:HA	1:A:61:LEU:HD22	1.93	0.49
2:B:37:LYS:HB2	2:B:46:ALA:HB3	1.95	0.49
3:C:111:ARG:NH1	3:C:183:HIS:O	2.45	0.49
7:H:10:VAL:HG23	7:H:17:ARG:O	2.12	0.49
27:X:2226:A:H2'	27:X:2227:C:C6	2.47	0.49
27:X:2605:C:H2'	27:X:2606:G:H8	1.76	0.49
1:A:161:THR:O	1:A:196:VAL:HG22	2.13	0.49
2:B:104:ALA:HB1	2:B:188:ILE:HD11	1.93	0.49
3:C:128:ALA:C	3:C:130:THR:H	2.16	0.49
8:I:42:GLY:N	8:I:45:LYS:HE3	2.27	0.49
17:R:84:VAL:HG11	17:R:89:GLY:HA2	1.95	0.49
18:S:155:PRO:HG2	18:S:158:CYS:SG	2.53	0.49
27:X:104:C:H2'	27:X:105:G:H8	1.78	0.49
27:X:1184:G:H3'	27:X:1185:C:H5''	1.95	0.49
27:X:1699:A:H2'	27:X:1700:C:C6	2.48	0.49
27:X:2198:U:C2	27:X:2199:C:H1'	2.48	0.49
26:3:42:ARG:NE	27:X:2328:G:OP1	2.46	0.49
27:X:2553:G:N1	27:X:2554:C:O2	2.45	0.49
27:X:346:C:C6	27:X:347:C:H5	2.30	0.49
27:X:538:A:N6	27:X:2025:A:H3'	2.28	0.49
27:X:960:U:H2'	27:X:961:G:C8	2.47	0.49
26:3:14:ILE:HG23	26:3:60:LEU:HD22	1.95	0.49
26:3:30:ARG:HB3	26:3:31:HIS:ND1	2.28	0.49
1:A:143:HIS:ND1	1:A:194:GLY:O	2.35	0.49
1:A:206:LEU:HD23	1:A:211:ARG:HD2	1.94	0.49
4:D:56:GLU:HA	4:D:59:LEU:HD12	1.95	0.49
5:E:24:PHE:HB2	5:E:37:TYR:HD1	1.76	0.49
10:K:12:ARG:HH11	10:K:12:ARG:HG2	1.78	0.49
17:R:62:MET:O	17:R:65:PRO:HA	2.12	0.49
27:X:1672:A:C6	27:X:1673:C:C2	3.00	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2427:A:HO2'	27:X:2428:U:H5	1.61	0.49
4:D:38:GLU:HB3	4:D:87:ILE:HB	1.95	0.49
7:H:28:GLY:O	7:H:35:THR:HG23	2.13	0.49
9:J:16:GLY:C	9:J:17:ARG:HD3	2.33	0.49
27:X:1802:A:H2'	27:X:1803:G:O4'	2.13	0.49
27:X:830:C:O2'	27:X:852:U:H5''	2.13	0.49
28:Y:15:A:O2'	28:Y:16:U:H5''	2.12	0.49
28:Y:39:C:H5'	28:Y:40:C:OP2	2.12	0.49
2:B:136:ARG:HG2	2:B:137:ARG:N	2.27	0.48
6:G:67:ARG:HG2	6:G:70:PHE:HA	1.95	0.48
6:G:69:ASP:H	6:G:76:GLN:NE2	2.10	0.48
11:L:32:TYR:O	11:L:38:ILE:HA	2.13	0.48
12:M:104:LEU:HA	12:M:106:TYR:CE2	2.47	0.48
17:R:86:PRO:HG2	17:R:90:LYS:HE2	1.95	0.48
27:X:1351:G:H2'	27:X:1352:G:C8	2.48	0.48
27:X:2543:A:C2	27:X:2626:U:H4'	2.47	0.48
28:Y:96:C:H2'	28:Y:97:C:C6	2.47	0.48
13:N:66:ASN:HB2	13:N:70:ARG:NH1	2.28	0.48
8:I:33:GLY:HA2	14:O:79:GLN:HG3	1.95	0.48
15:P:41:VAL:HG11	15:P:65:SER:HA	1.95	0.48
14:O:85:GLY:N	27:X:1238:A:H5'	2.27	0.48
27:X:2204:A:H4'	27:X:2205:C:O5'	2.13	0.48
27:X:2261:G:H5''	27:X:2262:C:O4'	2.14	0.48
2:B:145:LYS:HB2	27:X:2551:A:N7	2.29	0.48
27:X:836:G:H2'	27:X:837:U:H6	1.78	0.48
1:A:251:GLY:HA3	1:A:255:LYS:NZ	2.27	0.48
3:C:163:ASN:HD21	3:C:166:TRP:HB2	1.78	0.48
6:G:43:VAL:HG12	6:G:167:LYS:HE3	1.96	0.48
12:M:102:ALA:C	12:M:103:LYS:HD2	2.33	0.48
18:S:104:SER:HA	18:S:139:THR:HA	1.95	0.48
19:T:41:ARG:HA	19:T:41:ARG:HD2	1.52	0.48
27:X:1283:C:H5''	27:X:1284:G:C5'	2.42	0.48
27:X:2532:G:C2	27:X:2533:U:H1'	2.47	0.48
2:B:203:LYS:HG2	27:X:2713:A:H61	1.78	0.48
27:X:346:C:H2'	27:X:347:C:C5	2.48	0.48
27:X:38:G:H1	27:X:453:U:H3	1.61	0.48
27:X:514:G:H4'	27:X:515:A:OP2	2.11	0.48
27:X:543:G:C5	27:X:544:U:C4	3.02	0.48
27:X:558:G:C8	27:X:560:G:C8	3.01	0.48
24:I:30:ASN:OD1	24:I:31:THR:N	2.47	0.48
26:3:26:LYS:NZ	26:3:28:GLY:HA3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:80:ARG:NE	4:D:83:MET:SD	2.81	0.48
11:L:21:THR:O	11:L:25:GLY:N	2.33	0.48
27:X:165:G:H1	27:X:185:C:N4	2.11	0.48
27:X:2040:A:H2'	27:X:2041:A:H8	1.73	0.48
27:X:2278:A:H2'	27:X:2279:G:C8	2.47	0.48
27:X:2407:G:H5''	27:X:2408:G:O5'	2.12	0.48
27:X:2498:U:C5	27:X:2520:A:C6	3.01	0.48
27:X:2655:C:O2	27:X:2712:G:N2	2.38	0.48
27:X:736:G:H2'	27:X:737:C:O4'	2.14	0.48
26:3:58:MET:HA	26:3:61:MET:HB2	1.94	0.48
1:A:30:GLU:HB2	1:A:82:ILE:O	2.14	0.48
2:B:128:SER:HB2	2:B:129:HIS:ND1	2.29	0.48
2:B:172:VAL:HG22	2:B:182:ILE:HD11	1.96	0.48
3:C:182:ARG:NH1	3:C:183:HIS:HE1	2.10	0.48
9:J:99:LYS:HG3	9:J:100:PRO:HD2	1.94	0.48
16:Q:62:ARG:NH1	16:Q:73:ASN:HD21	2.11	0.48
27:X:1019:U:HO2'	27:X:1020:A:P	2.35	0.48
27:X:1437:A:H2'	27:X:1438:G:C8	2.47	0.48
27:X:1623:C:H4'	27:X:1624:A:O5'	2.13	0.48
27:X:224:G:H4'	27:X:399:G:C5	2.48	0.48
27:X:459:A:H4'	27:X:461:A:N7	2.28	0.48
28:Y:7:C:H2'	28:Y:8:C:C6	2.49	0.48
3:C:104:LEU:O	3:C:108:ILE:HG13	2.12	0.48
5:E:143:GLN:NE2	27:X:2724:G:H21	2.12	0.48
5:E:37:TYR:CZ	5:E:72:VAL:HG22	2.48	0.48
6:G:56:THR:HA	6:G:134:MET:HE1	1.96	0.48
7:H:14:SER:OG	7:H:98:ILE:HD12	2.13	0.48
16:Q:28:TRP:HZ3	16:Q:58:VAL:HG21	1.78	0.48
27:X:936:A:H2'	27:X:937:C:O4'	2.13	0.48
3:C:62:LYS:HD2	27:X:2044:G:OP1	2.13	0.48
15:P:39:ARG:HD2	15:P:97:VAL:HB	1.94	0.48
20:U:20:ARG:N	20:U:41:VAL:O	2.38	0.48
20:U:20:ARG:HH21	20:U:43:ARG:HG2	1.79	0.48
27:X:1653:C:H2'	27:X:1654:A:C8	2.49	0.48
27:X:1815:G:H2'	27:X:1816:G:H8	1.79	0.48
27:X:2013:A:H4'	27:X:2014:A:C8	2.49	0.48
9:J:57:ARG:NE	27:X:2448:A:O2'	2.38	0.48
27:X:537:C:O2'	27:X:538:A:C4	2.66	0.48
27:X:764:A:H2	27:X:802:A:HO2'	1.59	0.48
24:1:28:ARG:HB2	24:1:30:ASN:ND2	2.28	0.48
8:I:94:GLU:HA	8:I:97:ARG:NE	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:82:GLU:O	10:K:85:PRO:HD2	2.14	0.48
16:Q:58:VAL:HA	16:Q:59:PRO:HD2	1.61	0.48
17:R:61:SER:HA	17:R:65:PRO:CG	2.42	0.48
27:X:1333:G:N2	27:X:1344:C:N4	2.61	0.48
27:X:1404:C:C2	27:X:1406:A:N7	2.81	0.48
27:X:1451:C:H2'	27:X:1452:U:C6	2.47	0.48
27:X:1586:A:H2'	27:X:1587:A:C8	2.49	0.48
27:X:2199:C:H2'	27:X:2200:G:H8	1.79	0.48
27:X:2590:U:C1'	30:X:2902:ERY:H361	2.44	0.48
27:X:2657:G:H2'	27:X:2658:A:O4'	2.14	0.48
27:X:492:G:H2'	27:X:517:A:N1	2.29	0.48
27:X:603:C:H2'	27:X:604:U:H6	1.79	0.48
3:C:72:ARG:CZ	3:C:77:PHE:HE2	2.27	0.48
4:D:134:GLU:HG2	4:D:136:LEU:H	1.79	0.48
5:E:165:VAL:HB	5:E:166:GLY:H	1.46	0.48
5:E:24:PHE:CD1	5:E:37:TYR:HB2	2.49	0.48
6:G:137:LYS:HD2	27:X:2022:C:OP2	2.14	0.48
13:N:74:MET:HE1	13:N:113:SER:HB3	1.95	0.48
15:P:70:LYS:HE2	27:X:499:G:O2'	2.14	0.48
27:X:2260:C:O2'	27:X:2261:G:H5'	2.14	0.48
27:X:568:G:H2'	27:X:569:C:O4'	2.14	0.48
27:X:732:G:H2'	27:X:733:G:C8	2.48	0.48
1:A:200:GLU:HB2	1:A:203:ASN:ND2	2.29	0.48
1:A:206:LEU:HA	1:A:211:ARG:HH11	1.79	0.48
27:X:2190:A:H61	27:X:2196:U:H3	1.60	0.48
27:X:227:G:C6	27:X:228:A:C6	3.01	0.48
5:E:143:GLN:HG2	27:X:2725:C:H1'	1.95	0.48
23:Z:7:PRO:HA	27:X:2594:U:C6	2.49	0.48
24:1:36:GLU:HG3	24:1:53:LYS:HA	1.96	0.47
1:A:212:SER:OG	1:A:213:ARG:N	2.48	0.47
3:C:62:LYS:HE2	3:C:63:GLY:N	2.29	0.47
8:I:31:GLY:HA3	8:I:34:HIS:ND1	2.29	0.47
8:I:38:LYS:HG3	27:X:954:U:OP2	2.14	0.47
13:N:81:ASN:HD22	13:N:117:ARG:HH12	1.61	0.47
27:X:1107:A:H3'	27:X:1108:U:H5''	1.96	0.47
27:X:114:C:O2'	27:X:124:A:N3	2.43	0.47
27:X:824:U:O2	27:X:1263:G:H3'	2.14	0.47
27:X:1417:C:H2'	27:X:1418:C:H6	1.78	0.47
27:X:773:G:H2'	27:X:774:A:H5'	1.95	0.47
2:B:108:SER:HB3	2:B:163:GLU:H	1.79	0.47
8:I:38:LYS:HG3	27:X:954:U:P	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:28:VAL:HG11	9:J:135:ARG:HB3	1.95	0.47
18:S:67:LYS:NZ	18:S:92:VAL:HG21	2.28	0.47
30:X:2902:ERY:H2	30:X:2902:ERY:H312	1.63	0.47
27:X:66:U:H2'	27:X:67:G:C8	2.49	0.47
8:I:62:LYS:HB3	26:3:13:ARG:H	1.77	0.47
1:A:97:TYR:HE2	1:A:103:ARG:HB2	1.79	0.47
7:H:11:ALA:N	7:H:96:ALA:O	2.37	0.47
16:Q:59:PRO:HA	16:Q:74:ASP:OD1	2.15	0.47
19:T:83:ALA:HB1	19:T:85:GLN:HE21	1.79	0.47
21:V:46:LEU:O	21:V:50:VAL:HG23	2.14	0.47
27:X:1074:G:H1	27:X:1086:C:N4	2.12	0.47
27:X:1636:G:H2'	27:X:1637:U:C6	2.49	0.47
27:X:1655:C:H4'	27:X:2689:C:O2	2.14	0.47
27:X:1672:A:H3'	27:X:1673:C:C6	2.49	0.47
19:T:56:ASP:OD1	27:X:2343:C:H4'	2.15	0.47
27:X:2542:U:O2	27:X:2544:A:H8	1.98	0.47
2:B:136:ARG:HH21	2:B:157:ALA:H	1.62	0.47
8:I:128:ALA:HA	8:I:131:LYS:HB3	1.95	0.47
9:J:16:GLY:HA2	9:J:17:ARG:NH1	2.25	0.47
9:J:70:PHE:C	9:J:70:PHE:CD2	2.87	0.47
21:V:54:ASN:HB3	27:X:71:A:C5	2.49	0.47
27:X:1052:C:N4	27:X:1053:G:N7	2.63	0.47
27:X:1171:A:H2'	27:X:1172:U:C6	2.49	0.47
27:X:2184:C:H2'	27:X:2185:U:O4'	2.14	0.47
27:X:2258:G:C2	27:X:2259:G:C8	3.02	0.47
27:X:760:U:OP1	27:X:2591:C:H1'	2.15	0.47
27:X:2691:C:O2'	27:X:2693:U:H5'	2.13	0.47
27:X:2701:A:C2	27:X:2848:A:C4	3.03	0.47
27:X:333:A:H5'	27:X:351:A:H1'	1.95	0.47
27:X:91:A:H2'	27:X:92:U:C6	2.49	0.47
4:D:4:LEU:C	4:D:6:THR:H	2.18	0.47
27:X:2363:G:H3'	27:X:2365:U:OP1	2.14	0.47
27:X:525:A:N1	27:X:1273:G:O2'	2.40	0.47
27:X:540:G:C5	27:X:2005:U:H5''	2.49	0.47
23:Z:45:ILE:HD13	23:Z:57:VAL:HG23	1.96	0.47
8:I:56:LEU:CB	26:3:52:LYS:HZ1	2.25	0.47
4:D:153:ASP:OD1	27:X:2283:G:O2'	2.28	0.47
4:D:31:ILE:HA	4:D:158:THR:HA	1.97	0.47
15:P:122:LYS:HB3	15:P:124:THR:CG2	2.45	0.47
27:X:1468:A:H8	27:X:1468:A:P	2.38	0.47
27:X:2363:G:HO2'	27:X:2364:C:P	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2368:G:H5''	27:X:2369:U:H5'	1.97	0.47
27:X:2576:G:C6	27:X:2577:A:C6	3.03	0.47
27:X:1750:A:H4'	27:X:2695:C:O4'	2.14	0.47
15:P:21:ARG:HH21	27:X:506:G:H5'	1.79	0.47
27:X:552:C:H2'	27:X:553:C:H5''	1.96	0.47
27:X:682:G:H3'	27:X:683:A:C8	2.50	0.47
1:A:79:VAL:HB	1:A:114:GLY:H	1.80	0.47
7:H:110:VAL:HB	7:H:129:LEU:HB3	1.97	0.47
7:H:23:ARG:HD2	7:H:24:VAL:O	2.15	0.47
10:K:60:LEU:HD11	10:K:64:ARG:HH11	1.80	0.47
17:R:62:MET:H	17:R:65:PRO:HA	1.79	0.47
27:X:136:A:H2'	27:X:137:A:O4'	2.15	0.47
27:X:1353:A:H4'	27:X:1407:G:H1'	1.95	0.47
27:X:1779:C:O5'	27:X:1779:C:H6	1.97	0.47
27:X:2512:A:OP1	27:X:2644:A:O2'	2.26	0.47
27:X:2524:G:C6	27:X:2525:U:C4	3.02	0.47
27:X:2684:A:H2'	27:X:2685:A:O4'	2.14	0.47
15:P:47:GLY:H	15:P:92:VAL:CG2	2.27	0.47
27:X:1164:C:H2'	27:X:1165:G:O4'	2.15	0.47
27:X:1419:G:H2'	27:X:1420:A:C8	2.50	0.47
27:X:1673:C:C2	27:X:1674:C:C5	3.02	0.47
27:X:742:G:H2'	27:X:1766:U:H1'	1.96	0.47
27:X:536:A:N6	27:X:2605:C:H4'	2.30	0.47
27:X:2670:C:H5'	27:X:2847:G:H5''	1.97	0.47
27:X:469:G:N2	27:X:480:G:H2'	2.30	0.47
27:X:582:G:O2'	27:X:583:C:H3'	2.14	0.47
1:A:181:GLU:HG3	1:A:270:ILE:HA	1.95	0.47
2:B:32:PRO:O	2:B:49:ILE:HA	2.15	0.47
11:L:59:LEU:HD23	11:L:61:SER:HB3	1.97	0.47
11:L:8:ARG:HE	11:L:9:ARG:HG2	1.79	0.47
15:P:34:SER:O	15:P:37:LYS:HB3	2.15	0.47
16:Q:57:ASN:HD21	16:Q:76:LYS:HE3	1.80	0.47
27:X:1332:G:C6	27:X:1333:G:N1	2.82	0.47
27:X:1838:G:N2	27:X:1878:C:N3	2.63	0.47
27:X:2280:A:H2'	27:X:2281:C:C6	2.49	0.47
5:E:138:LYS:HG2	27:X:2726:U:H5''	1.97	0.47
27:X:343:A:H1'	27:X:346:C:N4	2.29	0.47
27:X:835:U:H2'	27:X:836:G:C8	2.50	0.47
28:Y:16:U:O2'	28:Y:110:U:H1'	2.15	0.47
26:3:23:MET:HB3	26:3:25:PHE:CE2	2.49	0.47
26:3:30:ARG:HB2	27:X:2372:A:OP1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:PRO:HG3	27:X:1586:A:H5'	1.97	0.47
3:C:54:THR:HG22	3:C:55:GLY:O	2.15	0.47
11:L:33:ARG:HH21	11:L:103:LEU:HD12	1.79	0.47
17:R:22:VAL:HG13	17:R:81:VAL:O	2.15	0.47
19:T:46:LYS:HE3	19:T:76:ALA:HA	1.96	0.47
27:X:1727:C:H2'	27:X:1728:A:C8	2.50	0.47
27:X:1813:A:H5''	27:X:1814:G:OP2	2.15	0.47
27:X:393:U:H2'	27:X:394:U:C6	2.49	0.47
27:X:640:C:H1'	27:X:650:U:H1'	1.97	0.47
1:A:118:ASN:HD22	1:A:119:ALA:N	2.12	0.47
3:C:129:LYS:O	3:C:131:LYS:N	2.47	0.47
6:G:151:TYR:HE1	6:G:161:GLN:HE21	1.63	0.47
9:J:28:VAL:HG21	9:J:135:ARG:HB3	1.97	0.47
14:O:88:GLN:HB3	14:O:88:GLN:HE21	1.48	0.47
15:P:9:ARG:HD2	15:P:13:GLN:HG3	1.96	0.47
18:S:1:MET:N	18:S:53:ASP:O	2.42	0.47
20:U:64:ALA:O	20:U:67:LEU:HB3	2.15	0.47
27:X:1643:A:N6	27:X:1656:U:H3	2.08	0.47
27:X:203:G:H21	27:X:205:A:H62	1.63	0.47
27:X:2266:A:H5''	27:X:2267:A:OP1	2.15	0.47
27:X:2781:G:H2'	27:X:2782:G:H5''	1.96	0.47
27:X:649:G:C5	27:X:650:U:C5	3.02	0.47
27:X:879:A:H2'	27:X:879:A:N3	2.30	0.47
28:Y:53:G:N3	28:Y:53:G:H2'	2.29	0.47
23:Z:42:SER:O	23:Z:44:HIS:CD2	2.67	0.47
26:3:6:THR:N	26:3:59:LYS:HB3	2.30	0.46
1:A:159:ALA:HA	1:A:198:ASN:CG	2.35	0.46
4:D:103:LEU:HG	4:D:108:LEU:HG	1.97	0.46
6:G:83:ILE:HG22	6:G:153:GLY:O	2.15	0.46
7:H:29:ILE:HB	7:H:34:LEU:HD23	1.96	0.46
8:I:102:LYS:C	8:I:104:ARG:H	2.17	0.46
9:J:21:ASP:OD1	9:J:21:ASP:N	2.36	0.46
7:H:132:GLU:HB2	12:M:73:PHE:CE1	2.49	0.46
15:P:45:ILE:O	15:P:48:LYS:HG2	2.15	0.46
27:X:1301:U:C2	27:X:1340:C:O2	2.68	0.46
27:X:1467:U:H3'	27:X:1467:U:H6	1.80	0.46
27:X:1448:A:H61	27:X:1574:A:H61	1.61	0.46
27:X:2170:C:H3'	27:X:2171:U:H5''	1.97	0.46
11:L:11:LEU:HD21	27:X:2273:C:H5''	1.97	0.46
1:A:133:LEU:HB3	1:A:173:VAL:HG21	1.97	0.46
1:A:18:THR:HG22	1:A:19:ALA:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:19:LEU:HA	3:C:20:PRO:C	2.34	0.46
5:E:84:THR:HG22	5:E:134:SER:OG	2.15	0.46
8:I:31:GLY:O	8:I:32:ARG:HD2	2.15	0.46
10:K:13:ASN:OD1	10:K:15:SER:N	2.43	0.46
10:K:78:LYS:O	10:K:83:VAL:HG23	2.15	0.46
12:M:99:VAL:HG21	12:M:104:LEU:HD11	1.97	0.46
27:X:1141:U:O2'	27:X:1142:G:O5'	2.23	0.46
27:X:1407:G:C6	27:X:1408:A:C6	3.03	0.46
27:X:1781:C:H2'	27:X:1782:A:C5	2.50	0.46
27:X:179:U:H2'	27:X:180:C:O4'	2.15	0.46
27:X:1919:A:C6	27:X:1928:G:C4	3.03	0.46
27:X:2312:A:H4'	27:X:2313:G:O5'	2.15	0.46
27:X:218:A:H61	27:X:232:A:H5''	1.80	0.46
27:X:522:G:OP1	27:X:1247:U:O2'	2.23	0.46
27:X:540:G:O2'	27:X:542:A:H2	1.97	0.46
27:X:687:G:N2	27:X:2423:G:O3'	2.48	0.46
27:X:747:A:H2'	27:X:748:A:O4'	2.14	0.46
27:X:758:G:H2'	27:X:759:C:H5'	1.98	0.46
26:3:6:THR:N	26:3:59:LYS:HD3	2.31	0.46
1:A:222:ARG:HD3	27:X:1820:G:O6	2.16	0.46
1:A:25:THR:HG22	1:A:26:LYS:N	2.30	0.46
3:C:5:ASN:OD1	3:C:5:ASN:N	2.48	0.46
5:E:68:THR:O	5:E:72:VAL:HG23	2.15	0.46
7:H:5:GLN:HG2	27:X:1685:A:H5''	1.97	0.46
9:J:37:ALA:O	9:J:100:PRO:HA	2.14	0.46
12:M:22:ARG:HH22	12:M:24:LEU:HD23	1.80	0.46
12:M:90:GLN:OE1	12:M:90:GLN:N	2.34	0.46
16:Q:8:GLN:O	21:V:29:ARG:HG2	2.15	0.46
27:X:1388:C:H2'	27:X:1389:C:C6	2.50	0.46
27:X:1840:A:H2'	27:X:1841:G:O4'	2.15	0.46
27:X:2020:G:C6	27:X:2021:G:C6	3.03	0.46
5:E:150:LYS:HZ1	27:X:2724:G:H1'	1.81	0.46
2:B:162:MET:SD	27:X:2796:A:H4'	2.55	0.46
6:G:31:THR:HG21	13:N:61:TRP:HE1	1.81	0.46
9:J:6:LYS:HE2	9:J:6:LYS:HB2	1.57	0.46
15:P:28:ALA:O	15:P:126:HIS:HA	2.16	0.46
27:X:1159:U:H2'	27:X:1160:C:C6	2.51	0.46
27:X:1975:G:H22	27:X:1979:C:H6	1.63	0.46
27:X:2026:C:H2'	27:X:2027:C:H6	1.80	0.46
27:X:2226:A:H2'	27:X:2227:C:H6	1.81	0.46
27:X:2605:C:H2'	27:X:2606:G:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:835:U:H2'	27:X:836:G:H8	1.80	0.46
27:X:962:C:H2'	27:X:963:G:H8	1.81	0.46
7:H:2:ILE:HG22	7:H:6:SER:HB3	1.98	0.46
13:N:74:MET:SD	13:N:110:VAL:HG13	2.55	0.46
14:O:5:ILE:N	14:O:10:LYS:HE2	2.30	0.46
14:O:20:ILE:HG22	14:O:21:ARG:H	1.80	0.46
14:O:68:LYS:HA	14:O:87:ARG:HG2	1.97	0.46
17:R:40:LEU:HB2	17:R:45:LYS:HB2	1.98	0.46
18:S:94:VAL:O	18:S:121:GLN:HA	2.15	0.46
19:T:74:LYS:HG2	19:T:77:ARG:NE	2.30	0.46
27:X:104:C:H2'	27:X:105:G:C8	2.50	0.46
27:X:2030:U:H2'	27:X:2031:A:H8	1.81	0.46
27:X:2406:C:H5''	27:X:2407:G:OP1	2.15	0.46
27:X:2425:G:C2	27:X:2480:C:C4	3.03	0.46
27:X:571:U:C2	27:X:581:A:C8	3.03	0.46
27:X:769:C:C4	27:X:770:U:C4	3.03	0.46
27:X:89:A:H4'	27:X:90:G:C5'	2.42	0.46
27:X:958:G:H2'	27:X:959:C:C6	2.51	0.46
8:I:118:VAL:HG23	8:I:133:VAL:HG13	1.98	0.46
9:J:37:ALA:HB2	9:J:104:MET:SD	2.55	0.46
14:O:15:SER:N	14:O:95:ILE:O	2.49	0.46
18:S:19:ILE:HG23	18:S:79:ILE:O	2.16	0.46
19:T:25:LYS:HD3	19:T:31:VAL:HG12	1.98	0.46
22:W:12:ARG:HG2	22:W:12:ARG:HH11	1.81	0.46
27:X:1018:C:H5''	27:X:1019:U:H5''	1.98	0.46
27:X:1030:U:H2'	27:X:1032:A:C2	2.48	0.46
27:X:1040:A:C8	27:X:1041:G:C8	3.04	0.46
27:X:1073:G:H8	27:X:1073:G:OP2	1.99	0.46
27:X:54:G:O2'	27:X:125:A:N1	2.43	0.46
27:X:1806:G:H5''	27:X:1807:A:H2'	1.97	0.46
27:X:2197:U:H2'	27:X:2198:U:C5	2.51	0.46
27:X:2485:U:O2	27:X:2485:U:H2'	2.15	0.46
27:X:2522:G:H2'	27:X:2523:G:H8	1.79	0.46
27:X:2692:A:H5''	27:X:2693:U:OP2	2.16	0.46
3:C:46:ARG:HD3	27:X:463:C:OP1	2.15	0.46
27:X:817:A:H2'	27:X:819:C:C4	2.50	0.46
27:X:824:U:H1'	27:X:1264:C:O4'	2.15	0.46
25:2:21:ARG:O	25:2:28:ARG:HD3	2.16	0.46
2:B:98:GLU:HA	2:B:172:VAL:HG12	1.97	0.46
3:C:58:MET:HB2	3:C:70:GLY:O	2.16	0.46
5:E:90:ARG:HB3	5:E:160:LYS:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:169:ILE:HD13	5:E:170:ALA:H	1.81	0.46
10:K:28:LEU:HD12	10:K:113:ILE:HG23	1.96	0.46
12:M:31:ASP:OD2	12:M:31:ASP:N	2.49	0.46
15:P:105:ARG:HG3	15:P:107:ILE:HB	1.97	0.46
15:P:89:ARG:HB3	15:P:133:GLU:HB3	1.97	0.46
27:X:1412:C:H2'	27:X:1412:C:H6	1.61	0.46
27:X:2051:U:H3	27:X:2409:A:H62	1.63	0.46
27:X:308:C:H2'	27:X:309:G:O4'	2.15	0.46
27:X:603:C:H2'	27:X:604:U:C6	2.51	0.46
26:3:29:LYS:HD2	26:3:33:ASN:O	2.16	0.46
4:D:22:TYR:OH	4:D:165:GLU:OE1	2.34	0.46
6:G:94:LYS:HE3	6:G:95:LEU:HG	1.98	0.46
7:H:132:GLU:HB2	12:M:73:PHE:HE1	1.80	0.46
27:X:1681:A:C2	27:X:2706:U:C2	3.04	0.46
2:B:129:HIS:CD2	27:X:1692:C:C2	3.03	0.46
27:X:839:U:H5''	27:X:2408:G:P	2.56	0.46
27:X:2516:U:H2'	27:X:2517:C:C6	2.51	0.46
27:X:2546:G:H2'	27:X:2547:C:C6	2.51	0.46
27:X:2696:A:O2'	27:X:2697:G:H5'	2.15	0.46
27:X:2753:C:H2'	27:X:2754:C:H6	1.81	0.46
27:X:82:G:N1	27:X:100:G:O2'	2.42	0.46
26:3:13:ARG:O	26:3:13:ARG:HG3	2.16	0.46
1:A:201:HIS:HA	1:A:204:ILE:HD12	1.97	0.46
3:C:59:TYR:CD2	3:C:64:THR:HG21	2.51	0.46
13:N:24:PHE:HB3	13:N:28:ARG:HB2	1.97	0.46
15:P:97:VAL:HG13	15:P:125:SER:O	2.16	0.46
16:Q:11:VAL:HG23	16:Q:27:PHE:HA	1.97	0.46
27:X:1096:A:H5''	27:X:1116:U:H4'	1.98	0.46
27:X:1223:G:H5'	27:X:1225:G:O4'	2.16	0.46
27:X:1770:U:C5	27:X:1775:A:N7	2.84	0.46
27:X:2309:G:H1	27:X:2364:C:H42	1.63	0.46
27:X:2453:C:H5'	27:X:2454:C:OP2	2.16	0.46
27:X:2526:U:H2'	27:X:2527:G:C8	2.50	0.46
27:X:312:G:C4	27:X:313:U:C5	3.04	0.46
27:X:330:C:H2'	27:X:331:U:O4'	2.16	0.46
1:A:252:LYS:NZ	1:A:253:PRO:HD2	2.31	0.46
2:B:37:LYS:NZ	2:B:80:GLU:OE2	2.42	0.46
3:C:34:GLN:NE2	3:C:176:ASN:OD1	2.49	0.46
12:M:16:ILE:HD12	12:M:16:ILE:H	1.81	0.46
27:X:1998:A:O5'	27:X:1998:A:H8	1.99	0.46
27:X:2372:A:H62	27:X:2401:A:N6	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2434:G:H2'	27:X:2435:C:C6	2.51	0.46
27:X:1981:A:O3'	27:X:2704:U:H4'	2.15	0.46
27:X:650:U:H2'	27:X:651:C:C6	2.51	0.46
27:X:820:U:H2'	27:X:821:A:C8	2.51	0.46
2:B:164:ARG:HD2	27:X:2753:C:H5''	1.98	0.45
10:K:89:GLU:O	10:K:91:PRO:HD3	2.15	0.45
12:M:104:LEU:HD23	12:M:106:TYR:CZ	2.51	0.45
27:X:1478:U:H2'	27:X:1479:G:C8	2.51	0.45
27:X:1782:A:N6	27:X:1820:G:O2'	2.49	0.45
27:X:1793:A:H2'	27:X:1794:A:C8	2.51	0.45
27:X:2048:C:H1'	27:X:2428:U:H3	1.81	0.45
27:X:658:G:H2'	27:X:659:G:H8	1.81	0.45
27:X:666:U:H2'	27:X:667:U:H5''	1.98	0.45
27:X:746:G:N7	27:X:774:A:C6	2.85	0.45
27:X:787:A:H2	27:X:800:U:HO2'	1.63	0.45
27:X:825:C:H5''	27:X:1263:G:HO2'	1.81	0.45
27:X:939:C:OP2	27:X:940:G:C8	2.70	0.45
27:X:984:A:O4'	27:X:1202:U:C6	2.69	0.45
28:Y:16:U:H4'	28:Y:72:C:O2	2.16	0.45
7:H:91:PHE:N	7:H:91:PHE:CD1	2.84	0.45
2:B:52:ALA:HB2	12:M:3:THR:HG23	1.98	0.45
13:N:8:ILE:HG22	13:N:11:ARG:NH2	2.31	0.45
16:Q:10:PRO:HA	16:Q:27:PHE:HB3	1.98	0.45
1:A:252:LYS:HD3	27:X:1817:U:O4'	2.16	0.45
27:X:2736:U:H4'	27:X:2737:A:OP1	2.17	0.45
27:X:2797:G:H2'	27:X:2798:A:H5''	1.99	0.45
27:X:2849:C:H2'	27:X:2850:U:C6	2.51	0.45
27:X:88:G:C3'	27:X:89:A:H5''	2.47	0.45
27:X:982:C:H2'	27:X:983:G:O4'	2.16	0.45
24:1:39:LYS:NZ	24:1:47:HIS:HA	2.31	0.45
25:2:38:GLY:HA3	27:X:469:G:H8	1.82	0.45
2:B:9:ILE:HD11	2:B:27:LEU:CB	2.43	0.45
5:E:150:LYS:NZ	27:X:2741:G:H21	2.13	0.45
8:I:94:GLU:HA	8:I:97:ARG:HG3	1.97	0.45
9:J:82:THR:HA	27:X:2474:G:C5'	2.34	0.45
15:P:104:LYS:HG3	15:P:106:LEU:H	1.82	0.45
16:Q:68:PHE:O	16:Q:70:GLY:N	2.42	0.45
27:X:115:G:P	27:X:117:A:HO2'	2.40	0.45
27:X:1230:C:H2'	27:X:1231:A:C8	2.52	0.45
27:X:1763:G:H2'	27:X:1764:A:H4'	1.97	0.45
8:I:59:ARG:CB	27:X:2371:A:H8	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2477:C:O2'	27:X:2478:C:H5'	2.15	0.45
15:P:99:ALA:CB	27:X:25:U:H5'	2.43	0.45
27:X:2640:G:H2'	27:X:2641:A:C8	2.51	0.45
27:X:324:C:H2'	27:X:325:U:O4'	2.17	0.45
1:A:206:LEU:HD22	1:A:211:ARG:HB3	1.98	0.45
2:B:69:LYS:HB3	2:B:69:LYS:HE2	1.80	0.45
3:C:133:PHE:CE1	3:C:161:ALA:HB2	2.51	0.45
5:E:44:ARG:NH2	5:E:51:LEU:HB3	2.32	0.45
9:J:13:GLN:HG3	9:J:14:PHE:CD1	2.51	0.45
12:M:50:PHE:CE2	12:M:70:LYS:HB2	2.52	0.45
27:X:2044:G:C8	27:X:2482:A:C8	3.04	0.45
27:X:2590:U:C5	30:X:2902:ERY:H312	2.51	0.45
27:X:2645:C:H3'	27:X:2646:C:H6	1.82	0.45
27:X:2674:C:H2'	27:X:2675:U:H6	1.81	0.45
13:N:45:TYR:HH	27:X:570:G:HO2'	1.64	0.45
27:X:577:U:H2'	27:X:579:G:OP2	2.17	0.45
27:X:768:U:C4	27:X:769:C:C4	3.05	0.45
28:Y:43:G:OP1	28:Y:45:C:N4	2.40	0.45
26:3:14:ILE:HD11	26:3:56:ALA:HB1	1.98	0.45
2:B:152:LYS:HB3	6:G:106:TYR:CB	2.44	0.45
7:H:24:VAL:HG22	7:H:45:ALA:HB2	1.97	0.45
8:I:56:LEU:HD21	8:I:59:ARG:HH21	1.82	0.45
17:R:105:ARG:HH22	17:R:112:LYS:HA	1.82	0.45
27:X:1083:C:H42	27:X:1103:C:N4	2.15	0.45
27:X:1225:G:H2'	27:X:1249:G:H22	1.81	0.45
27:X:1724:C:N3	27:X:1747:G:C6	2.85	0.45
27:X:172:A:H5''	27:X:173:A:OP2	2.17	0.45
27:X:1751:A:H2'	27:X:1752:U:C6	2.51	0.45
27:X:2519:C:O2	27:X:2720:A:H2	2.00	0.45
27:X:2499:C:C4	27:X:2546:G:C8	3.04	0.45
27:X:90:G:H3'	27:X:91:A:H8	1.80	0.45
9:J:42:TRP:CZ2	27:X:969:U:H5	2.35	0.45
25:2:25:LYS:HD3	25:2:25:LYS:HA	1.74	0.45
26:3:52:LYS:O	26:3:56:ALA:HB2	2.17	0.45
1:A:208:LYS:HD3	27:X:1782:A:H1'	1.99	0.45
1:A:231:HIS:CG	1:A:232:PRO:HD2	2.52	0.45
1:A:43:ARG:H	1:A:43:ARG:NH1	2.14	0.45
9:J:76:THR:HB	9:J:88:LYS:O	2.17	0.45
10:K:43:GLU:O	10:K:46:PRO:HD2	2.17	0.45
13:N:64:ARG:O	13:N:67:ALA:HB3	2.16	0.45
20:U:46:LEU:O	27:X:2209:G:O2'	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1223:G:N2	27:X:1249:G:O2'	2.49	0.45
27:X:1646:G:C5	27:X:1647:U:C5	3.04	0.45
27:X:16:G:H2'	27:X:17:G:H8	1.80	0.45
27:X:1736:C:H2'	27:X:1737:G:C8	2.52	0.45
27:X:2220:A:H2'	27:X:2221:G:H8	1.81	0.45
27:X:2306:A:O2'	27:X:2307:A:O5'	2.34	0.45
27:X:2579:A:H2'	27:X:2580:C:H6	1.81	0.45
27:X:725:C:H2'	27:X:726:G:C8	2.52	0.45
28:Y:71:G:C6	28:Y:72:C:C4	3.05	0.45
24:1:16:ALA:HB2	24:1:50:PHE:CE1	2.51	0.45
4:D:129:ASN:ND2	27:X:2282:G:O2'	2.49	0.45
2:B:145:LYS:HB2	27:X:2551:A:C8	2.51	0.45
27:X:36:G:N3	27:X:462:G:O2'	2.50	0.45
26:3:62:LEU:HA	26:3:62:LEU:HD12	1.86	0.45
3:C:65:GLY:O	15:P:112:ARG:NH2	2.50	0.45
5:E:25:LYS:HG3	5:E:34:THR:HG22	1.98	0.45
7:H:23:ARG:HH11	27:X:2541:U:H1'	1.82	0.45
10:K:98:LEU:O	10:K:111:ALA:HB1	2.17	0.45
20:U:78:ILE:HG12	20:U:79:GLU:H	1.81	0.45
21:V:15:ALA:O	21:V:18:ILE:HB	2.17	0.45
22:W:14:GLY:O	22:W:18:LYS:HG2	2.17	0.45
27:X:1098:G:C5	27:X:1100:G:H1'	2.51	0.45
27:X:1286:U:O2	27:X:1985:G:O2'	2.35	0.45
27:X:742:G:N2	27:X:1766:U:O4'	2.50	0.45
27:X:186:C:H2'	27:X:187:U:O4'	2.17	0.45
27:X:2368:G:H5''	27:X:2369:U:C5'	2.47	0.45
27:X:2513:A:C2	27:X:2514:G:H1'	2.50	0.45
27:X:2668:U:OP2	27:X:2847:G:N2	2.36	0.45
27:X:1982:C:OP1	27:X:2704:U:H5'	2.16	0.45
27:X:2859:U:C5	27:X:2860:C:C2	3.05	0.45
27:X:346:C:H2'	27:X:347:C:H6	1.80	0.45
27:X:231:G:H4'	27:X:397:U:H5''	1.99	0.45
27:X:242:A:C8	27:X:441:A:N6	2.84	0.45
27:X:587:A:OP1	27:X:1268:U:O2'	2.26	0.45
27:X:809:C:H2'	27:X:810:U:C6	2.52	0.45
27:X:828:C:H2'	27:X:829:C:H6	1.82	0.45
27:X:838:A:H2'	27:X:839:U:O4'	2.17	0.45
1:A:107:ALA:HA	1:A:108:PRO:HD2	1.82	0.45
6:G:124:GLU:O	6:G:128:GLU:HG2	2.17	0.45
9:J:15:ARG:NE	9:J:73:LYS:HZ2	2.15	0.45
11:L:88:VAL:HG11	27:X:2357:A:H1'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:120:ILE:HG12	27:X:1996:A:OP1	2.17	0.45
17:R:105:ARG:HH22	17:R:113:THR:N	2.10	0.45
17:R:38:LEU:HD22	17:R:40:LEU:HG	1.99	0.45
27:X:1418:C:H2'	27:X:1419:G:C8	2.52	0.45
27:X:1987:G:C6	27:X:1988:A:C4	3.05	0.45
26:3:7:HIS:NE2	27:X:220:U:OP2	2.47	0.45
27:X:658:G:H1'	27:X:2330:G:OP1	2.17	0.45
27:X:2579:A:H2'	27:X:2580:C:C6	2.52	0.45
27:X:2656:G:H1	27:X:2710:C:H42	1.63	0.45
27:X:2706:U:OP1	27:X:2706:U:C6	2.70	0.45
27:X:2738:A:H2'	27:X:2739:G:O4'	2.17	0.45
27:X:659:G:H2'	27:X:660:G:C8	2.51	0.45
24:1:9:ILE:HG13	24:1:10:VAL:N	2.32	0.45
2:B:109:LYS:NZ	27:X:2703:C:OP2	2.50	0.45
2:B:95:ILE:HA	2:B:95:ILE:HD13	1.82	0.45
3:C:17:LEU:HG	3:C:109:ALA:HB2	1.99	0.45
5:E:109:TYR:CD2	27:X:2646:C:H1'	2.51	0.45
14:O:83:ARG:HG2	27:X:1238:A:H4'	1.99	0.45
19:T:29:GLU:HG2	27:X:935:C:H1'	1.98	0.45
27:X:2034:A:H2	27:X:2035:G:O6	1.99	0.45
27:X:2796:A:O2'	27:X:2801:A:N1	2.46	0.45
27:X:2792:C:C2	27:X:2805:G:C2	3.05	0.45
27:X:513:A:H5''	27:X:514:G:H5'	1.99	0.45
27:X:699:G:H5''	27:X:699:G:H8	1.82	0.45
25:2:36:ALA:C	25:2:38:GLY:H	2.21	0.44
2:B:115:GLY:O	2:B:119:ARG:HB2	2.17	0.44
2:B:152:LYS:CB	6:G:106:TYR:HB2	2.45	0.44
6:G:94:LYS:HE2	6:G:94:LYS:HB3	1.48	0.44
8:I:22:GLY:HA3	27:X:674:U:O2'	2.17	0.44
13:N:93:LYS:H	13:N:93:LYS:HG3	1.49	0.44
20:U:49:LYS:HB2	20:U:61:TRP:HA	1.99	0.44
22:W:12:ARG:HA	22:W:13:PRO:HD3	1.83	0.44
27:X:1121:G:H2'	27:X:1122:A:C8	2.52	0.44
27:X:1468:A:OP2	27:X:1468:A:C8	2.69	0.44
20:U:37:ILE:HD12	27:X:177:U:O2'	2.17	0.44
27:X:2053:G:C2	27:X:2054:A:C4	3.05	0.44
27:X:2269:G:N2	27:X:2322:U:H1'	2.32	0.44
27:X:2495:G:C6	27:X:2548:G:C2	3.05	0.44
27:X:2864:C:H2'	27:X:2865:G:C8	2.52	0.44
27:X:577:U:O2'	27:X:579:G:N7	2.42	0.44
27:X:649:G:C8	27:X:650:U:H5	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:613:A:N7	27:X:668:A:H1'	2.31	0.44
28:Y:56:G:O5'	28:Y:56:G:H8	2.00	0.44
28:Y:80:A:H2'	28:Y:81:C:O4'	2.17	0.44
1:A:142:VAL:HG12	1:A:193:ILE:HA	1.98	0.44
1:A:32:ALA:HB3	1:A:83:GLU:CD	2.38	0.44
2:B:134:TRP:HB2	2:B:135:HIS:CD2	2.52	0.44
4:D:115:ARG:HH22	4:D:178:ARG:NH1	2.12	0.44
7:H:116:ARG:CZ	12:M:38:LYS:HD2	2.47	0.44
15:P:11:LYS:HD2	27:X:1225:G:N7	2.32	0.44
17:R:105:ARG:NH2	17:R:112:LYS:HA	2.32	0.44
17:R:14:LEU:HD21	17:R:41:PRO:HA	1.99	0.44
17:R:23:ILE:HG22	17:R:33:THR:HB	1.98	0.44
16:Q:10:PRO:HD3	21:V:30:PHE:CD2	2.52	0.44
27:X:1210:C:C2	27:X:1211:G:C8	3.05	0.44
27:X:1329:U:O2'	27:X:1330:G:H5'	2.17	0.44
27:X:2058:U:C4	27:X:2217:G:C6	3.05	0.44
27:X:205:A:H2'	27:X:206:U:H5'	1.99	0.44
27:X:2451:G:H22	27:X:2456:U:H5''	1.81	0.44
27:X:2728:A:H2'	27:X:2729:A:C8	2.51	0.44
27:X:495:C:H2'	27:X:496:C:C6	2.52	0.44
8:I:100:ARG:NH1	27:X:614:G:N7	2.64	0.44
1:A:24:LEU:HB3	1:A:25:THR:H	1.61	0.44
8:I:54:SER:HB3	8:I:55:ARG:HE	1.82	0.44
11:L:88:VAL:HG12	11:L:89:PHE:H	1.82	0.44
13:N:60:LEU:O	13:N:64:ARG:HG3	2.17	0.44
13:N:75:ASN:H	13:N:78:THR:HB	1.83	0.44
20:U:46:LEU:C	20:U:47:HIS:CG	2.90	0.44
27:X:588:G:C2	27:X:1275:A:C4	3.05	0.44
1:A:99:ASP:HB3	27:X:1507:A:O4'	2.17	0.44
27:X:2044:G:N2	27:X:2046:C:C2	2.85	0.44
11:L:91:ARG:HH22	27:X:2355:A:H61	1.66	0.44
27:X:2372:A:H62	27:X:2401:A:H61	1.65	0.44
27:X:2406:C:H5'	27:X:2408:G:H5'	1.99	0.44
27:X:354:C:H2'	27:X:355:G:H8	1.82	0.44
27:X:748:A:H5''	27:X:749:C:C5	2.52	0.44
28:Y:39:C:H5''	28:Y:40:C:C5	2.53	0.44
1:A:246:PRO:HG2	1:A:248:THR:O	2.18	0.44
1:A:16:MET:HE1	1:A:24:LEU:H	1.83	0.44
3:C:47:THR:N	3:C:51:VAL:HG21	2.32	0.44
3:C:39:ARG:HE	3:C:91:TYR:HD2	1.65	0.44
5:E:156:ALA:O	5:E:172:LYS:N	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:160:LYS:NZ	27:X:2637:C:H5'	2.32	0.44
8:I:73:GLU:OE2	8:I:73:GLU:N	2.50	0.44
18:S:3:LEU:HD11	18:S:33:ALA:H	1.81	0.44
16:Q:72:ARG:NH2	27:X:1324:G:O2'	2.51	0.44
27:X:1482:U:OP2	27:X:1562:G:O2'	2.35	0.44
27:X:2510:A:C2'	27:X:2511:G:H5'	2.48	0.44
27:X:1686:A:O3'	27:X:2528:G:H5'	2.17	0.44
23:Z:51:TYR:CD1	23:Z:55:ARG:HD3	2.53	0.44
1:A:208:LYS:O	1:A:211:ARG:HB2	2.18	0.44
5:E:88:GLU:HG3	5:E:130:ARG:HG2	1.99	0.44
6:G:134:MET:HG3	27:X:1148:G:O2'	2.17	0.44
6:G:151:TYR:HB2	6:G:157:PRO:HB3	1.99	0.44
7:H:8:LEU:HD22	7:H:94:ASN:HB3	2.00	0.44
12:M:22:ARG:NH1	12:M:22:ARG:HB3	2.32	0.44
27:X:1329:U:C2	27:X:1330:G:N7	2.85	0.44
27:X:1816:G:H2'	27:X:1817:U:H6	1.83	0.44
27:X:1882:G:N2	27:X:1885:C:N4	2.60	0.44
27:X:2495:G:O2'	27:X:2496:C:H5'	2.18	0.44
27:X:494:A:N7	27:X:507:A:H2	2.16	0.44
15:P:39:ARG:NH2	27:X:527:C:O2'	2.47	0.44
27:X:763:A:H2'	27:X:764:A:H5''	1.98	0.44
27:X:98:U:H4'	27:X:99:U:H5''	1.99	0.44
23:Z:4:HIS:HB3	27:X:2039:G:H22	1.83	0.44
26:3:57:ARG:O	26:3:61:MET:N	2.50	0.44
2:B:116:VAL:CG2	2:B:136:ARG:HG3	2.23	0.44
2:B:105:THR:CG2	2:B:197:VAL:HB	2.48	0.44
2:B:61:LYS:HB3	2:B:62:PRO:HD3	1.99	0.44
6:G:62:ILE:HG13	6:G:80:VAL:HG23	2.00	0.44
27:X:1065:A:H2'	27:X:1066:G:H8	1.83	0.44
27:X:2058:U:H1'	27:X:2576:G:H21	1.81	0.44
27:X:2251:U:H5''	27:X:2252:A:OP1	2.18	0.44
19:T:20:TYR:CD2	27:X:2335:U:H4'	2.52	0.44
27:X:2351:G:C2	27:X:2352:A:C5	3.06	0.44
27:X:245:C:H42	27:X:437:G:H1	1.64	0.44
27:X:748:A:H3'	27:X:749:C:C6	2.52	0.44
19:T:26:PHE:CD1	27:X:934:G:H1'	2.53	0.44
3:C:112:GLN:NE2	3:C:116:LYS:HD2	2.33	0.44
6:G:35:LYS:HA	6:G:35:LYS:HD3	1.44	0.44
7:H:17:ARG:H	7:H:58:ALA:HA	1.82	0.44
7:H:83:ARG:HD2	7:H:89:ILE:HD11	2.00	0.44
8:I:38:LYS:HG2	8:I:40:ARG:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:49:GLU:O	10:K:52:ILE:HG12	2.18	0.44
12:M:78:GLU:OE2	12:M:108:ARG:NE	2.48	0.44
16:Q:35:LYS:HB2	27:X:1614:C:H5''	2.00	0.44
27:X:1296:G:N2	27:X:1299:A:C8	2.85	0.44
27:X:1935:A:C6	27:X:1936:A:N1	2.85	0.44
27:X:2528:G:C2	27:X:2529:G:N7	2.85	0.44
27:X:2578:G:N2	27:X:2579:A:C4	2.86	0.44
27:X:448:C:H2'	27:X:449:C:O4'	2.18	0.44
27:X:580:A:H4'	27:X:581:A:OP1	2.17	0.44
27:X:840:U:H4'	27:X:841:G:N2	2.32	0.44
23:Z:16:ARG:HD3	23:Z:20:ARG:CZ	2.48	0.44
1:A:59:LYS:O	1:A:59:LYS:HG3	2.18	0.44
3:C:112:GLN:HE22	3:C:116:LYS:HD2	1.83	0.44
3:C:176:ASN:ND2	3:C:178:TYR:HB3	2.32	0.44
15:P:44:VAL:O	15:P:48:LYS:HD3	2.18	0.44
18:S:66:VAL:HG22	18:S:83:PHE:CE2	2.53	0.44
27:X:1679:U:O2	27:X:2666:U:H5''	2.18	0.44
27:X:1777:A:C4	27:X:1921:A:C6	3.06	0.44
27:X:1795:C:H2'	27:X:1796:A:C8	2.52	0.44
27:X:1810:U:HO2'	27:X:1811:A:P	2.40	0.44
27:X:2474:G:H2'	27:X:2475:C:O4'	2.18	0.44
27:X:2493:U:H2'	27:X:2494:C:H6	1.81	0.44
27:X:1773:C:H1'	27:X:2588:U:C5'	2.48	0.44
27:X:2634:G:O2'	27:X:2643:G:O6	2.28	0.44
27:X:586:G:C6	27:X:587:A:N6	2.86	0.44
27:X:616:U:O2'	27:X:671:A:H4'	2.18	0.44
27:X:753:U:H2'	27:X:754:G:C8	2.52	0.44
22:W:18:LYS:HB2	27:X:863:C:H4'	1.99	0.44
5:E:17:VAL:HG13	5:E:26:VAL:HG22	1.98	0.44
5:E:55:PRO:HD2	5:E:61:HIS:CD2	2.53	0.44
6:G:158:HIS:HA	6:G:161:GLN:HE22	1.83	0.44
15:P:27:VAL:CG1	27:X:504:G:H4'	2.48	0.44
15:P:29:LYS:HB3	15:P:30:TYR:CD2	2.52	0.44
27:X:1359:G:C6	27:X:1617:G:C6	3.06	0.44
27:X:1597:A:H2'	27:X:1598:C:C6	2.52	0.44
27:X:14:A:N6	27:X:15:G:C2	2.86	0.44
27:X:1698:C:O2'	27:X:1753:A:N3	2.42	0.44
27:X:2198:U:N3	27:X:2199:C:H1'	2.32	0.44
27:X:2201:G:H2'	27:X:2202:G:C8	2.51	0.44
27:X:226:C:H4'	27:X:227:G:O5'	2.18	0.44
27:X:796:A:H8	27:X:797:A:H4'	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LEU:HB2	1:A:187:SER:HA	2.00	0.43
1:A:222:ARG:HG3	27:X:1780:A:OP1	2.17	0.43
2:B:120:TRP:CE3	2:B:155:ARG:HD2	2.53	0.43
9:J:35:LEU:HD11	9:J:130:THR:HB	2.00	0.43
9:J:54:VAL:O	9:J:57:ARG:HB2	2.18	0.43
17:R:97:GLN:NE2	17:R:101:GLY:HA2	2.33	0.43
27:X:1026:U:H2'	27:X:1027:C:C6	2.53	0.43
27:X:1098:G:H22	27:X:1114:A:H1'	1.82	0.43
27:X:1043:A:H2	27:X:1133:G:H22	1.65	0.43
27:X:1580:C:H2'	27:X:1581:C:C6	2.53	0.43
27:X:1835:C:H2'	27:X:1836:C:C6	2.52	0.43
27:X:2670:C:H2'	27:X:2671:C:H6	1.83	0.43
27:X:1670:G:H5'	27:X:2797:G:N2	2.33	0.43
27:X:500:G:H2'	27:X:501:G:O4'	2.18	0.43
27:X:748:A:H3'	27:X:749:C:H6	1.83	0.43
27:X:957:G:H2'	27:X:958:G:H8	1.83	0.43
11:L:32:TYR:CZ	28:Y:9:G:H5'	2.53	0.43
8:I:56:LEU:HD22	26:3:52:LYS:HZ1	1.83	0.43
2:B:122:PHE:CE1	27:X:2491:C:H4'	2.53	0.43
2:B:95:ILE:HG22	2:B:96:PHE:CD1	2.53	0.43
4:D:12:VAL:HG22	4:D:172:SER:HB2	2.00	0.43
8:I:80:LEU:HD21	8:I:89:ASP:OD2	2.18	0.43
27:X:1141:U:HO2'	27:X:1142:G:P	2.39	0.43
27:X:1219:C:H2'	27:X:1220:G:O4'	2.18	0.43
27:X:1399:C:H2'	27:X:1400:A:C8	2.53	0.43
27:X:2307:A:H2'	27:X:2308:A:C8	2.53	0.43
27:X:2310:G:N2	27:X:2364:C:C4	2.86	0.43
27:X:2041:A:H61	30:X:2902:ERY:H282	1.83	0.43
27:X:649:G:H2'	27:X:650:U:H6	1.84	0.43
27:X:773:G:C2'	27:X:774:A:H5'	2.48	0.43
28:Y:64:C:H2'	28:Y:65:A:C8	2.52	0.43
1:A:108:PRO:HG2	1:A:111:LEU:HD12	2.00	0.43
1:A:254:THR:O	27:X:1836:C:H5'	2.19	0.43
8:I:63:ARG:HD3	26:3:30:ARG:HH22	1.82	0.43
11:L:8:ARG:HB2	11:L:8:ARG:CZ	2.48	0.43
12:M:103:LYS:O	12:M:104:LEU:HB2	2.18	0.43
13:N:81:ASN:ND2	27:X:1162:A:H4'	2.33	0.43
14:O:32:LYS:HD3	14:O:32:LYS:HA	1.77	0.43
14:O:39:PHE:CE2	14:O:46:VAL:HB	2.53	0.43
17:R:48:VAL:HG13	17:R:50:GLY:H	1.83	0.43
27:X:1336:G:O6	27:X:1337:G:C6	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1573:G:H3'	27:X:1574:A:H5''	2.00	0.43
27:X:1880:G:C6	27:X:1881:U:C4	3.06	0.43
27:X:2555:G:OP1	27:X:2555:G:H3'	2.19	0.43
26:3:15:LYS:HZ3	26:3:60:LEU:HD21	1.84	0.43
2:B:34:VAL:HG11	2:B:78:LEU:HD21	2.00	0.43
10:K:107:GLY:HA3	27:X:1992:G:H1'	2.00	0.43
21:V:41:HIS:CD2	27:X:95:G:H4'	2.52	0.43
27:X:1255:A:H2'	27:X:1256:C:H6	1.82	0.43
27:X:1712:G:H3'	27:X:1712:G:N3	2.34	0.43
27:X:1974:U:H6	27:X:1974:U:O5'	2.01	0.43
27:X:2017:U:H2'	27:X:2018:G:H5''	2.00	0.43
27:X:2048:C:H1'	27:X:2428:U:N3	2.33	0.43
27:X:2470:U:O2	27:X:2470:U:H2'	2.17	0.43
27:X:2511:G:C6	27:X:2512:A:C5	3.07	0.43
27:X:485:G:C6	27:X:520:C:N4	2.86	0.43
28:Y:27:A:N6	28:Y:55:C:H5''	2.34	0.43
28:Y:30:C:H2'	28:Y:31:A:C8	2.53	0.43
24:1:3:LYS:HB3	24:1:3:LYS:HE2	1.83	0.43
18:S:125:PRO:HA	18:S:158:CYS:SG	2.58	0.43
22:W:39:ALA:O	27:X:864:C:O2'	2.37	0.43
27:X:1493:A:H2'	27:X:1494:G:O4'	2.19	0.43
27:X:2027:C:C2'	27:X:2028:C:H5'	2.48	0.43
8:I:59:ARG:HA	27:X:2371:A:H8	1.81	0.43
27:X:2451:G:H2'	27:X:2454:C:H42	1.83	0.43
27:X:529:U:H2'	27:X:530:G:H8	1.83	0.43
27:X:611:C:N4	27:X:612:G:C5	2.86	0.43
27:X:754:G:H2'	27:X:755:C:C6	2.53	0.43
27:X:859:U:H3	27:X:944:A:H61	1.66	0.43
27:X:956:A:C4	27:X:2427:A:C2	3.06	0.43
23:Z:10:LYS:HG3	27:X:1276:U:O4'	2.18	0.43
25:2:8:ASN:HB3	25:2:11:LYS:HB3	2.00	0.43
25:2:42:LEU:H	25:2:42:LEU:HD12	1.83	0.43
2:B:54:LYS:HB3	2:B:74:PRO:HB2	2.00	0.43
4:D:52:LYS:HE3	4:D:147:ASP:HB2	2.01	0.43
4:D:66:ILE:HD12	28:Y:44:C:C6	2.54	0.43
5:E:103:LEU:HD21	5:E:105:MET:HG3	1.99	0.43
6:G:46:ALA:HB2	6:G:54:LEU:HD22	2.00	0.43
7:H:104:GLU:HB3	7:H:125:LYS:HD2	1.99	0.43
11:L:32:TYR:CG	28:Y:9:G:H4'	2.54	0.43
12:M:101:ARG:HG2	12:M:101:ARG:HH21	1.84	0.43
14:O:48:GLY:C	14:O:50:ASP:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:15:SER:OG	14:O:96:LEU:HD13	2.18	0.43
18:S:130:ILE:HD12	18:S:130:ILE:H	1.84	0.43
20:U:48:LYS:HE2	20:U:48:LYS:HB2	1.76	0.43
27:X:1574:A:H2'	27:X:1575:C:H5''	2.00	0.43
1:A:63:ARG:HH22	27:X:1584:G:P	2.42	0.43
1:A:258:LYS:HG3	27:X:1790:G:OP1	2.18	0.43
27:X:2224:U:H5''	27:X:2225:G:H5'	2.00	0.43
27:X:240:U:H2'	27:X:241:C:O4'	2.19	0.43
27:X:617:U:C5	27:X:632:A:N1	2.87	0.43
27:X:632:A:C2	27:X:633:G:C4	3.07	0.43
24:1:54:LYS:HB2	24:1:54:LYS:HE2	1.76	0.43
26:3:25:PHE:CG	26:3:46:LYS:HA	2.54	0.43
1:A:188:GLU:H	1:A:188:GLU:HG2	1.46	0.43
15:P:60:ILE:HA	15:P:61:PRO:HD3	1.67	0.43
19:T:57:HIS:N	19:T:57:HIS:CD2	2.87	0.43
27:X:1398:G:O2'	27:X:1399:C:O5'	2.36	0.43
27:X:1949:A:O2'	27:X:2572:U:H5'	2.18	0.43
27:X:2234:G:C6	27:X:2235:G:C4	3.06	0.43
27:X:2367:A:N7	27:X:2368:G:C5	2.87	0.43
27:X:734:G:C2	27:X:735:G:C8	3.07	0.43
1:A:91:ARG:NH1	1:A:109:GLU:HA	2.34	0.43
1:A:248:THR:HG22	1:A:249:PRO:HD2	2.01	0.43
7:H:7:ARG:HB3	7:H:18:GLU:OE2	2.18	0.43
11:L:33:ARG:HH11	11:L:99:ARG:HD2	1.84	0.43
12:M:104:LEU:HD23	12:M:106:TYR:CE2	2.54	0.43
15:P:109:ARG:HD2	15:P:109:ARG:O	2.19	0.43
18:S:49:THR:O	18:S:49:THR:OG1	2.37	0.43
27:X:1408:A:C6	27:X:1411:C:C2	3.07	0.43
27:X:1429:A:N6	27:X:1600:U:H4'	2.33	0.43
27:X:1769:U:H2'	27:X:1775:A:H62	1.83	0.43
27:X:187:U:H2'	27:X:188:G:C8	2.54	0.43
27:X:2262:C:C2	27:X:2368:G:C2	3.06	0.43
27:X:883:A:H2'	27:X:884:C:O4'	2.19	0.43
24:1:9:ILE:O	24:1:10:VAL:HB	2.17	0.43
1:A:124:GLU:HA	1:A:125:PRO:HD3	1.80	0.43
1:A:24:LEU:HD22	1:A:205:VAL:HG13	2.00	0.43
8:I:17:LYS:HB3	8:I:17:LYS:HE2	1.81	0.43
8:I:42:GLY:H	8:I:45:LYS:HE3	1.84	0.43
8:I:77:LEU:HB2	8:I:110:ALA:HA	2.01	0.43
9:J:136:GLU:OE1	9:J:137:VAL:HB	2.19	0.43
15:P:9:ARG:HB3	15:P:10:ASN:H	1.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:99:ALA:O	15:P:124:THR:HG22	2.19	0.43
27:X:1154:A:OP1	27:X:1154:A:H8	2.01	0.43
27:X:1370:U:H2'	27:X:1371:G:C8	2.53	0.43
27:X:172:A:H61	27:X:175:C:H3'	1.84	0.43
27:X:17:G:H1	27:X:533:C:H42	1.66	0.43
27:X:194:G:H3'	27:X:195:A:H8	1.84	0.43
27:X:1845:A:N1	27:X:2070:G:H1'	2.34	0.43
27:X:2574:G:N1	27:X:2578:G:C6	2.86	0.43
27:X:78:C:H2'	27:X:79:G:H8	1.84	0.43
23:Z:6:VAL:HG13	23:Z:7:PRO:O	2.19	0.43
26:3:13:ARG:HD2	26:3:24:ALA:HA	2.01	0.43
26:3:9:MET:N	26:3:9:MET:SD	2.92	0.43
1:A:39:LYS:HE2	1:A:87:ASN:HD21	1.84	0.43
1:A:87:ASN:O	27:X:1809:G:H5''	2.19	0.43
4:D:51:ASP:O	4:D:55:LYS:HG2	2.18	0.43
6:G:71:THR:HG22	6:G:76:GLN:OE1	2.17	0.43
9:J:126:LEU:HA	9:J:127:PRO:HD3	1.86	0.43
9:J:15:ARG:HE	9:J:73:LYS:NZ	2.17	0.43
12:M:38:LYS:HE2	12:M:38:LYS:HB3	1.78	0.43
13:N:101:ARG:O	13:N:103:PRO:HD3	2.18	0.43
13:N:20:ARG:HH22	14:O:72:ARG:HD3	1.83	0.43
19:T:40:GLN:HE21	19:T:57:HIS:HB3	1.84	0.43
27:X:1196:G:H2'	27:X:1197:U:O4'	2.19	0.43
23:Z:40:LYS:HD3	23:Z:46:CYS:HB2	1.99	0.43
26:3:23:MET:HB3	26:3:25:PHE:HE2	1.82	0.42
1:A:218:LYS:HD2	1:A:219:PRO:HD2	2.00	0.42
3:C:46:ARG:HD2	3:C:51:VAL:HG11	2.01	0.42
4:D:104:ILE:HD13	4:D:173:MET:HB3	2.01	0.42
4:D:65:PRO:HA	4:D:89:VAL:HG22	2.00	0.42
5:E:175:LYS:HD3	5:E:175:LYS:HA	1.74	0.42
7:H:3:MET:O	7:H:6:SER:HB3	2.19	0.42
9:J:61:ARG:NH1	18:S:175:ARG:HD3	2.34	0.42
18:S:141:MET:SD	18:S:147:ILE:HG12	2.59	0.42
20:U:17:SER:CB	20:U:44:ALA:HA	2.49	0.42
22:W:46:THR:HG22	22:W:47:VAL:HG13	2.01	0.42
27:X:69:G:H5''	27:X:111:G:H1'	2.01	0.42
27:X:1281:A:H2'	27:X:1282:A:O4'	2.19	0.42
27:X:149:A:H2'	27:X:150:A:C8	2.54	0.42
27:X:2044:G:H2'	27:X:2480:C:O2'	2.19	0.42
27:X:2331:A:C4	27:X:2345:A:C2	3.06	0.42
3:C:97:ARG:HA	3:C:100:ARG:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:40:PRO:HB3	9:J:99:LYS:HD2	2.00	0.42
10:K:20:LEU:HD23	10:K:21:ALA:N	2.35	0.42
12:M:104:LEU:HD22	12:M:107:LEU:HD11	2.01	0.42
13:N:24:PHE:O	13:N:29:SER:HB3	2.19	0.42
13:N:65:ILE:HD13	13:N:95:LEU:HD22	2.01	0.42
13:N:81:ASN:CG	27:X:1162:A:H4'	2.39	0.42
14:O:39:PHE:HE2	14:O:46:VAL:HB	1.84	0.42
14:O:72:ARG:HA	14:O:82:ARG:O	2.18	0.42
20:U:15:VAL:HG23	20:U:16:ASN:H	1.83	0.42
20:U:20:ARG:HD3	20:U:43:ARG:HD2	2.01	0.42
27:X:1260:A:C6	27:X:1262:U:C2	3.07	0.42
27:X:1330:G:H2'	27:X:1331:G:O4'	2.19	0.42
5:E:157:TYR:CZ	27:X:2510:A:H5'	2.53	0.42
27:X:2559:U:C2'	27:X:2560:G:H5'	2.49	0.42
27:X:565:A:O5'	27:X:565:A:H8	2.02	0.42
27:X:745:C:H2'	27:X:746:G:O4'	2.19	0.42
27:X:820:U:H1'	27:X:2424:G:OP1	2.19	0.42
24:1:8:ILE:HD13	24:1:8:ILE:H	1.85	0.42
1:A:133:LEU:HA	1:A:133:LEU:HD23	1.91	0.42
1:A:210:GLY:HA2	1:A:213:ARG:CG	2.45	0.42
1:A:183:ARG:NH2	1:A:263:ARG:HB3	2.34	0.42
5:E:106:ASN:HD22	5:E:112:PRO:HB3	1.84	0.42
7:H:109:ARG:HA	7:H:129:LEU:HD22	2.00	0.42
7:H:129:LEU:HD23	7:H:129:LEU:HA	1.74	0.42
14:O:26:GLN:HG2	14:O:27:GLY:N	2.34	0.42
14:O:85:GLY:H	27:X:1238:A:H5'	1.84	0.42
17:R:25:LEU:H	17:R:80:LYS:HA	1.83	0.42
20:U:68:ARG:O	20:U:72:LYS:HG2	2.19	0.42
27:X:1032:A:O2'	27:X:1134:C:H5''	2.19	0.42
27:X:105:G:C2	27:X:106:G:C8	3.07	0.42
27:X:1466:C:N4	27:X:1476:G:H1	2.16	0.42
27:X:1603:A:H2'	27:X:1604:A:H8	1.84	0.42
27:X:1742:G:C2	27:X:1743:C:C4	3.07	0.42
27:X:1832:G:H1	27:X:1885:C:H42	1.65	0.42
27:X:2011:U:H2'	27:X:2012:A:C8	2.54	0.42
27:X:2328:G:H1	27:X:2347:C:H42	1.66	0.42
27:X:2221:G:H22	27:X:2413:A:H2	1.67	0.42
27:X:488:A:H8	27:X:488:A:OP1	2.02	0.42
27:X:725:C:H2'	27:X:726:G:H8	1.84	0.42
27:X:795:A:OP2	27:X:1768:U:O2'	2.26	0.42
27:X:475:U:C2	27:X:801:A:C6	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:764:A:C2	27:X:802:A:C4	3.07	0.42
27:X:877:G:H1	27:X:924:C:H42	1.67	0.42
11:L:39:TYR:OH	28:Y:117:G:N2	2.52	0.42
1:A:16:MET:HE1	1:A:23:GLY:HA2	2.01	0.42
4:D:4:LEU:CG	4:D:5:LYS:H	2.27	0.42
15:P:119:ILE:HG13	15:P:120:ILE:N	2.35	0.42
15:P:73:ASN:O	15:P:77:ALA:N	2.42	0.42
2:B:147:PRO:HD3	27:X:1141:U:C5	2.54	0.42
27:X:1227:A:H4'	27:X:1252:C:H4'	2.02	0.42
25:2:44:VAL:HG11	27:X:124:A:OP1	2.19	0.42
27:X:1469:U:H5'	27:X:1470:G:OP2	2.20	0.42
27:X:2780:A:N3	27:X:2780:A:H2'	2.35	0.42
28:Y:39:C:N4	28:Y:50:U:O2'	2.53	0.42
4:D:90:THR:OG1	28:Y:44:C:N3	2.42	0.42
28:Y:42:U:O2'	28:Y:45:C:N4	2.53	0.42
27:X:930:A:C2	28:Y:82:U:H4'	2.55	0.42
2:B:131:SER:C	2:B:134:TRP:HE1	2.19	0.42
3:C:156:ASN:HA	3:C:159:ARG:HH21	1.84	0.42
4:D:118:ASN:HB3	4:D:122:PHE:HZ	1.85	0.42
6:G:119:LEU:HA	6:G:119:LEU:HD13	1.64	0.42
8:I:90:ARG:HA	8:I:121:HIS:CG	2.54	0.42
9:J:53:ILE:O	9:J:57:ARG:HG2	2.20	0.42
10:K:60:LEU:CG	10:K:64:ARG:HD2	2.36	0.42
14:O:6:GLN:HB2	14:O:7:THR:H	1.66	0.42
15:P:64:ALA:O	15:P:67:PRO:HD2	2.20	0.42
16:Q:43:GLN:HG2	16:Q:48:VAL:O	2.20	0.42
17:R:52:ASN:HB2	17:R:73:GLU:HA	2.01	0.42
27:X:1086:C:H2'	27:X:1087:C:H5''	2.01	0.42
27:X:14:A:C5	27:X:536:A:C2	3.07	0.42
27:X:2284:U:H5'	27:X:2286:G:N1	2.32	0.42
27:X:2432:A:O2'	27:X:2551:A:H1'	2.19	0.42
27:X:2817:A:H2'	27:X:2818:G:O4'	2.19	0.42
27:X:398:C:N4	27:X:424:G:H1	2.18	0.42
27:X:54:G:H2'	27:X:55:A:H8	1.83	0.42
27:X:564:U:H2'	27:X:565:A:C8	2.54	0.42
27:X:748:A:H5''	27:X:749:C:H5	1.84	0.42
2:B:5:LEU:CD2	2:B:195:LEU:HD11	2.49	0.42
3:C:128:ALA:O	3:C:130:THR:N	2.51	0.42
3:C:48:ARG:H	3:C:48:ARG:HG3	1.45	0.42
4:D:105:ASN:O	4:D:109:PRO:HG2	2.19	0.42
4:D:161:LYS:HG3	4:D:162:THR:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:17:LYS:HG3	8:I:19:VAL:N	2.31	0.42
9:J:123:GLY:HA2	9:J:126:LEU:HD12	2.01	0.42
14:O:26:GLN:HG3	14:O:63:HIS:HD2	1.85	0.42
15:P:109:ARG:HG3	15:P:109:ARG:H	1.64	0.42
17:R:52:ASN:HB2	17:R:72:ARG:O	2.20	0.42
22:W:38:PRO:HB2	27:X:865:A:O2'	2.20	0.42
6:G:103:TYR:CD2	27:X:1142:G:O4'	2.73	0.42
27:X:1016:C:C2	27:X:1154:A:C5	3.07	0.42
27:X:1437:A:H2'	27:X:1438:G:H8	1.85	0.42
27:X:1562:G:H8	27:X:1562:G:OP2	2.03	0.42
27:X:2424:G:O2'	27:X:2425:G:H5'	2.19	0.42
20:U:68:ARG:NH1	27:X:413:G:N7	2.67	0.42
27:X:427:C:H2'	27:X:428:A:C8	2.54	0.42
27:X:340:G:O4'	27:X:488:A:H1'	2.20	0.42
27:X:788:G:C4	27:X:807:A:C8	3.08	0.42
27:X:802:A:OP2	27:X:802:A:H8	2.02	0.42
24:1:17:GLY:O	24:1:19:GLY:N	2.51	0.42
1:A:207:GLY:O	27:X:1782:A:O2'	2.35	0.42
1:A:94:LEU:HD12	1:A:95:LEU:N	2.35	0.42
1:A:96:HIS:HE1	1:A:100:GLY:HA2	1.84	0.42
10:K:39:THR:OG1	27:X:1668:G:H5'	2.20	0.42
12:M:19:ASP:OD2	12:M:19:ASP:N	2.33	0.42
13:N:89:ASP:HB3	13:N:91:ASN:HB2	2.02	0.42
14:O:10:LYS:HE3	14:O:13:ARG:NH2	2.35	0.42
14:O:6:GLN:HG2	27:X:1007:A:O2'	2.19	0.42
14:O:82:ARG:HD3	14:O:82:ARG:HA	1.56	0.42
17:R:15:HIS:HE1	17:R:80:LYS:HE2	1.84	0.42
27:X:102:C:C4	27:X:103:U:C4	3.08	0.42
27:X:1454:U:H2'	27:X:1455:C:H6	1.83	0.42
27:X:2327:U:H6	27:X:2327:U:O5'	2.03	0.42
27:X:590:C:H2'	27:X:591:G:H8	1.84	0.42
27:X:964:A:H2'	27:X:965:G:O4'	2.19	0.42
24:1:8:ILE:O	24:1:9:ILE:HG12	2.20	0.42
25:2:3:ARG:HD3	25:2:3:ARG:HA	1.51	0.42
2:B:103:ASP:O	2:B:199:ARG:HG3	2.20	0.42
3:C:45:THR:HG21	3:C:85:GLY:HA3	2.00	0.42
5:E:130:ARG:CZ	5:E:130:ARG:HB3	2.49	0.42
6:G:43:VAL:HG21	6:G:158:HIS:CE1	2.53	0.42
11:L:97:HIS:CG	11:L:98:GLY:N	2.85	0.42
13:N:72:HIS:CD2	13:N:110:VAL:HG21	2.55	0.42
14:O:64:GLY:HA3	14:O:90:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:4:TYR:HB3	21:V:26:MET:HE2	2.02	0.42
27:X:1730:G:N2	27:X:1736:C:O2	2.51	0.42
27:X:1812:U:H2'	27:X:1812:U:O2	2.20	0.42
27:X:2043:A:O4'	27:X:2481:G:H1'	2.20	0.42
27:X:2263:C:O2'	27:X:2267:A:N6	2.53	0.42
27:X:2696:A:H2'	27:X:2697:G:H8	1.84	0.42
27:X:459:A:N1	27:X:466:A:O2'	2.45	0.42
27:X:591:G:H3'	27:X:592:G:C8	2.42	0.42
1:A:67:PHE:CE2	1:A:106:LEU:HD11	2.54	0.42
2:B:133:LYS:C	2:B:134:TRP:CD1	2.93	0.42
2:B:195:LEU:HB3	12:M:2:GLN:HE21	1.84	0.42
9:J:64:LYS:O	9:J:107:VAL:HA	2.19	0.42
14:O:78:VAL:HG22	27:X:1202:U:H5'	2.02	0.42
27:X:762:A:H4'	27:X:1284:G:N3	2.34	0.42
16:Q:64:ARG:HH21	27:X:1349:A:H5'	1.84	0.42
27:X:1484:G:H2'	27:X:1485:U:H6	1.85	0.42
27:X:1505:U:H1'	27:X:1506:C:C5	2.55	0.42
27:X:1810:U:O2'	27:X:1811:A:O5'	2.36	0.42
27:X:459:A:O4'	27:X:461:A:N6	2.53	0.42
27:X:485:G:C5	27:X:520:C:N4	2.88	0.42
27:X:615:C:H1'	27:X:670:U:H1'	2.00	0.42
27:X:797:A:N7	27:X:805:G:C4	2.88	0.42
28:Y:58:G:H5"	28:Y:59:A:OP1	2.20	0.42
25:2:4:THR:O	27:X:700:C:H5'	2.19	0.42
3:C:176:ASN:HD22	3:C:178:TYR:HB3	1.85	0.42
5:E:44:ARG:HH22	5:E:51:LEU:HD23	1.85	0.42
6:G:116:ARG:HE	6:G:126:VAL:HG13	1.85	0.42
8:I:84:GLU:OE2	8:I:87:THR:OG1	2.30	0.42
9:J:119:PHE:CD1	9:J:132:MET:HB2	2.55	0.42
27:X:1212:U:H2'	27:X:1213:U:C6	2.55	0.42
13:N:10:ARG:HG3	27:X:1264:C:OP1	2.19	0.42
27:X:48:A:H61	27:X:154:U:H2'	1.85	0.42
27:X:2321:C:O2'	27:X:2353:G:H5"	2.20	0.42
25:2:24:THR:OG1	25:2:25:LYS:N	2.53	0.41
25:2:25:LYS:O	25:2:29:ASN:HB2	2.20	0.41
1:A:118:ASN:HD22	1:A:119:ALA:H	1.68	0.41
1:A:69:ARG:NH1	1:A:128:GLY:O	2.40	0.41
2:B:17:ASN:HB3	2:B:18:ASP:H	1.57	0.41
2:B:48:GLN:NE2	27:X:2614:A:O2'	2.53	0.41
12:M:44:ARG:NH2	12:M:46:ARG:HE	2.18	0.41
20:U:49:LYS:HB3	20:U:61:TRP:CE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:742:G:C2	27:X:1766:U:C6	3.08	0.41
27:X:1788:C:C4	27:X:1789:U:C4	3.07	0.41
27:X:2048:C:H1'	27:X:2428:U:C2	2.55	0.41
27:X:2189:A:H61	27:X:2190:A:N6	2.18	0.41
27:X:2338:C:H2'	27:X:2339:A:C8	2.55	0.41
27:X:2553:G:C2	27:X:2554:C:O2	2.73	0.41
27:X:502:A:H2'	27:X:503:G:O4'	2.19	0.41
27:X:753:U:H2'	27:X:754:G:H8	1.85	0.41
28:Y:75:A:H4'	28:Y:75:A:OP1	2.19	0.41
18:S:79:ILE:HD11	28:Y:78:A:O2'	2.19	0.41
26:3:50:LEU:HD23	26:3:53:ALA:CB	2.50	0.41
1:A:133:LEU:HD23	1:A:136:VAL:HG21	2.01	0.41
3:C:10:ASN:OD1	3:C:13:ARG:NH1	2.53	0.41
6:G:116:ARG:HD2	6:G:119:LEU:HG	2.02	0.41
7:H:101:ASN:N	7:H:101:ASN:HD22	2.18	0.41
9:J:75:VAL:HG21	9:J:93:TYR:HE1	1.86	0.41
13:N:66:ASN:HB2	13:N:70:ARG:HH11	1.85	0.41
15:P:35:PRO:O	15:P:39:ARG:HD3	2.20	0.41
17:R:96:LYS:O	17:R:104:VAL:HA	2.20	0.41
27:X:1137:A:H4'	27:X:1138:A:O5'	2.19	0.41
27:X:1615:C:H2'	27:X:1616:C:C6	2.55	0.41
27:X:1793:A:N1	27:X:1814:G:H1'	2.35	0.41
27:X:2188:A:H2'	27:X:2189:A:N7	2.36	0.41
27:X:627:A:C6	27:X:628:A:C6	3.08	0.41
27:X:837:U:H2'	27:X:838:A:C8	2.54	0.41
9:J:12:LYS:HD3	27:X:923:A:N7	2.34	0.41
22:W:22:ALA:HA	27:X:942:U:O2'	2.20	0.41
24:1:28:ARG:O	24:1:33:ALA:HB2	2.20	0.41
2:B:136:ARG:O	2:B:137:ARG:C	2.59	0.41
3:C:178:TYR:OH	27:X:1216:G:O2'	2.32	0.41
3:C:180:ILE:HG22	3:C:186:LEU:HD13	2.03	0.41
4:D:102:LYS:O	4:D:106:ILE:HB	2.21	0.41
5:E:11:VAL:HA	5:E:12:PRO:HD2	1.95	0.41
8:I:44:GLY:HA2	27:X:684:C:H5	1.84	0.41
8:I:86:THR:HG21	8:I:117:ALA:O	2.20	0.41
12:M:8:ASN:HA	27:X:2851:G:O5'	2.21	0.41
14:O:93:ILE:HG13	14:O:95:ILE:HD11	2.02	0.41
17:R:84:VAL:HB	17:R:88:THR:O	2.20	0.41
27:X:1030:U:C4	27:X:1031:C:H5	2.38	0.41
27:X:1447:U:HO2'	27:X:1448:A:H8	1.69	0.41
27:X:182:G:HO2'	27:X:183:U:P	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2499:C:N3	27:X:2546:G:C8	2.88	0.41
27:X:2578:G:C2	27:X:2579:A:C4	3.08	0.41
27:X:2705:A:H8	27:X:2706:U:O2'	2.03	0.41
3:C:162:ARG:NH2	27:X:331:U:O2'	2.54	0.41
28:Y:53:G:H2'	28:Y:54:U:H5''	2.02	0.41
1:A:257:LEU:HB3	27:X:1794:A:O3'	2.21	0.41
1:A:49:ILE:HG22	27:X:792:U:OP1	2.20	0.41
4:D:79:LEU:HA	4:D:79:LEU:HD23	1.92	0.41
9:J:49:GLU:OE2	9:J:52:ARG:NH2	2.54	0.41
10:K:28:LEU:CD2	10:K:115:LEU:HG	2.49	0.41
10:K:73:LYS:HA	10:K:76:VAL:HG12	2.03	0.41
17:R:40:LEU:HA	17:R:41:PRO:HD2	1.95	0.41
27:X:1228:G:C6	27:X:1229:C:C4	3.08	0.41
27:X:1841:G:H1	27:X:1876:C:H42	1.68	0.41
27:X:2046:C:O2	27:X:2430:A:C2	2.74	0.41
27:X:2283:G:N3	27:X:2283:G:H2'	2.35	0.41
27:X:2447:G:O2'	27:X:2448:A:H8	1.85	0.41
27:X:2705:A:O2'	27:X:2706:U:O5'	2.33	0.41
27:X:640:C:H5''	27:X:660:G:O2'	2.20	0.41
27:X:671:A:H2'	27:X:672:C:O4'	2.20	0.41
23:Z:36:CYS:HB3	23:Z:49:CYS:HB3	1.94	0.41
1:A:157:ARG:HH11	1:A:157:ARG:HB2	1.85	0.41
5:E:86:ASN:O	5:E:165:VAL:HG22	2.20	0.41
5:E:95:ARG:HH22	5:E:97:LYS:HD3	1.86	0.41
6:G:67:ARG:HB2	6:G:67:ARG:HH11	1.86	0.41
8:I:62:LYS:HB3	26:3:13:ARG:N	2.35	0.41
8:I:62:LYS:HG3	8:I:63:ARG:N	2.35	0.41
9:J:14:PHE:HE1	9:J:90:ALA:HA	1.86	0.41
11:L:14:ARG:HB2	11:L:14:ARG:HE	1.50	0.41
13:N:99:ALA:HB2	13:N:106:PHE:CE1	2.56	0.41
19:T:23:VAL:HB	19:T:26:PHE:CE2	2.54	0.41
19:T:37:LEU:HD11	19:T:61:ALA:HB2	2.03	0.41
27:X:1010:U:O2'	27:X:1011:A:H5'	2.20	0.41
27:X:1024:G:H2'	27:X:1025:A:C8	2.55	0.41
27:X:1278:A:H2	27:X:1997:A:N6	2.09	0.41
27:X:1462:C:C2	27:X:1480:G:N2	2.89	0.41
27:X:1642:G:H8	27:X:1642:G:O5'	2.03	0.41
7:H:37:GLY:O	27:X:2542:U:H5''	2.20	0.41
27:X:2667:C:N4	27:X:2700:U:OP2	2.41	0.41
27:X:525:A:C8	27:X:526:C:C6	3.09	0.41
8:I:74:VAL:HG11	27:X:638:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:726:G:H1'	27:X:731:A:H61	1.86	0.41
23:Z:15:LYS:O	23:Z:18:MET:HB3	2.19	0.41
1:A:124:GLU:O	1:A:126:LYS:N	2.52	0.41
2:B:5:LEU:HD21	2:B:79:ARG:CG	2.50	0.41
3:C:152:THR:OG1	3:C:153:ASP:N	2.53	0.41
4:D:132:ILE:HG13	4:D:154:ILE:HD13	2.03	0.41
6:G:134:MET:HE3	6:G:134:MET:HB3	1.58	0.41
11:L:12:ARG:HG3	11:L:13:THR:N	2.35	0.41
8:I:33:GLY:CA	14:O:79:GLN:HG3	2.49	0.41
15:P:72:LEU:HA	15:P:129:ILE:HD12	2.01	0.41
15:P:27:VAL:HG23	15:P:128:THR:HG22	2.02	0.41
21:V:41:HIS:ND1	27:X:94:C:O2'	2.33	0.41
27:X:1031:C:OP1	27:X:1045:G:N2	2.30	0.41
16:Q:64:ARG:NH1	27:X:1348:C:H4'	2.35	0.41
27:X:176:A:H2	27:X:2061:C:HO2'	1.65	0.41
27:X:2557:G:OP1	27:X:2593:A:N6	2.53	0.41
27:X:2733:A:H2'	27:X:2734:U:O4'	2.20	0.41
2:B:62:PRO:HG3	27:X:2767:C:H1'	2.01	0.41
30:X:2902:ERY:H71	30:X:2902:ERY:H4	1.92	0.41
27:X:645:G:H2'	27:X:646:C:C6	2.55	0.41
27:X:828:C:C2	27:X:1207:G:C2	3.08	0.41
1:A:44:ASN:CB	1:A:49:ILE:HA	2.51	0.41
1:A:89:SER:O	1:A:198:ASN:ND2	2.46	0.41
1:A:77:ALA:HB2	1:A:97:TYR:CD1	2.56	0.41
3:C:48:ARG:C	3:C:50:GLN:N	2.74	0.41
3:C:98:GLN:HE21	3:C:98:GLN:HB3	1.56	0.41
6:G:41:TRP:CZ3	6:G:79:PHE:CG	3.09	0.41
8:I:58:ALA:HA	26:3:12:ARG:NH1	2.35	0.41
9:J:39:GLU:HA	9:J:40:PRO:HD3	1.79	0.41
12:M:9:ARG:O	12:M:13:LEU:HB2	2.21	0.41
15:P:119:ILE:O	15:P:120:ILE:HG12	2.21	0.41
27:X:1398:G:O2'	27:X:1399:C:O4'	2.25	0.41
27:X:2042:A:C6	27:X:2482:A:C2	3.08	0.41
27:X:2510:A:H2'	27:X:2511:G:H5'	2.02	0.41
27:X:2522:G:H2'	27:X:2523:G:O4'	2.21	0.41
27:X:2679:G:H1	27:X:2686:C:N4	2.16	0.41
27:X:2751:C:H2'	27:X:2752:C:C6	2.55	0.41
27:X:665:A:N7	27:X:666:U:H1'	2.36	0.41
27:X:754:G:C2	27:X:755:C:C4	3.08	0.41
8:I:30:ALA:N	27:X:824:U:H2'	2.35	0.41
27:X:922:A:N7	27:X:923:A:C6	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:944:A:C2	27:X:945:G:C8	3.09	0.41
1:A:27:LYS:HZ3	1:A:29:PRO:CB	2.33	0.41
3:C:68:ARG:HH12	27:X:687:G:H1'	1.83	0.41
7:H:100:ASN:C	7:H:100:ASN:OD1	2.59	0.41
7:H:2:ILE:HG12	7:H:45:ALA:O	2.21	0.41
8:I:99:VAL:O	8:I:101:ARG:HG2	2.21	0.41
11:L:15:ARG:HA	11:L:15:ARG:HD3	1.57	0.41
11:L:39:TYR:HD2	11:L:41:GLN:HG3	1.86	0.41
14:O:23:GLU:CB	14:O:91:THR:HG21	2.48	0.41
15:P:41:VAL:O	15:P:44:VAL:HG22	2.21	0.41
17:R:85:ASP:O	17:R:87:GLU:N	2.46	0.41
19:T:45:PHE:HE2	19:T:77:ARG:CZ	2.33	0.41
21:V:2:LYS:HE3	21:V:2:LYS:HB2	1.90	0.41
21:V:43:VAL:O	21:V:47:ARG:HG2	2.21	0.41
14:O:65:ARG:NH2	27:X:1237:G:OP2	2.53	0.41
27:X:1533:G:H2'	27:X:1534:A:H8	1.85	0.41
27:X:2394:G:C2	27:X:2395:C:C2	3.08	0.41
27:X:2050:G:C6	27:X:2423:G:C6	3.09	0.41
27:X:2663:U:H3	27:X:2705:A:H62	1.66	0.41
27:X:457:C:O2'	27:X:458:G:H5'	2.21	0.41
27:X:998:C:O2	27:X:1011:A:H2	2.04	0.41
2:B:59:VAL:CG1	2:B:64:GLN:HG3	2.51	0.41
10:K:12:ARG:HG2	10:K:12:ARG:NH1	2.36	0.41
11:L:42:ILE:HD13	11:L:42:ILE:HA	1.90	0.41
13:N:86:ALA:C	13:N:88:ILE:N	2.73	0.41
19:T:56:ASP:OD1	19:T:58:THR:OG1	2.34	0.41
20:U:51:ILE:HG23	20:U:59:THR:HG22	2.03	0.41
6:G:111:LYS:HG2	27:X:1142:G:H5''	2.01	0.41
27:X:1250:A:H5'	27:X:1250:A:C8	2.54	0.41
27:X:1365:U:O2'	27:X:1586:A:N3	2.43	0.41
27:X:1609:G:H2'	27:X:1610:A:O4'	2.21	0.41
27:X:1816:G:H2'	27:X:1817:U:C6	2.56	0.41
27:X:216:U:H2'	27:X:217:U:C6	2.56	0.41
4:D:77:PHE:HB2	27:X:2289:A:N1	2.36	0.41
27:X:2432:A:N6	27:X:2479:U:H3	2.15	0.41
27:X:2579:A:O2'	27:X:2580:C:H5'	2.21	0.41
27:X:2838:U:H2'	27:X:2839:G:H8	1.86	0.41
27:X:224:G:H4'	27:X:399:G:C6	2.56	0.41
27:X:487:G:N2	27:X:489:A:H3'	2.35	0.41
27:X:534:U:P	27:X:549:G:H21	2.43	0.41
27:X:717:G:N3	27:X:739:G:C2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:41:SER:HB2	27:X:844:G:O3'	2.21	0.41
1:A:69:ARG:NH2	1:A:192:THR:OG1	2.54	0.41
1:A:36:ALA:CB	1:A:63:ARG:HA	2.50	0.41
2:B:9:ILE:HG13	2:B:25:VAL:O	2.21	0.41
6:G:62:ILE:HG22	6:G:135:LEU:HD21	2.02	0.41
9:J:55:MET:HG3	9:J:122:ALA:HB2	2.03	0.41
7:H:113:PRO:HD3	12:M:73:PHE:HB2	2.03	0.41
13:N:72:HIS:HD2	13:N:110:VAL:HG21	1.86	0.41
13:N:33:ARG:HG2	13:N:33:ARG:H	1.46	0.41
15:P:113:ALA:HB1	15:P:114:ARG:HD2	2.02	0.41
17:R:56:LYS:HD3	17:R:69:GLN:NE2	2.35	0.41
27:X:1385:C:H2'	27:X:1386:A:O4'	2.21	0.41
27:X:1779:C:H2'	27:X:1780:A:C8	2.56	0.41
27:X:1869:A:H2'	27:X:1870:U:O4'	2.21	0.41
27:X:1991:C:H2'	27:X:1992:G:C8	2.53	0.41
27:X:2185:U:H2'	27:X:2186:G:C8	2.56	0.41
27:X:2355:A:H8	27:X:2355:A:OP1	2.04	0.41
27:X:242:A:N6	27:X:441:A:C8	2.89	0.41
27:X:2443:C:H2'	27:X:2444:C:H6	1.86	0.41
27:X:2501:U:O2'	27:X:2626:U:OP1	2.32	0.41
27:X:2702:G:H2'	27:X:2703:C:O4'	2.21	0.41
27:X:2772:U:H2'	27:X:2773:G:C8	2.56	0.41
27:X:474:G:C6	27:X:478:G:O6	2.74	0.41
27:X:481:A:H3'	27:X:482:A:C8	2.56	0.41
24:1:10:VAL:HG22	24:1:11:LYS:N	2.36	0.41
7:H:116:ARG:HD3	12:M:40:ARG:HB2	2.03	0.41
7:H:127:VAL:HG22	7:H:133:VAL:HG21	2.03	0.41
6:G:56:THR:HG21	27:X:1016:C:O2'	2.21	0.41
27:X:1123:G:C6	27:X:1124:U:N3	2.89	0.41
27:X:1417:C:H2'	27:X:1418:C:C6	2.56	0.41
27:X:1717:A:H5'	27:X:1718:A:OP2	2.20	0.41
3:C:65:GLY:CA	27:X:2042:A:H5''	2.50	0.41
27:X:923:A:N3	27:X:2243:C:H1'	2.36	0.41
27:X:2712:G:H3'	27:X:2713:A:O4'	2.21	0.41
27:X:617:U:H5	27:X:632:A:N1	2.19	0.41
27:X:215:G:H1'	27:X:619:A:H1'	2.03	0.41
27:X:830:C:H3'	27:X:831:G:H8	1.86	0.41
9:J:24:GLY:HA3	27:X:920:G:P	2.61	0.41
28:Y:32:C:O5'	28:Y:32:C:H6	2.03	0.41
3:C:165:SER:HB3	3:C:166:TRP:CE3	2.56	0.40
3:C:17:LEU:HA	3:C:17:LEU:HD12	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:101:ARG:HH22	27:X:1745:C:P	2.43	0.40
17:R:14:LEU:HA	17:R:14:LEU:HD23	1.85	0.40
20:U:28:GLY:HA3	20:U:32:ARG:HG2	2.03	0.40
27:X:1754:G:H4'	27:X:1754:G:OP1	2.21	0.40
2:B:148:GLY:HA3	27:X:2036:G:C4'	2.51	0.40
27:X:2220:A:H2'	27:X:2221:G:C8	2.56	0.40
27:X:2288:A:C5	27:X:2289:A:N7	2.89	0.40
27:X:2616:U:H5''	27:X:2617:G:OP2	2.21	0.40
27:X:1671:A:O4'	27:X:2798:A:H5'	2.21	0.40
10:K:96:ARG:HB2	27:X:2857:C:H5'	2.03	0.40
25:2:35:ARG:NH1	27:X:53:G:H1'	2.36	0.40
27:X:877:G:C6	27:X:878:C:N4	2.89	0.40
23:Z:52:TYR:CE1	27:X:2859:U:N3	2.88	0.40
26:3:15:LYS:HD3	26:3:15:LYS:HA	1.70	0.40
8:I:56:LEU:HD22	26:3:52:LYS:NZ	2.37	0.40
3:C:163:ASN:ND2	3:C:166:TRP:HB2	2.36	0.40
3:C:189:ASP:HB3	3:C:190:ALA:H	1.65	0.40
4:D:35:VAL:HB	4:D:155:THR:OG1	2.21	0.40
6:G:139:ARG:HB2	27:X:567:G:OP1	2.21	0.40
6:G:52:GLY:HA3	27:X:1150:C:H5'	2.04	0.40
7:H:88:THR:O	12:M:79:ARG:HG2	2.22	0.40
9:J:26:ASP:OD1	9:J:28:VAL:N	2.52	0.40
13:N:52:ASN:O	13:N:55:ARG:N	2.55	0.40
15:P:125:SER:OG	15:P:126:HIS:N	2.53	0.40
18:S:152:ILE:HD11	18:S:168:VAL:HB	2.03	0.40
18:S:1:MET:HB3	18:S:2:GLU:H	1.70	0.40
20:U:10:LYS:HD3	20:U:11:LYS:N	2.37	0.40
20:U:33:LYS:HD3	20:U:33:LYS:HA	1.72	0.40
22:W:47:VAL:HG23	22:W:51:LEU:HD21	2.03	0.40
27:X:951:G:N3	27:X:1205:G:H4'	2.35	0.40
27:X:1251:G:O2'	27:X:1252:C:H5'	2.21	0.40
27:X:1531:C:H5'	27:X:1532:A:OP1	2.21	0.40
27:X:1882:G:N2	27:X:1886:G:C6	2.89	0.40
27:X:2609:G:H21	27:X:2866:A:H1'	1.85	0.40
27:X:350:U:H6	27:X:350:U:O5'	2.04	0.40
13:N:2:PRO:HD3	27:X:456:C:O5'	2.22	0.40
27:X:825:C:C6	27:X:1263:G:C5	3.10	0.40
28:Y:31:A:N3	28:Y:58:G:N2	2.69	0.40
26:3:32:GLN:H	26:3:32:GLN:HG3	1.67	0.40
2:B:37:LYS:HD2	2:B:42:ASP:OD1	2.22	0.40
3:C:147:LYS:O	3:C:185:ARG:N	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:84:PHE:CD2	27:X:597:U:H1'	2.57	0.40
3:C:86:PRO:C	3:C:87:LYS:HD2	2.42	0.40
8:I:43:ALA:HB1	27:X:684:C:H41	1.85	0.40
15:P:30:TYR:HB3	15:P:123:ARG:CZ	2.51	0.40
27:X:1026:U:H2'	27:X:1027:C:H6	1.86	0.40
27:X:1080:A:N7	27:X:1084:A:N6	2.69	0.40
27:X:1742:G:H2'	27:X:1743:C:C6	2.56	0.40
27:X:1850:G:C1'	27:X:1867:A:H62	2.35	0.40
27:X:45:C:OP2	27:X:192:G:H2'	2.21	0.40
27:X:2013:A:H4'	27:X:2014:A:H8	1.87	0.40
27:X:538:A:N3	27:X:2025:A:C6	2.89	0.40
27:X:2262:C:H2'	27:X:2263:C:O4'	2.21	0.40
27:X:2455:A:N3	27:X:2460:G:N1	2.62	0.40
27:X:312:G:O2'	27:X:313:U:H6	2.03	0.40
27:X:494:A:C8	27:X:495:C:C5	3.09	0.40
27:X:676:G:C6	27:X:677:G:C5	3.10	0.40
28:Y:36:A:N6	28:Y:46:G:H2'	2.36	0.40
24:1:11:LYS:HE3	24:1:26:LYS:HD3	2.03	0.40
25:2:19:ARG:O	25:2:22:MET:HB3	2.22	0.40
26:3:25:PHE:CD2	26:3:25:PHE:N	2.88	0.40
2:B:136:ARG:CZ	2:B:157:ALA:HB2	2.51	0.40
2:B:109:LYS:HE2	2:B:191:ALA:HB2	2.02	0.40
5:E:67:LEU:O	5:E:71:LEU:HG	2.22	0.40
6:G:111:LYS:HE2	27:X:1142:G:H5''	2.03	0.40
7:H:3:MET:HG2	7:H:44:TYR:CE1	2.57	0.40
8:I:56:LEU:HD21	8:I:59:ARG:NH2	2.35	0.40
12:M:103:LYS:N	12:M:103:LYS:HD2	2.36	0.40
16:Q:20:MET:HG3	16:Q:25:TYR:CD1	2.57	0.40
20:U:53:GLU:HB2	20:U:56:GLN:O	2.21	0.40
13:N:13:ARG:NH2	27:X:1264:C:OP1	2.53	0.40
10:K:36:THR:OG1	27:X:1291:G:OP1	2.16	0.40
27:X:1354:A:H2'	27:X:1410:U:O2	2.21	0.40
27:X:1473:U:O2	27:X:1474:A:N6	2.55	0.40
1:A:222:ARG:NH2	27:X:1819:U:OP2	2.53	0.40
27:X:192:G:H4'	27:X:193:A:H4'	2.04	0.40
27:X:2030:U:H2'	27:X:2031:A:C8	2.57	0.40
27:X:2281:C:N4	27:X:2293:G:H1	2.04	0.40
27:X:2533:U:H2'	27:X:2534:U:C6	2.56	0.40
27:X:1773:C:H2'	27:X:2587:G:O2'	2.22	0.40
27:X:2609:G:N3	27:X:2866:A:O2'	2.53	0.40
5:E:143:GLN:HE21	27:X:2724:G:H21	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2827:G:C6	27:X:2828:C:N3	2.90	0.40
27:X:573:C:H2'	27:X:574:C:O4'	2.21	0.40
27:X:600:G:C6	27:X:602:C:C4	3.09	0.40
27:X:692:C:H2'	27:X:693:A:C8	2.56	0.40
27:X:836:G:C4	27:X:837:U:C5	3.10	0.40
28:Y:119:G:C6	28:Y:120:G:C5	3.10	0.40
15:P:51:GLN:HE22	23:Z:39:LYS:NZ	2.20	0.40
2:B:114:GLN:C	27:X:1672:A:H4'	2.42	0.40
2:B:147:PRO:HB2	2:B:149:ARG:HG2	2.03	0.40
6:G:131:VAL:O	6:G:134:MET:N	2.41	0.40
9:J:6:LYS:HB2	9:J:7:ARG:H	1.68	0.40
10:K:45:ARG:O	10:K:49:GLU:HG3	2.21	0.40
15:P:31:VAL:O	15:P:125:SER:HB3	2.21	0.40
15:P:12:LYS:HA	15:P:15:LYS:HB2	2.04	0.40
17:R:14:LEU:HD13	17:R:16:PHE:CZ	2.57	0.40
18:S:116:VAL:N	18:S:168:VAL:O	2.49	0.40
21:V:18:ILE:HG23	21:V:22:LYS:HE2	2.04	0.40
27:X:1174:G:N2	27:X:1175:A:C5	2.89	0.40
27:X:1413:U:H2'	27:X:1414:G:H8	1.87	0.40
27:X:1662:G:H8	27:X:1662:G:O5'	2.04	0.40
10:K:9:LYS:HE2	27:X:1669:A:OP1	2.22	0.40
27:X:1695:U:H2'	27:X:1696:C:O4'	2.21	0.40
27:X:2212:U:H2'	27:X:2213:G:C8	2.56	0.40
27:X:2528:G:C2	27:X:2529:G:C5	3.09	0.40
27:X:2662:C:C4	27:X:2663:U:C5	3.10	0.40
27:X:2698:G:H2'	27:X:2699:G:O4'	2.21	0.40
27:X:2763:U:H2'	27:X:2764:U:C6	2.51	0.40
27:X:2821:G:H2'	27:X:2822:U:O4'	2.20	0.40
27:X:2825:A:N3	27:X:2825:A:H2'	2.35	0.40
27:X:759:C:C2	30:X:2902:ERY:H371	2.56	0.40
27:X:354:C:H2'	27:X:355:G:C8	2.55	0.40
23:Z:8:LYS:O	27:X:2000:U:H4'	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	258/275 (94%)	221 (86%)	34 (13%)	3 (1%)	13	52
2	B	203/211 (96%)	178 (88%)	24 (12%)	1 (0%)	29	68
3	C	192/205 (94%)	164 (85%)	26 (14%)	2 (1%)	15	55
4	D	175/180 (97%)	155 (89%)	19 (11%)	1 (1%)	25	65
5	E	169/185 (91%)	157 (93%)	11 (6%)	1 (1%)	25	65
6	G	140/174 (80%)	127 (91%)	13 (9%)	0	100	100
7	H	132/134 (98%)	120 (91%)	11 (8%)	1 (1%)	19	60
8	I	132/156 (85%)	102 (77%)	26 (20%)	4 (3%)	4	33
9	J	134/141 (95%)	113 (84%)	21 (16%)	0	100	100
10	K	111/116 (96%)	102 (92%)	8 (7%)	1 (1%)	17	58
11	L	102/114 (90%)	86 (84%)	16 (16%)	0	100	100
12	M	106/165 (64%)	99 (93%)	6 (6%)	1 (1%)	17	58
13	N	115/118 (98%)	103 (90%)	10 (9%)	2 (2%)	9	45
14	O	92/100 (92%)	82 (89%)	10 (11%)	0	100	100
15	P	128/137 (93%)	109 (85%)	15 (12%)	4 (3%)	4	32
16	Q	91/95 (96%)	76 (84%)	12 (13%)	3 (3%)	4	31
17	R	108/115 (94%)	91 (84%)	16 (15%)	1 (1%)	17	58
18	S	173/237 (73%)	154 (89%)	19 (11%)	0	100	100
19	T	72/91 (79%)	62 (86%)	9 (12%)	1 (1%)	11	48
20	U	70/81 (86%)	52 (74%)	14 (20%)	4 (6%)	1	18
21	V	63/67 (94%)	58 (92%)	5 (8%)	0	100	100
22	W	53/55 (96%)	48 (91%)	5 (9%)	0	100	100
23	Z	54/60 (90%)	48 (89%)	6 (11%)	0	100	100
24	1	51/55 (93%)	38 (74%)	10 (20%)	3 (6%)	1	17
25	2	44/47 (94%)	41 (93%)	3 (7%)	0	100	100
26	3	57/65 (88%)	46 (81%)	10 (18%)	1 (2%)	8	43
All	All	3025/3379 (90%)	2632 (87%)	359 (12%)	34 (1%)	14	54

All (34) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
15	P	120	ILE
16	Q	6	ILE
16	Q	69	ILE
1	A	24	LEU
1	A	25	THR
13	N	94	VAL
16	Q	59	PRO
24	1	9	ILE
24	1	10	VAL
15	P	125	SER
20	U	60	VAL
5	E	165	VAL
7	H	42	LYS
8	I	39	SER
8	I	103	ASN
15	P	119	ILE
20	U	15	VAL
20	U	39	LYS
10	K	18	VAL
15	P	99	ALA
19	T	19	LYS
24	1	18	THR
2	B	121	ASN
4	D	8	TYR
13	N	8	ILE
17	R	80	LYS
26	3	37	SER
1	A	219	PRO
3	C	15	ILE
12	M	29	PRO
20	U	30	VAL
3	C	22	VAL
8	I	61	PRO
8	I	68	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	
1	A	202/216 (94%)	163 (81%)	39 (19%)	1	8
2	B	155/157 (99%)	127 (82%)	28 (18%)	1	10
3	C	154/163 (94%)	131 (85%)	23 (15%)	3	19
4	D	153/156 (98%)	140 (92%)	13 (8%)	10	40
5	E	136/144 (94%)	115 (85%)	21 (15%)	2	18
6	G	118/146 (81%)	93 (79%)	25 (21%)	1	6
7	H	103/103 (100%)	88 (85%)	15 (15%)	3	19
8	I	101/121 (84%)	82 (81%)	19 (19%)	1	9
9	J	110/115 (96%)	87 (79%)	23 (21%)	1	7
10	K	90/93 (97%)	70 (78%)	20 (22%)	1	5
11	L	74/82 (90%)	57 (77%)	17 (23%)	1	5
12	M	94/133 (71%)	71 (76%)	23 (24%)	0	4
13	N	96/97 (99%)	81 (84%)	15 (16%)	2	17
14	O	75/79 (95%)	61 (81%)	14 (19%)	1	9
15	P	112/118 (95%)	87 (78%)	25 (22%)	1	5
16	Q	75/76 (99%)	61 (81%)	14 (19%)	1	9
17	R	91/96 (95%)	72 (79%)	19 (21%)	1	7
18	S	149/192 (78%)	135 (91%)	14 (9%)	8	37
19	T	55/67 (82%)	44 (80%)	11 (20%)	1	8
20	U	57/66 (86%)	45 (79%)	12 (21%)	1	7
21	V	53/55 (96%)	46 (87%)	7 (13%)	4	23
22	W	48/48 (100%)	39 (81%)	9 (19%)	1	9
23	Z	50/53 (94%)	44 (88%)	6 (12%)	5	27
24	1	46/48 (96%)	32 (70%)	14 (30%)	0	3
25	2	39/40 (98%)	28 (72%)	11 (28%)	0	3
26	3	46/51 (90%)	36 (78%)	10 (22%)	1	6
All	All	2482/2715 (91%)	2035 (82%)	447 (18%)	1	10

All (447) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	14	ARG
1	A	16	MET

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Mol	Chain	Res	Type
1	A	26	LYS
1	A	34	THR
1	A	40	THR
1	A	43	ARG
1	A	48	ARG
1	A	49	ILE
1	A	53	PHE
1	A	65	ILE
1	A	68	LYS
1	A	84	TYR
1	A	104	TYR
1	A	111	LEU
1	A	118	ASN
1	A	122	GLU
1	A	151	LYS
1	A	157	ARG
1	A	161	THR
1	A	164	GLN
1	A	165	VAL
1	A	186	HIS
1	A	188	GLU
1	A	198	ASN
1	A	201	HIS
1	A	206	LEU
1	A	211	ARG
1	A	214	TRP
1	A	215	LEU
1	A	218	LYS
1	A	220	HIS
1	A	229	VAL
1	A	240	THR
1	A	244	ARG
1	A	247	VAL
1	A	248	THR
1	A	252	LYS
1	A	269	PHE
2	B	9	ILE
2	B	12	THR
2	B	19	ARG
2	B	56	GLU
2	B	66	HIS
2	B	69	LYS

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Mol	Chain	Res	Type
2	B	72	VAL
2	B	79	ARG
2	B	82	ARG
2	B	84	PHE
2	B	87	ASP
2	B	92	ASN
2	B	107	THR
2	B	118	LYS
2	B	119	ARG
2	B	128	SER
2	B	137	ARG
2	B	140	SER
2	B	143	GLN
2	B	150	VAL
2	B	155	ARG
2	B	156	MET
2	B	162	MET
2	B	164	ARG
2	B	173	VAL
2	B	188	ILE
2	B	198	LEU
2	B	199	ARG
3	C	5	ASN
3	C	14	THR
3	C	17	LEU
3	C	24	SER
3	C	31	VAL
3	C	45	THR
3	C	48	ARG
3	C	51	VAL
3	C	52	SER
3	C	62	LYS
3	C	64	THR
3	C	74	VAL
3	C	76	THR
3	C	98	GLN
3	C	116	LYS
3	C	120	VAL
3	C	143	ASP
3	C	150	LEU
3	C	152	THR
3	C	155	GLU

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Mol	Chain	Res	Type
3	C	157	THR
3	C	165	SER
3	C	188	ILE
4	D	46	ASP
4	D	62	LEU
4	D	66	ILE
4	D	67	ILE
4	D	74	ILE
4	D	80	ARG
4	D	90	THR
4	D	112	ARG
4	D	128	TYR
4	D	130	LEU
4	D	143	TYR
4	D	146	VAL
4	D	150	ARG
5	E	20	GLN
5	E	32	GLU
5	E	43	VAL
5	E	44	ARG
5	E	57	ASP
5	E	61	HIS
5	E	70	THR
5	E	86	ASN
5	E	90	ARG
5	E	105	MET
5	E	113	VAL
5	E	116	GLU
5	E	129	THR
5	E	130	ARG
5	E	136	ILE
5	E	155	ASP
5	E	164	PHE
5	E	165	VAL
5	E	167	GLU
5	E	168	GLN
5	E	169	ILE
6	G	31	THR
6	G	32	TYR
6	G	39	GLN
6	G	41	TRP
6	G	56	THR

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Mol	Chain	Res	Type
6	G	61	ARG
6	G	62	ILE
6	G	63	ARG
6	G	67	ARG
6	G	69	ASP
6	G	76	GLN
6	G	83	ILE
6	G	90	LEU
6	G	91	THR
6	G	93	LYS
6	G	99	VAL
6	G	101	THR
6	G	102	ARG
6	G	111	LYS
6	G	116	ARG
6	G	132	PHE
6	G	145	HIS
6	G	150	VAL
6	G	161	GLN
6	G	171	LEU
7	H	23	ARG
7	H	25	LEU
7	H	41	ASN
7	H	47	VAL
7	H	78	SER
7	H	93	ARG
7	H	102	GLN
7	H	104	GLU
7	H	108	THR
7	H	114	VAL
7	H	117	GLU
7	H	119	ARG
7	H	120	ASP
7	H	126	ILE
7	H	127	VAL
8	I	13	ARG
8	I	18	ARG
8	I	21	ARG
8	I	32	ARG
8	I	39	SER
8	I	49	PHE
8	I	50	GLU

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Mol	Chain	Res	Type
8	I	53	ARG
8	I	59	ARG
8	I	60	LEU
8	I	73	GLU
8	I	78	SER
8	I	80	LEU
8	I	88	PHE
8	I	89	ASP
8	I	96	TYR
8	I	103	ASN
8	I	114	ILE
8	I	141	VAL
9	J	6	LYS
9	J	7	ARG
9	J	8	THR
9	J	10	PHE
9	J	11	ARG
9	J	17	ARG
9	J	21	ASP
9	J	27	TYR
9	J	28	VAL
9	J	44	LYS
9	J	54	VAL
9	J	60	ARG
9	J	64	LYS
9	J	68	ARG
9	J	69	ILE
9	J	88	LYS
9	J	93	TYR
9	J	103	VAL
9	J	111	THR
9	J	130	THR
9	J	132	MET
9	J	133	VAL
9	J	135	ARG
10	K	5	LYS
10	K	8	ARG
10	K	9	LYS
10	K	11	ASN
10	K	12	ARG
10	K	14	SER
10	K	17	ARG

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Mol	Chain	Res	Type
10	K	33	ARG
10	K	35	GLN
10	K	48	VAL
10	K	51	LEU
10	K	59	ASP
10	K	64	ARG
10	K	94	TYR
10	K	95	THR
10	K	98	LEU
10	K	99	ARG
10	K	109	THR
10	K	110	MET
10	K	112	LEU
11	L	8	ARG
11	L	11	LEU
11	L	17	VAL
11	L	31	VAL
11	L	33	ARG
11	L	37	HIS
11	L	38	ILE
11	L	39	TYR
11	L	43	ILE
11	L	45	ASP
11	L	59	LEU
11	L	67	THR
11	L	87	VAL
11	L	88	VAL
11	L	91	ARG
11	L	93	SER
11	L	100	VAL
12	M	2	GLN
12	M	5	ILE
12	M	16	ILE
12	M	19	ASP
12	M	21	THR
12	M	22	ARG
12	M	24	LEU
12	M	29	PRO
12	M	31	ASP
12	M	33	VAL
12	M	34	ARG
12	M	37	THR

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Mol	Chain	Res	Type
12	M	39	VAL
12	M	40	ARG
12	M	45	THR
12	M	50	PHE
12	M	72	SER
12	M	79	ARG
12	M	87	LEU
12	M	88	VAL
12	M	91	VAL
12	M	101	ARG
12	M	103	LYS
13	N	3	ARG
13	N	5	LYS
13	N	8	ILE
13	N	11	ARG
13	N	18	LEU
13	N	22	LYS
13	N	28	ARG
13	N	30	LYS
13	N	33	ARG
13	N	37	GLN
13	N	84	LYS
13	N	90	LEU
13	N	93	LYS
13	N	102	GLU
13	N	117	ARG
14	O	12	TYR
14	O	13	ARG
14	O	14	VAL
14	O	21	ARG
14	O	34	GLU
14	O	47	PHE
14	O	67	LYS
14	O	69	ILE
14	O	72	ARG
14	O	76	SER
14	O	81	ARG
14	O	82	ARG
14	O	88	GLN
14	O	91	THR
15	P	9	ARG
15	P	12	LYS

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Mol	Chain	Res	Type
15	P	20	LEU
15	P	21	ARG
15	P	32	ARG
15	P	39	ARG
15	P	43	ASP
15	P	48	LYS
15	P	86	LEU
15	P	88	ASP
15	P	91	PHE
15	P	92	VAL
15	P	93	LYS
15	P	96	TYR
15	P	98	ASP
15	P	102	THR
15	P	103	LEU
15	P	104	LYS
15	P	105	ARG
15	P	106	LEU
15	P	109	ARG
15	P	114	ARG
15	P	122	LYS
15	P	128	THR
15	P	131	VAL
16	Q	5	ASP
16	Q	6	ILE
16	Q	7	LEU
16	Q	12	ILE
16	Q	26	SER
16	Q	27	PHE
16	Q	56	MET
16	Q	58	VAL
16	Q	62	ARG
16	Q	63	LYS
16	Q	67	ARG
16	Q	73	ASN
16	Q	80	VAL
16	Q	84	GLU
17	R	5	SER
17	R	10	HIS
17	R	11	ASN
17	R	18	LYS
17	R	38	LEU

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Mol	Chain	Res	Type
17	R	52	ASN
17	R	53	VAL
17	R	54	ILE
17	R	55	THR
17	R	56	LYS
17	R	62	MET
17	R	64	ASN
17	R	83	LEU
17	R	88	THR
17	R	92	THR
17	R	95	ARG
17	R	97	GLN
17	R	106	VAL
17	R	112	LYS
18	S	25	ASN
18	S	26	LYS
18	S	28	ASN
18	S	34	LEU
18	S	49	THR
18	S	52	PHE
18	S	53	ASP
18	S	71	MET
18	S	79	ILE
18	S	83	PHE
18	S	99	HIS
18	S	120	LEU
18	S	130	ILE
18	S	168	VAL
19	T	14	ARG
19	T	19	LYS
19	T	25	LYS
19	T	41	ARG
19	T	46	LYS
19	T	49	GLN
19	T	55	ARG
19	T	56	ASP
19	T	62	LEU
19	T	64	ASP
19	T	71	ASN
20	U	8	THR
20	U	13	LEU
20	U	19	ILE

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Mol	Chain	Res	Type
20	U	21	ARG
20	U	23	LYS
20	U	32	ARG
20	U	34	THR
20	U	35	THR
20	U	37	ILE
20	U	47	HIS
20	U	63	SER
20	U	70	LEU
21	V	7	ARG
21	V	19	ASP
21	V	25	LEU
21	V	26	MET
21	V	29	ARG
21	V	37	LEU
21	V	42	ARG
22	W	4	LYS
22	W	6	VAL
22	W	9	VAL
22	W	23	LEU
22	W	31	SER
22	W	34	VAL
22	W	37	THR
22	W	45	LYS
22	W	51	LEU
23	Z	6	VAL
23	Z	11	THR
23	Z	25	LEU
23	Z	29	ASN
23	Z	41	LEU
23	Z	44	HIS
24	1	4	ASP
24	1	8	ILE
24	1	20	PHE
24	1	21	TYR
24	1	22	TYR
24	1	26	LYS
24	1	27	ASN
24	1	28	ARG
24	1	36	GLU
24	1	41	ASP
24	1	43	VAL

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Mol	Chain	Res	Type
24	1	47	HIS
24	1	48	VAL
24	1	54	LYS
25	2	3	ARG
25	2	4	THR
25	2	10	ARG
25	2	14	LYS
25	2	19	ARG
25	2	22	MET
25	2	28	ARG
25	2	29	ASN
25	2	40	HIS
25	2	42	LEU
25	2	44	VAL
26	3	6	THR
26	3	11	LYS
26	3	19	THR
26	3	31	HIS
26	3	32	GLN
26	3	36	LYS
26	3	39	ASP
26	3	46	LYS
26	3	55	TRP
26	3	57	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	198	ASN
2	B	35	GLN
2	B	48	GLN
2	B	135	HIS
2	B	169	ASN
3	C	34	GLN
3	C	98	GLN
3	C	112	GLN
3	C	163	ASN
4	D	37	ASN
4	D	129	ASN
4	D	135	GLN
4	D	171	GLN

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Mol	Chain	Res	Type
5	E	61	HIS
5	E	65	HIS
5	E	74	ASN
5	E	106	ASN
5	E	168	GLN
6	G	39	GLN
6	G	76	GLN
6	G	84	ASN
6	G	158	HIS
6	G	161	GLN
7	H	101	ASN
8	I	66	ASN
8	I	79	GLN
8	I	103	ASN
9	J	58	HIS
10	K	3	HIS
10	K	11	ASN
11	L	37	HIS
11	L	86	GLN
12	M	2	GLN
12	M	20	HIS
13	N	37	GLN
13	N	41	ASN
13	N	52	ASN
13	N	63	GLN
13	N	72	HIS
13	N	81	ASN
14	O	88	GLN
15	P	16	GLN
15	P	51	GLN
15	P	78	ASN
15	P	81	HIS
15	P	118	ASN
16	Q	44	GLN
16	Q	57	ASN
16	Q	71	GLN
16	Q	73	ASN
16	Q	94	GLN
17	R	10	HIS
17	R	15	HIS
17	R	32	GLN
17	R	69	GLN

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Mol	Chain	Res	Type
17	R	71	GLN
17	R	97	GLN
18	S	118	HIS
19	T	71	ASN
19	T	85	GLN
21	V	10	GLN
22	W	15	ASN
22	W	49	HIS
23	Z	44	HIS
24	1	32	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	X	2673/2880 (92%)	638 (23%)	40 (1%)
28	Y	121/124 (97%)	29 (23%)	1 (0%)
All	All	2794/3004 (93%)	667 (23%)	41 (1%)

All (667) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
27	X	3	U
27	X	4	C
27	X	13	A
27	X	14	A
27	X	17	G
27	X	34	U
27	X	37	C
27	X	39	C
27	X	45	C
27	X	49	U
27	X	50	G
27	X	51	A
27	X	59	G
27	X	60	A
27	X	63	A
27	X	69	G
27	X	70	A
27	X	73	A
27	X	74	G
27	X	83	A

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Mol	Chain	Res	Type
27	X	88	G
27	X	89	A
27	X	90	G
27	X	91	A
27	X	98	U
27	X	100	G
27	X	107	G
27	X	108	G
27	X	116	A
27	X	118	U
27	X	123	A
27	X	124	A
27	X	129	A
27	X	135	U
27	X	136	A
27	X	143	A
27	X	146	C
27	X	151	G
27	X	173	A
27	X	176	A
27	X	178	C
27	X	181	A
27	X	192	G
27	X	193	A
27	X	199	A
27	X	205	A
27	X	206	U
27	X	207	U
27	X	209	G
27	X	210	A
27	X	220	U
27	X	221	A
27	X	222	G
27	X	225	G
27	X	227	G
27	X	229	G
27	X	238	G
27	X	242	A
27	X	243	G
27	X	246	C
27	X	248	A
27	X	304	A

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Mol	Chain	Res	Type
27	X	305	A
27	X	310	A
27	X	312	G
27	X	319	G
27	X	321	A
27	X	322	A
27	X	323	G
27	X	335	A
27	X	340	G
27	X	341	A
27	X	342	G
27	X	343	A
27	X	360	A
27	X	393	U
27	X	399	G
27	X	400	U
27	X	408	U
27	X	409	G
27	X	414	A
27	X	419	G
27	X	421	G
27	X	424	G
27	X	425	A
27	X	429	C
27	X	433	G
27	X	441	A
27	X	453	U
27	X	456	C
27	X	459	A
27	X	463	C
27	X	467	U
27	X	469	G
27	X	490	A
27	X	491	A
27	X	492	G
27	X	493	A
27	X	494	A
27	X	504	G
27	X	514	G
27	X	515	A
27	X	518	A
27	X	519	C

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Mol	Chain	Res	Type
27	X	520	C
27	X	537	C
27	X	538	A
27	X	539	A
27	X	540	G
27	X	541	C
27	X	542	A
27	X	543	G
27	X	554	U
27	X	555	U
27	X	556	A
27	X	557	U
27	X	559	C
27	X	560	G
27	X	564	U
27	X	572	G
27	X	582	G
27	X	584	A
27	X	587	A
27	X	591	G
27	X	595	A
27	X	596	C
27	X	613	A
27	X	614	G
27	X	616	U
27	X	624	A
27	X	625	A
27	X	626	A
27	X	627	A
27	X	628	A
27	X	631	G
27	X	632	A
27	X	633	G
27	X	642	A
27	X	645	G
27	X	648	A
27	X	649	G
27	X	651	C
27	X	654	A
27	X	655	A
27	X	656	U
27	X	657	A

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Mol	Chain	Res	Type
27	X	658	G
27	X	664	C
27	X	665	A
27	X	666	U
27	X	667	U
27	X	668	A
27	X	677	G
27	X	682	G
27	X	690	A
27	X	695	G
27	X	697	G
27	X	699	G
27	X	703	A
27	X	725	C
27	X	729	A
27	X	731	A
27	X	732	G
27	X	743	A
27	X	749	C
27	X	753	U
27	X	759	C
27	X	760	U
27	X	761	G
27	X	766	A
27	X	774	A
27	X	784	U
27	X	789	G
27	X	790	A
27	X	795	A
27	X	797	A
27	X	798	G
27	X	801	A
27	X	802	A
27	X	803	C
27	X	804	C
27	X	805	G
27	X	806	A
27	X	814	G
27	X	818	G
27	X	824	U
27	X	825	C
27	X	830	C

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Mol	Chain	Res	Type
27	X	832	A
27	X	840	U
27	X	841	G
27	X	843	G
27	X	859	U
27	X	872	G
27	X	879	A
27	X	891	A
27	X	914	C
27	X	922	A
27	X	931	G
27	X	938	G
27	X	939	C
27	X	940	G
27	X	943	U
27	X	944	A
27	X	952	A
27	X	956	A
27	X	957	G
27	X	966	A
27	X	967	G
27	X	969	U
27	X	972	C
27	X	973	U
27	X	976	C
27	X	979	A
27	X	985	G
27	X	992	A
27	X	999	A
27	X	1000	G
27	X	1006	C
27	X	1007	A
27	X	1016	C
27	X	1018	C
27	X	1019	U
27	X	1020	A
27	X	1022	A
27	X	1023	U
27	X	1024	G
27	X	1033	G
27	X	1034	U
27	X	1035	G

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Mol	Chain	Res	Type
27	X	1037	U
27	X	1044	U
27	X	1046	U
27	X	1051	U
27	X	1054	C
27	X	1055	A
27	X	1056	U
27	X	1058	G
27	X	1060	C
27	X	1071	U
27	X	1073	G
27	X	1081	A
27	X	1082	G
27	X	1083	C
27	X	1086	C
27	X	1087	C
27	X	1096	A
27	X	1097	A
27	X	1099	A
27	X	1101	U
27	X	1105	U
27	X	1108	U
27	X	1109	A
27	X	1113	C
27	X	1120	C
27	X	1121	G
27	X	1123	G
27	X	1127	C
27	X	1128	G
27	X	1140	A
27	X	1142	G
27	X	1145	C
27	X	1146	G
27	X	1149	G
27	X	1152	C
27	X	1153	A
27	X	1183	C
27	X	1185	C
27	X	1187	A
27	X	1189	G
27	X	1194	U
27	X	1195	U

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Mol	Chain	Res	Type
27	X	1200	G
27	X	1203	A
27	X	1208	A
27	X	1209	G
27	X	1217	U
27	X	1223	G
27	X	1225	G
27	X	1240	G
27	X	1249	G
27	X	1250	A
27	X	1251	G
27	X	1260	A
27	X	1261	G
27	X	1262	U
27	X	1263	G
27	X	1266	G
27	X	1269	G
27	X	1278	A
27	X	1279	G
27	X	1284	G
27	X	1285	A
27	X	1286	U
27	X	1288	A
27	X	1289	A
27	X	1301	U
27	X	1302	C
27	X	1313	U
27	X	1314	A
27	X	1315	A
27	X	1321	A
27	X	1325	U
27	X	1332	G
27	X	1334	A
27	X	1341	G
27	X	1342	U
27	X	1347	C
27	X	1349	A
27	X	1354	A
27	X	1358	C
27	X	1365	U
27	X	1378	A
27	X	1379	A

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Mol	Chain	Res	Type
27	X	1381	G
27	X	1391	A
27	X	1392	U
27	X	1393	G
27	X	1397	A
27	X	1398	G
27	X	1404	C
27	X	1408	A
27	X	1409	U
27	X	1413	U
27	X	1428	G
27	X	1429	A
27	X	1430	G
27	X	1432	G
27	X	1433	A
27	X	1434	U
27	X	1435	G
27	X	1441	A
27	X	1442	C
27	X	1443	G
27	X	1459	U
27	X	1460	G
27	X	1465	G
27	X	1467	U
27	X	1468	A
27	X	1469	U
27	X	1470	G
27	X	1475	U
27	X	1482	U
27	X	1490	U
27	X	1497	C
27	X	1498	G
27	X	1508	G
27	X	1517	C
27	X	1518	C
27	X	1524	C
27	X	1525	A
27	X	1527	G
27	X	1528	C
27	X	1541	G
27	X	1551	U
27	X	1552	C

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Mol	Chain	Res	Type
27	X	1553	G
27	X	1554	G
27	X	1562	G
27	X	1571	G
27	X	1574	A
27	X	1575	C
27	X	1582	A
27	X	1585	A
27	X	1600	U
27	X	1601	U
27	X	1602	G
27	X	1603	A
27	X	1608	U
27	X	1624	A
27	X	1625	A
27	X	1626	A
27	X	1629	G
27	X	1631	C
27	X	1632	A
27	X	1634	A
27	X	1641	C
27	X	1648	C
27	X	1651	U
27	X	1656	U
27	X	1661	C
27	X	1664	G
27	X	1665	C
27	X	1666	G
27	X	1667	A
27	X	1668	G
27	X	1682	A
27	X	1688	U
27	X	1691	G
27	X	1710	U
27	X	1711	C
27	X	1713	G
27	X	1719	G
27	X	1732	U
27	X	1735	G
27	X	1747	G
27	X	1754	G
27	X	1755	G

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Mol	Chain	Res	Type
27	X	1760	G
27	X	1764	A
27	X	1771	A
27	X	1775	A
27	X	1776	A
27	X	1782	A
27	X	1790	G
27	X	1791	C
27	X	1792	C
27	X	1793	A
27	X	1799	A
27	X	1801	C
27	X	1807	A
27	X	1808	C
27	X	1811	A
27	X	1812	U
27	X	1813	A
27	X	1819	U
27	X	1821	A
27	X	1830	C
27	X	1831	G
27	X	1859	A
27	X	1861	G
27	X	1867	A
27	X	1868	A
27	X	1882	G
27	X	1884	A
27	X	1910	A
27	X	1912	G
27	X	1919	A
27	X	1920	A
27	X	1921	A
27	X	1922	U
27	X	1923	U
27	X	1924	C
27	X	1930	C
27	X	1938	U
27	X	1946	U
27	X	1947	G
27	X	1948	C
27	X	1949	A
27	X	1950	C

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Mol	Chain	Res	Type
27	X	1951	G
27	X	1953	A
27	X	1954	A
27	X	1955	G
27	X	1958	G
27	X	1965	U
27	X	1974	U
27	X	1976	U
27	X	1980	A
27	X	2001	G
27	X	2003	A
27	X	2004	U
27	X	2006	G
27	X	2014	A
27	X	2015	G
27	X	2016	A
27	X	2018	G
27	X	2023	C
27	X	2025	A
27	X	2026	C
27	X	2028	C
27	X	2032	G
27	X	2035	G
27	X	2038	C
27	X	2039	G
27	X	2043	A
27	X	2044	G
27	X	2045	A
27	X	2052	G
27	X	2059	U
27	X	2075	U
27	X	2083	G
27	X	2089	C
27	X	2171	U
27	X	2172	U
27	X	2182	A
27	X	2189	A
27	X	2190	A
27	X	2191	A
27	X	2192	U
27	X	2193	C
27	X	2196	U

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Mol	Chain	Res	Type
27	X	2197	U
27	X	2198	U
27	X	2199	C
27	X	2200	G
27	X	2204	A
27	X	2205	C
27	X	2217	G
27	X	2218	G
27	X	2247	A
27	X	2252	A
27	X	2259	G
27	X	2262	C
27	X	2265	A
27	X	2266	A
27	X	2267	A
27	X	2272	A
27	X	2284	U
27	X	2285	U
27	X	2286	G
27	X	2287	G
27	X	2290	A
27	X	2291	U
27	X	2298	U
27	X	2299	A
27	X	2300	G
27	X	2301	A
27	X	2306	A
27	X	2307	A
27	X	2311	U
27	X	2312	A
27	X	2313	G
27	X	2315	A
27	X	2324	G
27	X	2326	C
27	X	2327	U
27	X	2330	G
27	X	2333	A
27	X	2351	G
27	X	2358	C
27	X	2362	G
27	X	2364	C
27	X	2367	A

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Mol	Chain	Res	Type
27	X	2368	G
27	X	2369	U
27	X	2375	G
27	X	2381	A
27	X	2385	U
27	X	2386	G
27	X	2397	A
27	X	2398	U
27	X	2401	A
27	X	2402	U
27	X	2404	A
27	X	2405	A
27	X	2406	C
27	X	2407	G
27	X	2408	G
27	X	2410	U
27	X	2413	A
27	X	2420	C
27	X	2424	G
27	X	2426	G
27	X	2427	A
27	X	2429	A
27	X	2441	U
27	X	2449	G
27	X	2452	U
27	X	2453	C
27	X	2455	A
27	X	2460	G
27	X	2463	G
27	X	2470	U
27	X	2471	U
27	X	2477	C
27	X	2480	C
27	X	2481	G
27	X	2482	A
27	X	2484	G
27	X	2485	U
27	X	2497	A
27	X	2498	U
27	X	2504	G
27	X	2508	G
27	X	2511	G

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Mol	Chain	Res	Type
27	X	2521	A
27	X	2545	A
27	X	2546	G
27	X	2552	C
27	X	2553	G
27	X	2557	G
27	X	2564	U
27	X	2581	A
27	X	2582	G
27	X	2588	U
27	X	2591	C
27	X	2593	A
27	X	2594	U
27	X	2600	A
27	X	2601	C
27	X	2608	A
27	X	2617	G
27	X	2624	G
27	X	2625	U
27	X	2633	A
27	X	2639	A
27	X	2642	G
27	X	2650	G
27	X	2664	G
27	X	2666	U
27	X	2668	U
27	X	2670	C
27	X	2677	U
27	X	2688	G
27	X	2691	C
27	X	2692	A
27	X	2693	U
27	X	2694	G
27	X	2698	G
27	X	2706	U
27	X	2707	G
27	X	2711	G
27	X	2713	A
27	X	2724	G
27	X	2728	A
27	X	2732	C
27	X	2737	A

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Mol	Chain	Res	Type
27	X	2738	A
27	X	2744	A
27	X	2745	A
27	X	2757	G
27	X	2758	A
27	X	2759	U
27	X	2760	G
27	X	2761	A
27	X	2769	C
27	X	2771	C
27	X	2782	G
27	X	2793	G
27	X	2795	A
27	X	2796	A
27	X	2798	A
27	X	2807	U
27	X	2808	U
27	X	2809	A
27	X	2811	G
27	X	2814	G
27	X	2825	A
27	X	2832	G
27	X	2847	G
27	X	2849	C
27	X	2851	G
27	X	2855	C
27	X	2858	A
27	X	2861	A
27	X	2866	A
27	X	2868	G
28	Y	14	C
28	Y	15	A
28	Y	17	A
28	Y	22	U
28	Y	26	G
28	Y	28	A
28	Y	29	C
28	Y	37	C
28	Y	39	C
28	Y	40	C
28	Y	43	G
28	Y	44	C

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Mol	Chain	Res	Type
28	Y	46	G
28	Y	47	A
28	Y	49	C
28	Y	52	G
28	Y	54	U
28	Y	56	G
28	Y	59	A
28	Y	69	G
28	Y	75	A
28	Y	86	A
28	Y	99	G
28	Y	102	A
28	Y	108	G
28	Y	111	C
28	Y	112	A
28	Y	115	G
28	Y	123	U

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	X	38	G
27	X	50	G
27	X	537	C
27	X	538	A
27	X	542	A
27	X	557	U
27	X	760	U
27	X	788	G
27	X	789	G
27	X	956	A
27	X	1019	U
27	X	1053	G
27	X	1059	A
27	X	1096	A
27	X	1141	U
27	X	1182	U
27	X	1250	A
27	X	1313	U
27	X	1391	A
27	X	1441	A
27	X	1496	G

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Mol	Chain	Res	Type
27	X	1607	A
27	X	1625	A
27	X	1664	G
27	X	1810	U
27	X	1919	A
27	X	1923	U
27	X	1975	G
27	X	2204	A
27	X	2299	A
27	X	2312	A
27	X	2363	G
27	X	2404	A
27	X	2409	A
27	X	2452	U
27	X	2705	A
27	X	2736	U
27	X	2756	A
27	X	2824	C
27	X	2846	G
28	Y	58	G

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 71 ligands modelled in this entry, 70 are monoatomic - leaving 1 for Mogul analysis.

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



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	ERY	X	2902	-	53,53,53	0.85	1 (1%)	82,82,82	1.29	7 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	ERY	X	2902	-	-	3/72/107/107	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	X	2902	ERY	O2-C13	2.06	1.50	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	X	2902	ERY	O8-C23-C22	-2.50	103.96	110.05
30	X	2902	ERY	C2-C3-C4	-2.46	105.94	113.05
30	X	2902	ERY	C30-C2-C1	-2.30	103.83	109.02
30	X	2902	ERY	C16-C15-C14	-2.20	111.25	115.07
30	X	2902	ERY	C34-C10-C11	-2.16	111.69	114.38
30	X	2902	ERY	C13-O2-C1	-2.15	114.36	118.18
30	X	2902	ERY	O10-C6-C7	2.09	113.80	108.40

There are no chirality outliers.

All (3) torsion outliers are listed below:

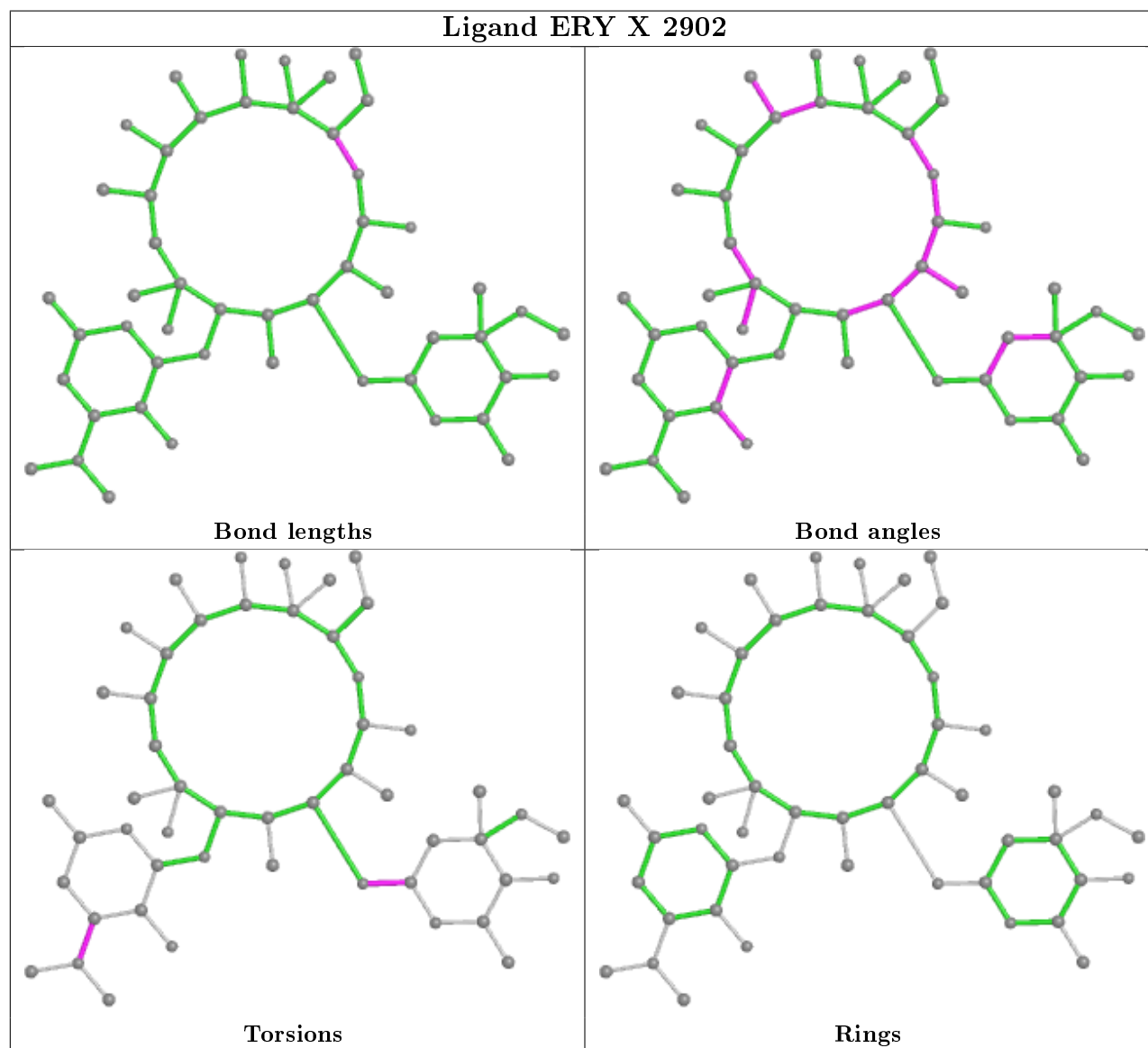
Mol	Chain	Res	Type	Atoms
30	X	2902	ERY	C15-C14-O3-C3
30	X	2902	ERY	O4-C14-O3-C3
30	X	2902	ERY	C25-C24-N1-C28

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	X	2902	ERY	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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	260/275 (94%)	0.01	4 (1%) 73 61	48, 104, 163, 221	0
2	B	205/211 (97%)	-0.33	5 (2%) 59 45	27, 50, 107, 233	0
3	C	194/205 (94%)	0.02	9 (4%) 32 23	39, 102, 180, 292	0
4	D	177/180 (98%)	0.15	11 (6%) 20 15	114, 175, 232, 282	0
5	E	171/185 (92%)	-0.28	4 (2%) 60 46	57, 131, 192, 243	0
6	G	142/174 (81%)	-0.01	8 (5%) 24 17	38, 77, 160, 339	0
7	H	134/134 (100%)	-0.40	2 (1%) 73 61	33, 45, 87, 135	0
8	I	134/156 (85%)	0.19	4 (2%) 50 37	55, 126, 192, 315	0
9	J	136/141 (96%)	-0.00	4 (2%) 51 38	56, 94, 163, 214	0
10	K	113/116 (97%)	-0.47	0 100 100	27, 32, 67, 100	0
11	L	104/114 (91%)	0.08	6 (5%) 23 16	130, 161, 200, 243	0
12	M	108/165 (65%)	-0.48	0 100 100	30, 43, 95, 242	0
13	N	117/118 (99%)	-0.20	2 (1%) 70 57	41, 76, 133, 232	0
14	O	94/100 (94%)	-0.26	4 (4%) 35 25	52, 94, 178, 204	0
15	P	130/137 (94%)	-0.40	0 100 100	33, 51, 147, 188	0
16	Q	93/95 (97%)	-0.39	1 (1%) 80 69	49, 94, 162, 192	0
17	R	110/115 (95%)	0.02	3 (2%) 54 41	65, 100, 189, 259	0
18	S	175/237 (73%)	0.39	20 (11%) 5 5	93, 144, 224, 285	0
19	T	74/91 (81%)	0.11	5 (6%) 17 13	72, 112, 158, 228	0
20	U	72/81 (88%)	0.37	4 (5%) 24 17	75, 119, 185, 238	0
21	V	65/67 (97%)	-0.26	2 (3%) 49 36	76, 115, 164, 208	0
22	W	55/55 (100%)	0.10	0 100 100	72, 91, 128, 190	0
23	Z	56/60 (93%)	-0.42	0 100 100	32, 40, 80, 152	0
24	1	53/55 (96%)	0.42	5 (9%) 8 6	102, 129, 217, 266	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	2	46/47 (97%)	0.11	1 (2%) 62 48	38, 67, 122, 169	0
26	3	59/65 (90%)	0.42	5 (8%) 10 9	81, 100, 172, 278	0
27	X	2680/2880 (93%)	-0.13	84 (3%) 49 36	26, 76, 186, 299	0
28	Y	122/124 (98%)	-0.09	4 (3%) 46 34	74, 153, 190, 332	0
All	All	5879/6383 (92%)	-0.10	197 (3%) 45 33	26, 89, 188, 339	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	S	15	ASP	7.4
27	X	1072	U	7.1
18	S	23	ALA	7.1
18	S	22	VAL	7.0
27	X	731	A	6.6
27	X	1071	U	6.2
4	D	153	ASP	6.0
27	X	1913	G	5.8
28	Y	123	U	5.7
20	U	28	GLY	5.6
27	X	1086	C	5.6
27	X	1073	G	5.5
27	X	1099	A	5.5
3	C	44	SER	5.2
27	X	1060	C	5.2
27	X	1070	G	5.1
4	D	43	SER	5.1
4	D	134	GLU	4.7
20	U	27	ASP	4.6
27	X	1115	C	4.6
18	S	14	LEU	4.6
11	L	52	ALA	4.4
3	C	19	LEU	4.4
20	U	26	ALA	4.4
4	D	23	SER	4.3
27	X	1069	G	4.3
9	J	84	MET	4.3
27	X	1954	A	4.3
24	1	35	LEU	4.1
8	I	75	VAL	4.1
25	2	1	MET	4.0
8	I	74	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
27	X	728	G	4.0
27	X	1188	A	3.9
1	A	236	GLY	3.8
17	R	83	LEU	3.8
27	X	1055	A	3.8
3	C	47	THR	3.8
27	X	2444	C	3.8
6	G	97	ASP	3.6
27	X	1090	C	3.5
11	L	53	ALA	3.5
18	S	68	ALA	3.5
27	X	200	A	3.5
27	X	424	G	3.5
27	X	1068	A	3.5
26	3	38	GLY	3.5
6	G	129	HIS	3.5
27	X	1912	G	3.4
27	X	1085	G	3.4
27	X	727	U	3.4
4	D	22	TYR	3.4
14	O	47	PHE	3.3
14	O	23	GLU	3.3
27	X	2287	G	3.3
27	X	1114	A	3.3
27	X	730	C	3.3
27	X	2082	C	3.2
18	S	83	PHE	3.2
4	D	75	SER	3.2
24	1	27	ASN	3.2
28	Y	68	A	3.2
27	X	75	C	3.1
27	X	1098	G	3.1
11	L	40	ALA	3.1
27	X	1951	G	3.1
4	D	42	SER	3.1
18	S	171	VAL	3.1
27	X	426	C	3.0
17	R	102	LYS	3.0
19	T	16	SER	3.0
5	E	174	GLY	3.0
19	T	15	ASP	3.0
27	X	425	A	3.0

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Mol	Chain	Res	Type	RSRZ
18	S	21	ALA	3.0
27	X	1091	C	3.0
27	X	2171	U	3.0
27	X	2731	G	3.0
18	S	91	PRO	2.9
18	S	92	VAL	2.9
5	E	175	LYS	2.9
27	X	1059	A	2.9
9	J	79	PRO	2.9
18	S	32	PHE	2.9
27	X	1087	C	2.9
19	T	73	GLY	2.9
8	I	54	SER	2.9
1	A	237	GLU	2.9
27	X	2090	U	2.9
27	X	420	C	2.8
27	X	1524	C	2.8
3	C	91	TYR	2.8
27	X	1104	G	2.8
4	D	25	VAL	2.8
4	D	132	ILE	2.8
18	S	30	VAL	2.8
19	T	14	ARG	2.8
2	B	136	ARG	2.8
27	X	1950	C	2.8
18	S	86	VAL	2.7
20	U	29	GLY	2.7
11	L	39	TYR	2.7
18	S	124	ALA	2.7
11	L	33	ARG	2.7
27	X	248	A	2.7
6	G	159	SER	2.7
28	Y	6	C	2.7
27	X	2381	A	2.6
27	X	74	G	2.6
27	X	2089	C	2.6
27	X	1186	G	2.6
26	3	55	TRP	2.6
17	R	55	THR	2.5
2	B	205	SER	2.5
27	X	2359	U	2.5
24	1	40	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
27	X	435	A	2.5
27	X	1187	A	2.5
27	X	1089	C	2.4
27	X	361	G	2.4
27	X	1062	G	2.4
27	X	2270	U	2.4
18	S	82	ASP	2.4
27	X	1067	G	2.4
13	N	91	ASN	2.4
14	O	11	GLN	2.4
4	D	152	MET	2.4
3	C	20	PRO	2.4
3	C	166	TRP	2.4
6	G	168	THR	2.4
27	X	434	C	2.4
27	X	2290	A	2.4
9	J	77	LYS	2.4
18	S	114	ASP	2.4
27	X	2083	G	2.4
21	V	48	ARG	2.4
26	3	37	SER	2.4
1	A	220	HIS	2.4
6	G	156	HIS	2.4
27	X	1846	A	2.4
27	X	225	G	2.3
27	X	2289	A	2.3
27	X	1888	C	2.3
3	C	81	GLY	2.3
9	J	78	LYS	2.3
27	X	1432	G	2.3
27	X	1955	G	2.3
27	X	1190	C	2.3
18	S	54	ILE	2.3
5	E	173	ALA	2.3
27	X	1074	G	2.3
27	X	1483	G	2.3
24	1	14	SER	2.3
7	H	19	ILE	2.3
27	X	2037	A	2.2
28	Y	2	C	2.2
26	3	39	ASP	2.2
27	X	2390	A	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	203	LYS	2.2
11	L	54	ALA	2.2
2	B	34	VAL	2.2
26	3	63	PRO	2.2
8	I	76	LYS	2.2
3	C	45	THR	2.2
27	X	1515	U	2.2
5	E	64	LEU	2.2
27	X	2170	C	2.2
27	X	1847	G	2.2
4	D	154	ILE	2.2
27	X	729	A	2.2
27	X	1887	G	2.2
18	S	69	VAL	2.2
27	X	1919	A	2.1
27	X	1390	G	2.1
3	C	193	LEU	2.1
6	G	66	HIS	2.1
13	N	92	ARG	2.1
27	X	1593	C	2.1
6	G	105	GLY	2.1
2	B	135	HIS	2.1
27	X	1588	A	2.1
18	S	143	ILE	2.1
6	G	44	VAL	2.1
27	X	423	G	2.1
24	1	4	ASP	2.1
19	T	17	ASN	2.1
27	X	1801	C	2.1
27	X	1084	A	2.1
27	X	2340	C	2.0
18	S	31	SER	2.0
7	H	8	LEU	2.0
27	X	2385	U	2.0
1	A	249	PRO	2.0
21	V	52	GLN	2.0
27	X	2173	G	2.0
16	Q	15	LYS	2.0
14	O	46	VAL	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
29	MG	K	202	1/1	0.77	0.83	27,27,27,27	0
29	MG	B	301	1/1	0.79	0.78	34,34,34,34	0
29	MG	X	2930	1/1	0.80	0.99	29,29,29,29	0
29	MG	X	2958	1/1	0.82	0.48	44,44,44,44	0
29	MG	X	2919	1/1	0.82	0.10	62,62,62,62	0
29	MG	X	2915	1/1	0.83	0.17	63,63,63,63	0
29	MG	X	2906	1/1	0.85	0.85	28,28,28,28	0
29	MG	K	201	1/1	0.86	0.49	27,27,27,27	0
29	MG	X	2933	1/1	0.86	0.65	36,36,36,36	0
29	MG	X	2931	1/1	0.87	0.57	46,46,46,46	0
29	MG	X	2907	1/1	0.90	0.77	28,28,28,28	0
29	MG	X	2963	1/1	0.90	0.31	56,56,56,56	0
29	MG	X	2917	1/1	0.91	0.86	40,40,40,40	0
29	MG	X	2911	1/1	0.91	0.53	56,56,56,56	0
29	MG	X	2925	1/1	0.91	1.04	31,31,31,31	0
29	MG	X	2952	1/1	0.91	0.44	29,29,29,29	0
29	MG	X	2946	1/1	0.91	0.19	46,46,46,46	0
29	MG	X	2965	1/1	0.91	0.91	43,43,43,43	0
29	MG	X	2951	1/1	0.92	0.76	32,32,32,32	0
29	MG	X	2943	1/1	0.92	0.95	42,42,42,42	0
29	MG	X	2960	1/1	0.92	0.32	61,61,61,61	0
29	MG	X	2939	1/1	0.93	0.60	50,50,50,50	0
29	MG	X	2964	1/1	0.93	0.90	28,28,28,28	0
29	MG	X	2961	1/1	0.93	1.07	56,56,56,56	0
29	MG	X	2916	1/1	0.93	0.87	41,41,41,41	0
29	MG	X	2926	1/1	0.93	0.91	44,44,44,44	0
29	MG	X	2957	1/1	0.93	0.85	52,52,52,52	0

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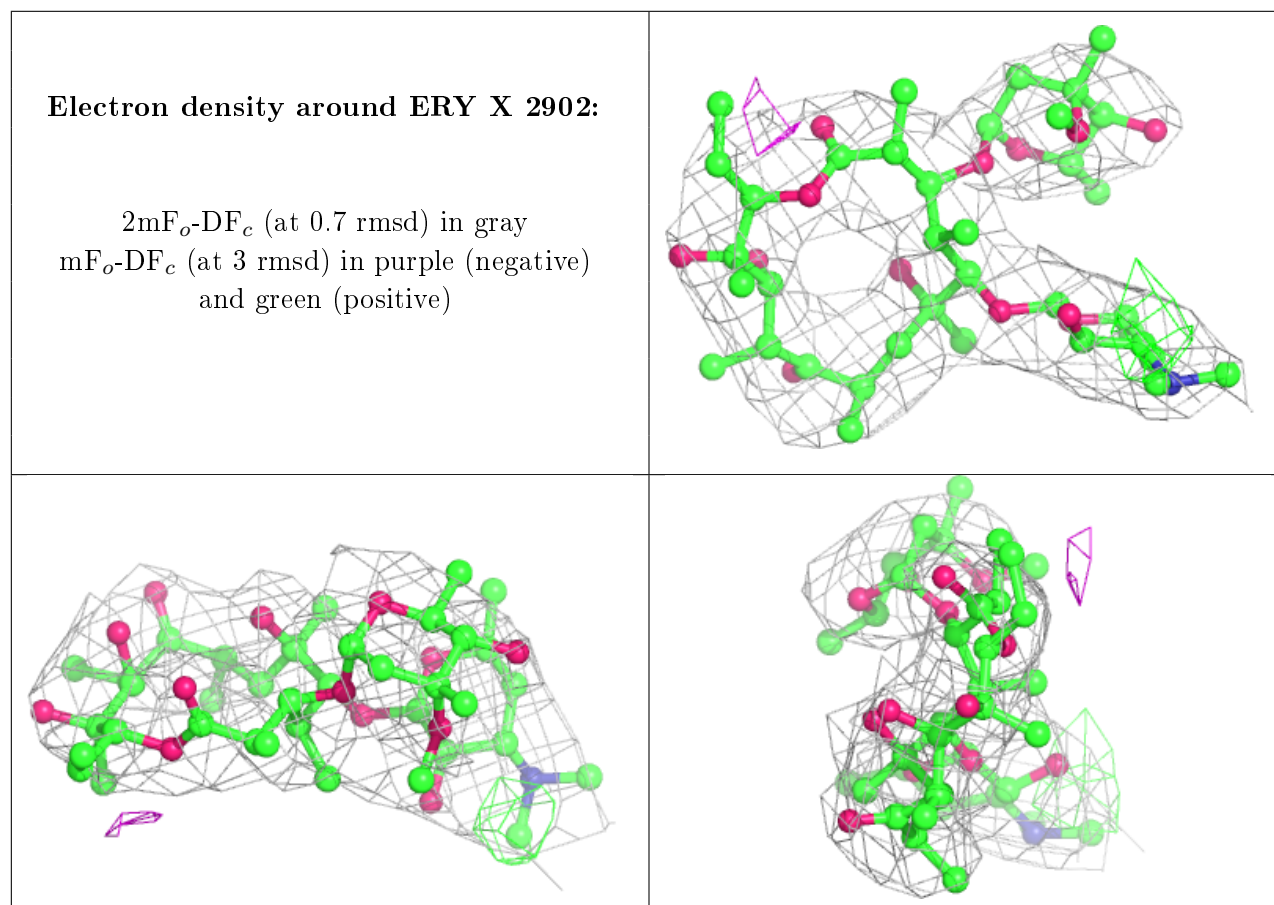
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
29	MG	A	301	1/1	0.93	0.39	54,54,54,54	0
30	ERY	X	2902	51/51	0.94	0.23	31,34,36,36	0
29	MG	X	2923	1/1	0.94	0.40	40,40,40,40	0
29	MG	X	2962	1/1	0.94	0.13	69,69,69,69	0
29	MG	X	2956	1/1	0.94	0.52	27,27,27,27	0
29	MG	X	2901	1/1	0.94	0.39	69,69,69,69	0
29	MG	X	2908	1/1	0.94	0.61	32,32,32,32	0
29	MG	X	2904	1/1	0.95	0.56	32,32,32,32	0
29	MG	X	2950	1/1	0.95	0.40	32,32,32,32	0
29	MG	X	2903	1/1	0.95	0.66	30,30,30,30	0
29	MG	X	2934	1/1	0.95	0.25	29,29,29,29	0
29	MG	X	2905	1/1	0.95	0.50	31,31,31,31	0
29	MG	X	2927	1/1	0.95	0.34	29,29,29,29	0
29	MG	X	2937	1/1	0.95	0.69	44,44,44,44	0
29	MG	X	2921	1/1	0.95	0.34	28,28,28,28	0
29	MG	X	2912	1/1	0.96	0.14	27,27,27,27	0
29	MG	X	2910	1/1	0.96	0.64	56,56,56,56	0
29	MG	X	2936	1/1	0.96	0.65	45,45,45,45	0
29	MG	X	2948	1/1	0.96	0.28	34,34,34,34	0
29	MG	X	2947	1/1	0.96	0.26	34,34,34,34	0
29	MG	X	2920	1/1	0.96	0.46	52,52,52,52	0
29	MG	X	2913	1/1	0.96	0.46	43,43,43,43	0
29	MG	X	2955	1/1	0.97	0.48	30,30,30,30	0
29	MG	X	2909	1/1	0.97	0.45	28,28,28,28	0
29	MG	M	202	1/1	0.97	0.35	35,35,35,35	0
29	MG	X	2954	1/1	0.97	0.44	45,45,45,45	0
29	MG	X	2935	1/1	0.97	0.47	34,34,34,34	0
29	MG	X	2942	1/1	0.97	0.66	46,46,46,46	0
29	MG	X	2944	1/1	0.97	0.41	35,35,35,35	0
29	MG	X	2941	1/1	0.97	0.46	38,38,38,38	0
29	MG	X	2959	1/1	0.97	0.64	41,41,41,41	0
29	MG	X	2922	1/1	0.97	0.34	29,29,29,29	0
29	MG	M	201	1/1	0.97	0.35	35,35,35,35	0
29	MG	X	2945	1/1	0.97	0.14	38,38,38,38	0
29	MG	X	2932	1/1	0.98	0.40	37,37,37,37	0
29	MG	X	2918	1/1	0.98	0.80	43,43,43,43	0
29	MG	X	2938	1/1	0.98	0.79	31,31,31,31	0
29	MG	X	2929	1/1	0.98	0.14	30,30,30,30	0
29	MG	X	2949	1/1	0.98	0.44	42,42,42,42	0
29	MG	X	2940	1/1	0.98	0.36	36,36,36,36	0
29	MG	X	2928	1/1	0.98	0.39	55,55,55,55	0
29	MG	X	2953	1/1	0.99	0.39	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
29	MG	X	2924	1/1	0.99	0.22	38,38,38,38	0
29	MG	X	2914	1/1	0.99	0.57	27,27,27,27	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.