



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 06:12 AM EDT

PDB ID : 4U67 / pdb_00004u67
Title : Crystal structure of the large ribosomal subunit (50S) of *Deinococcus radiodurans* containing a three residue insertion in L22
Authors : Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.
Deposited on : 2014-07-28
Resolution : 3.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

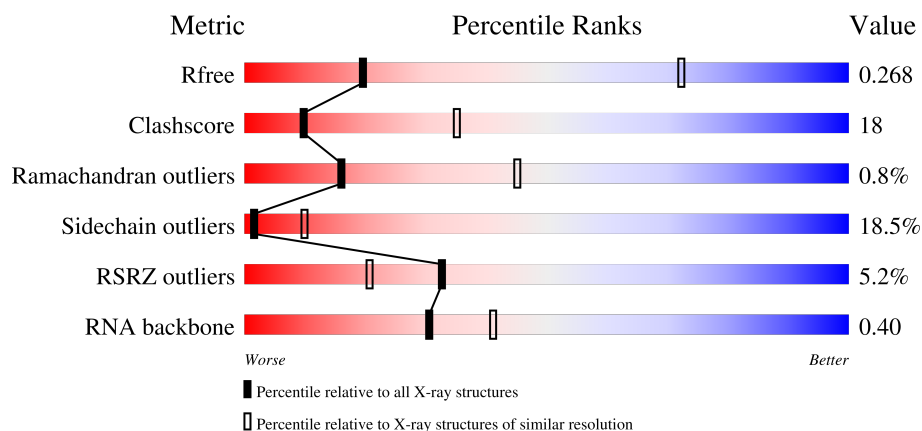
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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}	180053	1062 (3.78-3.54)
Clashscore	190562	1009 (3.76-3.56)
Ramachandran outliers	187476	1054 (3.78-3.54)
Sidechain outliers	187428	1052 (3.78-3.54)
RSRZ outliers	180081	1061 (3.78-3.54)
RNA backbone	3983	1027 (4.26-3.06)

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

Mol	Chain	Length	Quality of chain
1	A	275	
2	B	211	
3	C	205	
4	D	180	

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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	166	
13	N	118	
14	O	100	
15	P	137	
16	Q	95	
17	R	114	
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	66	
27	X	2880	
28	Y	123	

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	X	2908	-	-	-	X
29	MG	X	2910	-	-	-	X
29	MG	X	2924	-	-	-	X
29	MG	X	2926	-	-	-	X
29	MG	X	2944	-	-	-	X
29	MG	X	2948	-	-	-	X

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 83768 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.

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	-	insertion	UNP Q9RXJ7
P	111	PRO	-	insertion	UNP Q9RXJ7
P	112	ARG	-	insertion	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 RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	X	2667	Total	C	N	O	P	0	0	0
			57254	25538	10574	18475	2667			

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 RNA.

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

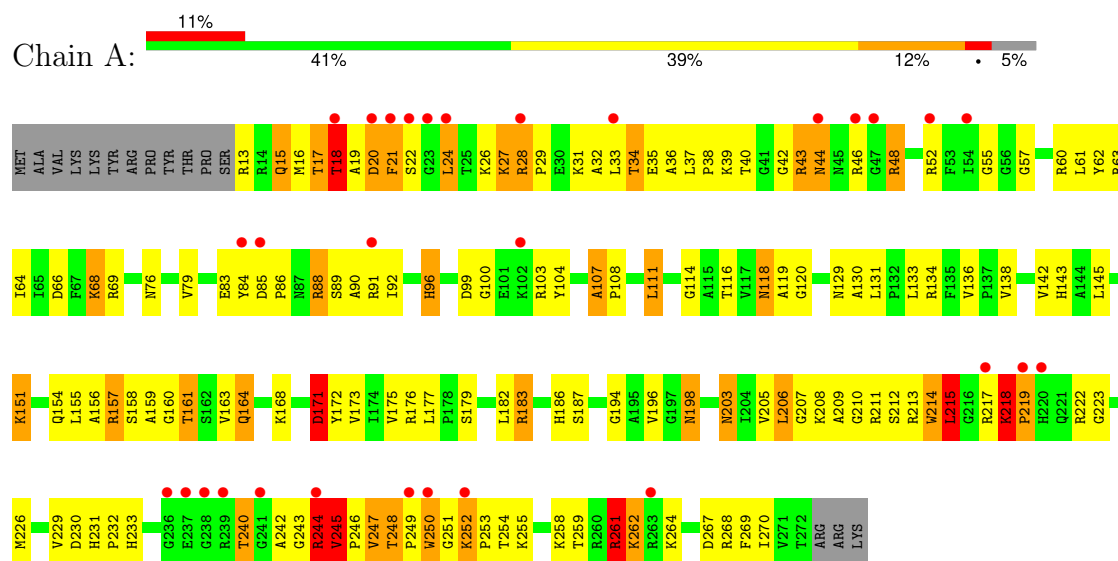
- Molecule 29 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	K	1	Total	Mg	0	0
			1	1		
29	X	50	Total	Mg	0	0
			50	50		

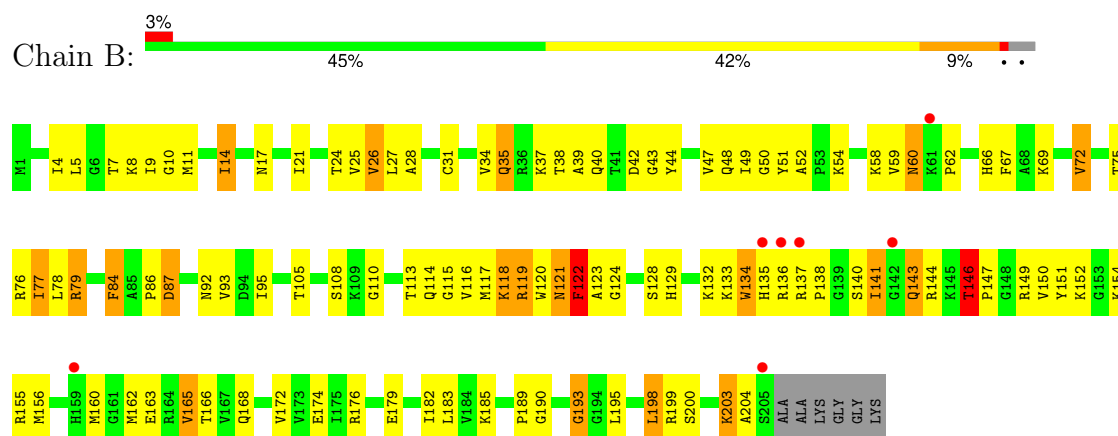
3 Residue-property plots [i](#)

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

• Molecule 1: 50S ribosomal protein L2

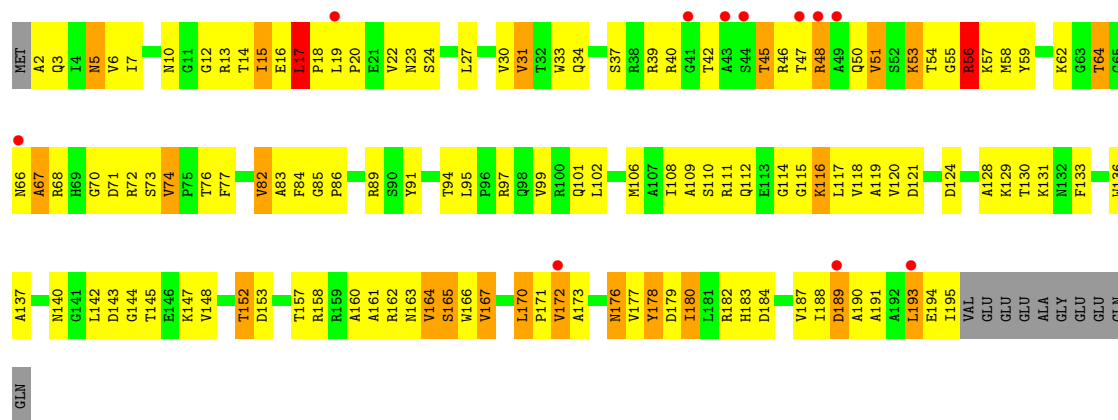


• Molecule 2: 50S ribosomal protein L3

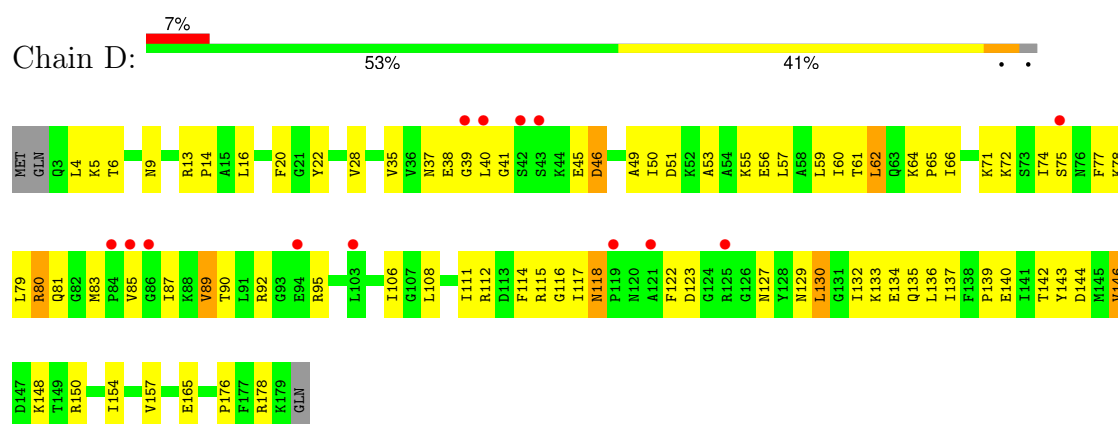


• Molecule 3: 50S ribosomal protein L4

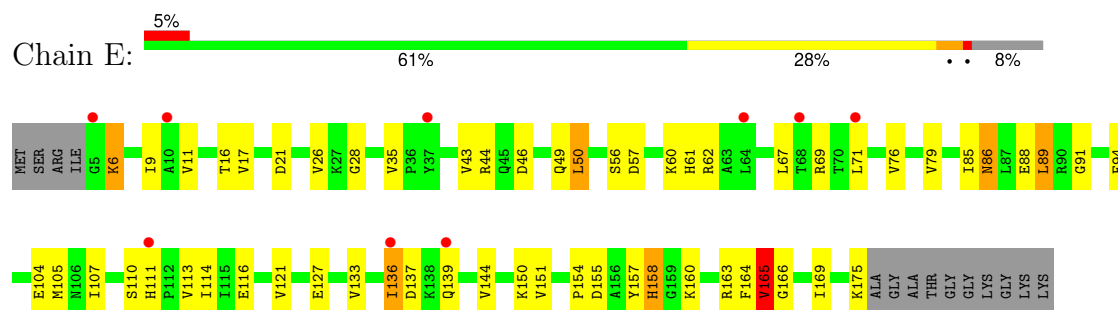




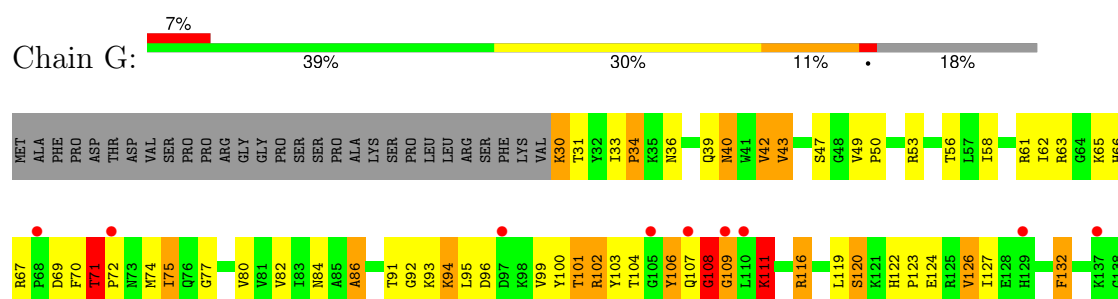
- Molecule 4: 50S ribosomal protein L5



- Molecule 5: 50S ribosomal protein L6



- Molecule 6: 50S ribosomal protein L13

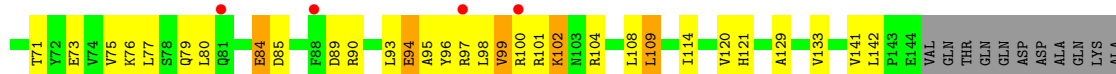
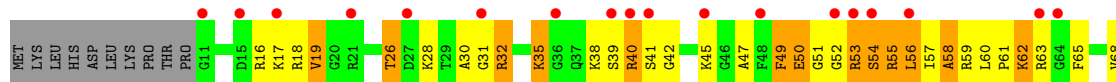
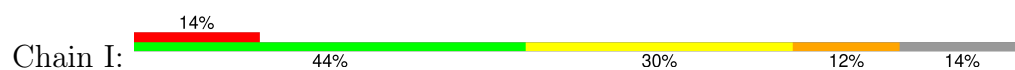




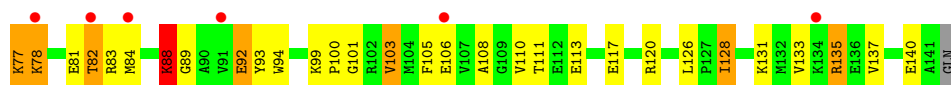
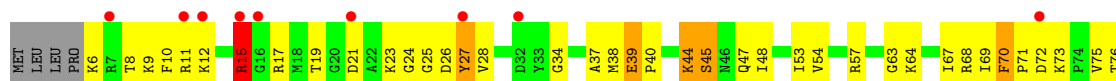
• Molecule 7: 50S ribosomal protein L14



• Molecule 8: 50S ribosomal protein L15



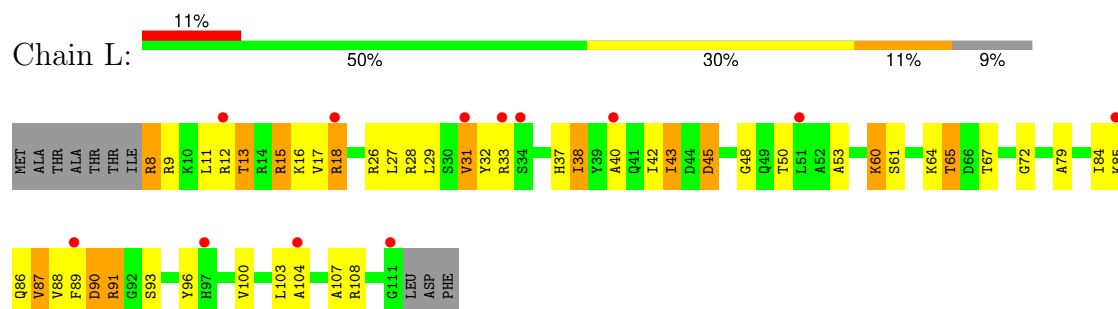
• Molecule 9: 50S ribosomal protein L16



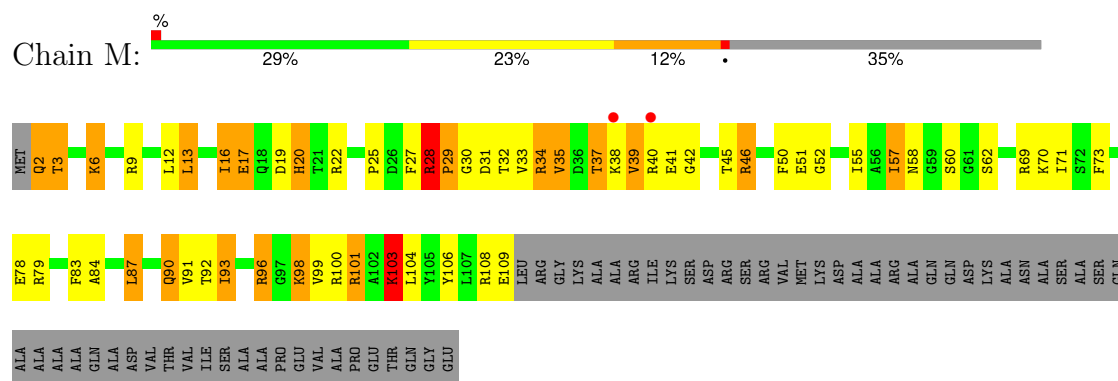
• Molecule 10: 50S ribosomal protein L17



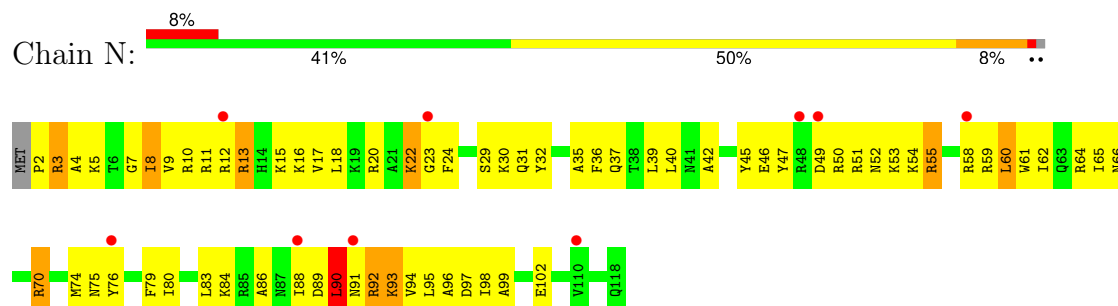
- Molecule 11: 50S ribosomal protein L18



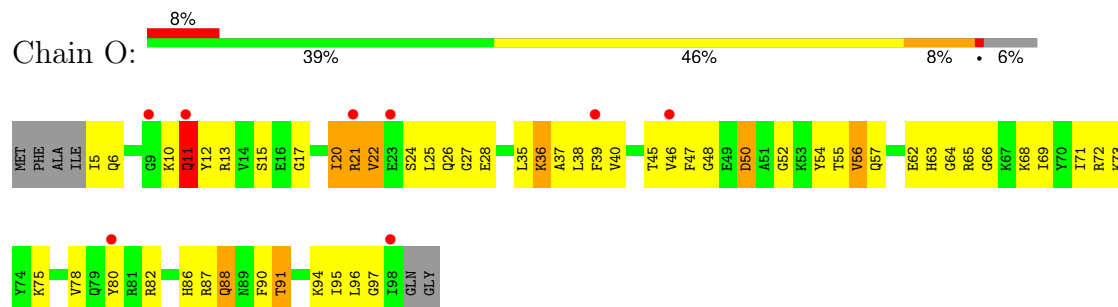
- Molecule 12: 50S ribosomal protein L19



- Molecule 13: 50S ribosomal protein L20

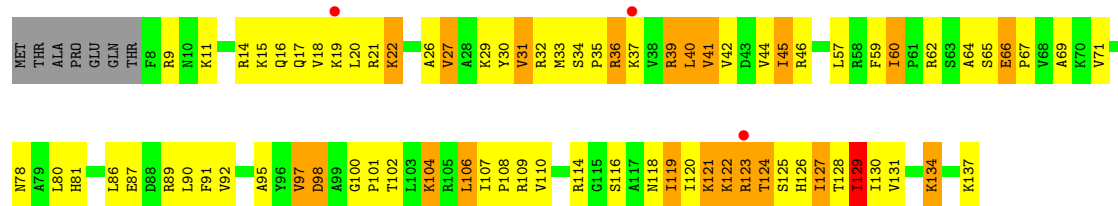


- Molecule 14: 50S ribosomal protein L21

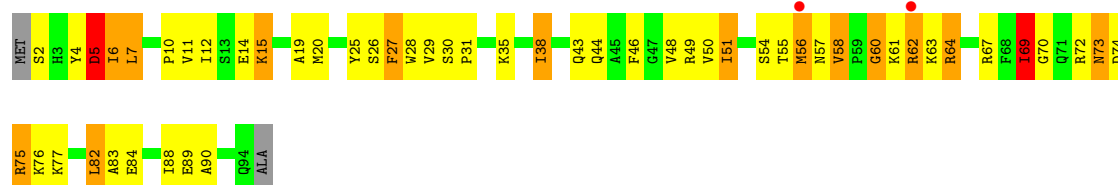


- Molecule 15: 50S ribosomal protein L22

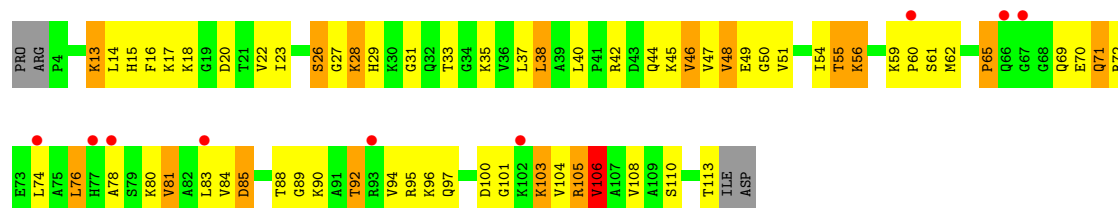




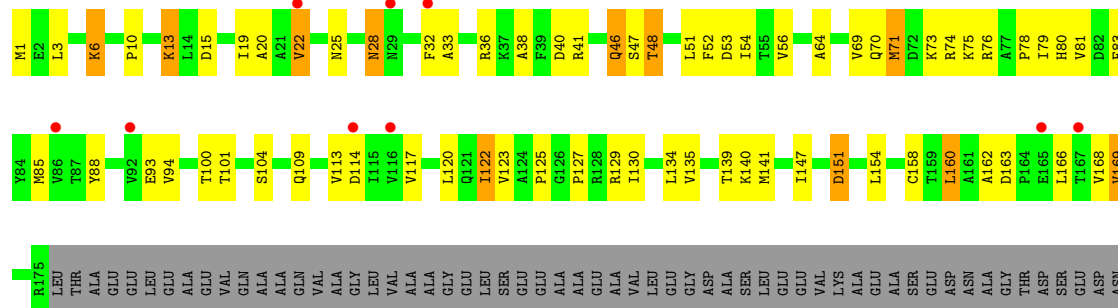
- Molecule 16: 50S ribosomal protein L23



- Molecule 17: 50S ribosomal protein L24

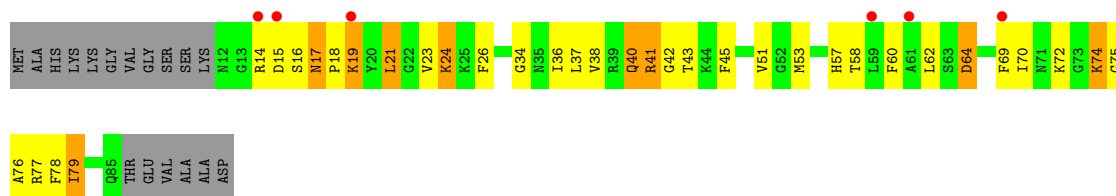


- Molecule 18: 50S ribosomal protein L25

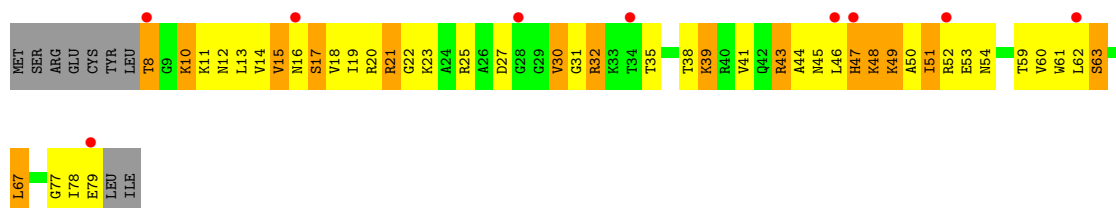


- Molecule 19: 50S ribosomal protein L27

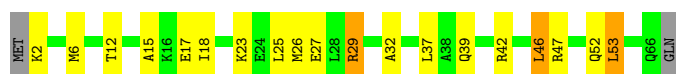




- Molecule 20: 50S ribosomal protein L28



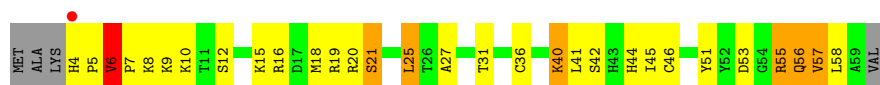
- Molecule 21: 50S ribosomal protein L29



- Molecule 22: 50S ribosomal protein L30



- Molecule 23: 50S ribosomal protein L32

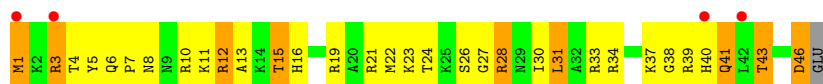


- Molecule 24: 50S ribosomal protein L33

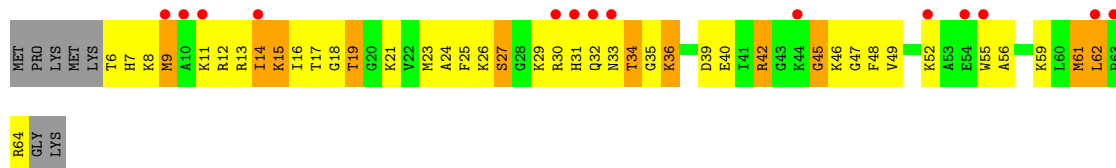


- Molecule 25: 50S ribosomal protein L34

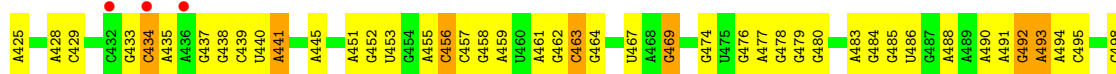
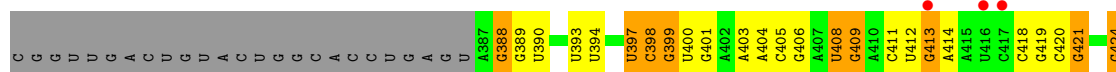
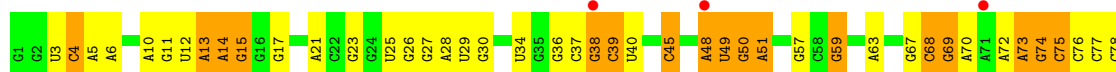




• Molecule 26: 50S ribosomal protein L35

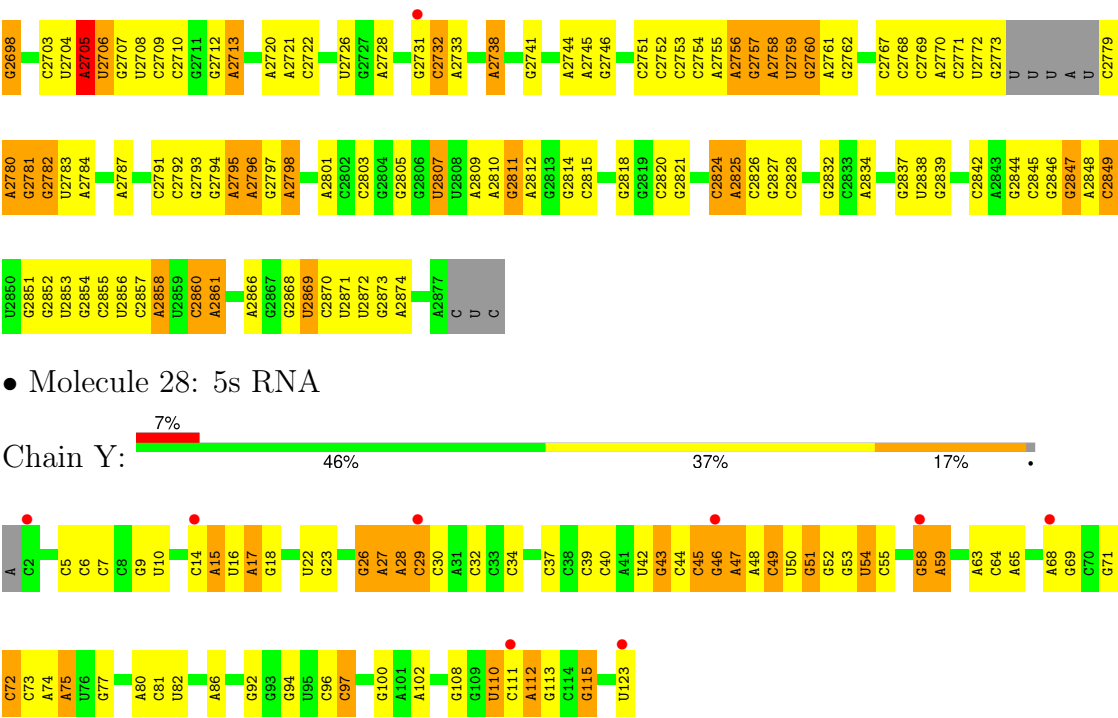


• Molecule 27: 23s RNA





G2620	G2621	G2624	G2625	G2626	G2627	G2628	G2629	A2633	G2634	G2635	A2636	G2637	G2640	A2641	G2642	G2645	G2646	G2650	G2651	G2652	A2653	G2654	G2655	G2656	G2657	A2658	G2659	G2660	G2662	G2663	G2664	G2665	G2666	G2667	G2668	A2690	G2691	A2692	U2693	G2694	G2695	A2696	G2697																																																						
C2547	C2548	G2549	C2550	A2551	G2552	G2553	G2554	G2555	A2556	G2557	G2558	G2559	G2560	G2561	G2562	U2563	U2564	G2565	A2566	G2571	U2572	G2573	G2576	A2577	G2578	A2579	G2580	A2581	G2582	U2583	G2587	U2588	C2591	G2592	A2593	U2594	G2595	G2596	U2597	G2598	G2599	A2600	G2604	G2605	G2606	G2607	A2608																																																		
C2477	U2478	U2479	C2480	G2481	A2482	U2483	G2484	U2485	G2486	G2487	G2488	G2489	U2490	G2491	G2492	U2493	C2494	G2495	G2496	A2497	U2498	G2499	C2500	G2504	G2508	A2509	A2510	A2513	G2514	G2515	U2516	C2517	C2518	U2519	C2520	A2521	G2522	G2523	U2526	G2527	G2528	U2529	C2530	U2531	G2532	U2533	U2534	A2540	U2541	U2542	A2543	A2544	U2545	G2546																																											
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C2260	G2261	C2262	C2263	C2264	A2265	A2266	G2267	G2268	G2269	U2270	C2271	A2272	A2277	A2278	G2281	G2282	U2283	U2284	U2285	G2286	G2287	A2288	A2289	A2290	U2291	G2292	G2293	U2294	G2297	U2298	A2299	G2300	A2301	G2302	C2303	G2304	C2305	A2306	A2307	A2308	G2309	U2310	U2311	A2312	G2313	A2314	A2315	U2318	U2323	U2324	A2325	G2326	U2327	G2328																																											
U2180	A2181	U2185	G2186	A2187	A2188	A2189	A2190	A2191	U2192	C2193	A2194	C2195	U2196	U2197	U2198	C2199	G2200	G2201	G2202	G2203	A2204	C2205	U2212	G2213	G2217	G2218	U2222	U2223	U2224	G2225	A2226	C2227	U2228	G2229	G2230	G2234	G2235	U2236	C2237	U2241	C2242	C2243	C2244	A2245	A2246	A2247	G2250	U2251	A2252	A2253	C2254																																														
A	C	U	G	G	C	U	U	U	U	G	G	G	G	G	U	C	G	U	U	G	G	C	A	C	C	U	U	C	A	A	C	U	C	U	C	A	C	C	U	G	A2165	A2166	A2167	A2168	A2169	C2170	U2171	G2174	A2175	U2176	U2177	U2178	C2179																																												
G1983	A1984	G1985	G1986	G1987	A1988	C1989	U1990	C1991	G1992	G1993	U1994	G1995	A1996	A1997	U1998	U1999	U2000	G2001	A2002	A2003	U2004	U2005	G2006	G2007	C2008	U2009	G2010	U2011	A2012	A2013	G2014	G2015	U2016	U2017	G2018	C2019	G2020	G2021	C2022	G2023	A2024	A2025	C2026	C2027	A2031	G2032	C2033	A2034	G2035	C2038	G2039	A2040	A2041	A2042	A2043	A2045																																									
U1833	G1834	G1835	C1836	A1840	G1841	G1842	G1843	A1844	U1845	A1846	G1850	A1851	G1852	C1853	G1854	G1855	U1856	G1857	C1858	A1859	A1860	G1861	C1865	G1866	G1867	A1868	G1871	A1872	G1873	U1874	A1875	G1876	G1877	G1879	G1882	C1885	G1886	G1887	C1888	G1889	A1891	U1892	A1893	G1894	G1895	C1896	U1897	A1898	G1899	U1909	A1910	A1911	G1912	U1913	U1914	A1919	A1920	A1921	U1922	U1923	U1924	C1925	U1926	A1935	A1936	G1937	U1938	U1939	A1943	G1944	C1945	U1946	G1947	C1948	A1949	C1950	A1953	A1954	G1955	G1958	U1959	A1963	A1964	U1965	C1966	U1967	G1968	G1969	G1970	C1973	U1974	U1975	U1976	C1979	A1980	U1981	C1982
U1688	U1768	U1769	U1770	C1773	A1774	A1775	A1776	U1777	U1778	C1779	A1780	C1781	A1782	U1785	C1786	U1787	G1788	U1789	G1790	C1791	C1792	A1793	A1794	C1795	A1796	C1797	G1798	A1799	A1800	C1801	A1802	U1803	U1804	G1805	A1806	A1807	C1808	G1809	A1810	A1811	U1812	A1813	G1814	G1815	C1816	U1817	G1818	U1819	A1820	A1821	C1824	U1825	U1826	G1827	A1831	U1832																																									



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.72Å 412.59Å 696.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.65 19.99 – 3.65	Depositor EDS
% Data completeness (in resolution range)	95.9 (19.99-3.65) 95.3 (19.99-3.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.226 , 0.270 0.227 , 0.268	Depositor DCC
R_{free} test set	13171 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	108.4	Xtriage
Anisotropy	0.636	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	83768	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.61	1/2025 (0.0%)	1.25	33/2726 (1.2%)
2	B	0.69	0/1567	1.18	8/2105 (0.4%)
3	C	0.58	0/1504	1.15	13/2036 (0.6%)
4	D	0.37	0/1419	0.86	2/1903 (0.1%)
5	E	0.40	0/1308	0.94	5/1771 (0.3%)
6	G	0.61	0/1138	1.29	15/1539 (1.0%)
7	H	0.75	1/1007 (0.1%)	1.17	6/1352 (0.4%)
8	I	0.63	0/1022	1.21	9/1366 (0.7%)
9	J	0.64	0/1113	1.29	22/1486 (1.5%)
10	K	0.79	0/886	1.26	8/1188 (0.7%)
11	L	0.45	0/785	0.95	1/1048 (0.1%)
12	M	0.79	2/884 (0.2%)	1.28	10/1186 (0.8%)
13	N	0.56	0/994	1.03	2/1323 (0.2%)
14	O	0.50	0/750	1.11	5/1000 (0.5%)
15	P	0.74	0/1052	1.27	9/1409 (0.6%)
16	Q	0.54	0/737	1.18	7/988 (0.7%)
17	R	0.60	0/835	1.16	10/1121 (0.9%)
18	S	0.43	0/1370	0.91	2/1862 (0.1%)
19	T	0.54	0/563	1.14	7/747 (0.9%)
20	U	0.59	0/556	1.07	2/741 (0.3%)
21	V	0.39	0/529	0.99	4/704 (0.6%)
22	W	0.48	0/426	0.93	2/568 (0.4%)
23	Z	0.66	0/455	1.20	4/611 (0.7%)
24	1	0.56	0/438	1.27	5/583 (0.9%)
25	2	0.56	0/387	1.22	6/509 (1.2%)
26	3	0.63	0/468	1.36	8/614 (1.3%)
27	X	0.32	0/64113	0.52	5/99999 (0.0%)
28	Y	0.22	0/2907	0.40	0/4529
All	All	0.41	4/91238 (0.0%)	0.72	210/137014 (0.2%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	2
6	G	0	4
7	H	0	1
8	I	0	2
10	K	0	1
17	R	0	2
20	U	0	1
26	3	0	1
All	All	0	15

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	29	PRO	CA-C	6.04	1.60	1.52
7	H	2	ILE	CA-CB	-5.23	1.48	1.54
1	A	20	ASP	CA-C	5.21	1.58	1.52
12	M	35	VAL	CA-CB	5.13	1.59	1.53

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	69	ILE	N-CA-C	12.65	124.19	112.29
16	Q	61	LYS	N-CA-C	12.42	125.44	110.91
8	I	52	GLY	N-CA-C	11.67	123.94	112.04
15	P	60	ILE	CA-C-N	10.65	130.32	119.56
15	P	60	ILE	C-N-CA	10.65	130.32	119.56
10	K	92	GLY	N-CA-C	-10.56	98.39	110.96
6	G	106	TYR	N-CA-C	-10.51	94.93	110.48
1	A	24	LEU	N-CA-C	10.11	122.73	110.91
12	M	103	LYS	N-CA-C	10.11	126.59	112.04
2	B	193	GLY	N-CA-C	-9.90	101.47	115.43
16	Q	74	ASP	N-CA-C	9.33	121.82	110.91
6	G	33	ILE	CA-C-N	9.18	130.39	120.11
6	G	33	ILE	C-N-CA	9.18	130.39	120.11
3	C	56	ARG	N-CA-C	9.05	124.51	113.38
24	1	5	GLY	CA-C-N	9.04	128.68	119.82
24	1	5	GLY	C-N-CA	9.04	128.68	119.82
25	2	38	GLY	N-CA-C	-8.99	100.19	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	108	GLY	N-CA-C	-8.75	101.57	112.77
1	A	245	VAL	CA-C-N	8.73	130.75	119.84
1	A	245	VAL	C-N-CA	8.73	130.75	119.84
1	A	35	GLU	N-CA-C	8.71	121.10	110.91
26	3	24	ALA	N-CA-C	-8.70	97.36	110.14
19	T	17	ASN	CA-C-N	8.65	128.28	118.85
19	T	17	ASN	C-N-CA	8.65	128.28	118.85
6	G	122	HIS	CA-C-N	8.60	128.24	119.56
6	G	122	HIS	C-N-CA	8.60	128.24	119.56
6	G	86	ALA	N-CA-C	-8.55	101.90	111.82
1	A	244	ARG	N-CA-C	8.34	121.45	111.02
12	M	57	ILE	N-CA-C	8.32	120.11	112.29
26	3	45	GLY	N-CA-C	8.24	122.68	112.79
8	I	58	ALA	N-CA-C	-8.22	100.30	110.41
2	B	122	PHE	CB-CA-C	-8.09	105.21	115.89
1	A	218	LYS	CA-C-N	8.07	129.93	119.84
1	A	218	LYS	C-N-CA	8.07	129.93	119.84
1	A	242	ALA	N-CA-C	8.04	121.70	107.80
1	A	211	ARG	N-CA-C	-7.96	102.58	111.82
10	K	90	ARG	CA-C-N	7.87	128.60	119.47
10	K	90	ARG	C-N-CA	7.87	128.60	119.47
9	J	19	THR	N-CA-C	7.86	121.30	108.26
2	B	146	THR	CA-C-N	-7.84	110.04	119.84
2	B	146	THR	C-N-CA	-7.84	110.04	119.84
3	C	17	LEU	CA-C-N	7.82	127.86	119.89
3	C	17	LEU	C-N-CA	7.82	127.86	119.89
9	J	81	GLU	N-CA-C	7.77	119.94	108.60
1	A	179	SER	N-CA-C	-7.76	103.39	113.17
10	K	58	GLY	N-CA-C	7.43	125.40	115.59
7	H	43	ARG	N-CA-C	7.37	120.18	111.71
3	C	170	LEU	CA-C-N	7.35	127.31	120.03
3	C	170	LEU	C-N-CA	7.35	127.31	120.03
6	G	40	ASN	N-CA-C	7.28	120.95	110.24
8	I	102	LYS	CB-CA-C	-7.27	106.29	115.89
9	J	25	GLY	N-CA-C	-7.23	102.36	110.96
9	J	63	GLY	N-CA-C	-7.16	104.96	115.63
1	A	107	ALA	CA-C-N	7.15	128.12	120.11
1	A	107	ALA	C-N-CA	7.15	128.12	120.11
2	B	134	TRP	N-CA-C	-7.12	98.25	108.07
12	M	58	ASN	N-CA-C	7.08	120.22	110.24
1	A	34	THR	N-CA-C	7.05	119.96	108.26
1	A	240	THR	N-CA-C	7.02	117.14	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	83	VAL	N-CA-C	7.00	117.11	110.53
12	M	39	VAL	N-CA-C	-6.98	104.77	112.80
7	H	130	ALA	CA-C-N	6.96	127.25	119.32
7	H	130	ALA	C-N-CA	6.96	127.25	119.32
6	G	109	GLY	N-CA-C	-6.91	105.67	114.37
8	I	50	GLU	N-CA-C	6.90	121.15	112.87
1	A	17	THR	N-CA-C	6.81	119.69	108.99
23	Z	6	VAL	CA-C-N	6.77	126.53	119.76
23	Z	6	VAL	C-N-CA	6.77	126.53	119.76
6	G	142	ARG	N-CA-C	-6.77	102.98	111.11
10	K	13	ASN	N-CA-C	6.75	118.71	110.41
14	O	52	GLY	N-CA-C	-6.68	106.38	114.66
6	G	165	VAL	N-CA-C	6.66	118.55	112.29
9	J	70	PHE	CA-C-N	6.58	127.56	120.13
9	J	70	PHE	C-N-CA	6.58	127.56	120.13
14	O	11	GLN	N-CA-C	6.57	117.73	108.00
13	N	90	LEU	N-CA-C	-6.55	105.16	113.02
17	R	85	ASP	N-CA-C	6.55	121.12	112.35
5	E	21	ASP	CB-CA-C	-6.54	109.02	116.54
1	A	171	ASP	N-CA-C	-6.51	104.96	113.17
1	A	18	THR	N-CA-C	6.45	124.54	110.80
2	B	179	GLU	N-CA-C	-6.44	105.05	113.17
8	I	89	ASP	N-CA-C	6.41	118.84	111.02
3	C	47	THR	N-CA-C	-6.39	103.60	111.40
6	G	42	VAL	N-CA-C	6.38	117.54	108.42
6	G	71	THR	CA-C-N	6.38	126.59	119.32
6	G	71	THR	C-N-CA	6.38	126.59	119.32
4	D	118	ASN	CA-C-N	6.34	125.96	119.56
4	D	118	ASN	C-N-CA	6.34	125.96	119.56
5	E	111	HIS	CA-C-N	6.30	126.67	119.92
5	E	111	HIS	C-N-CA	6.30	126.67	119.92
16	Q	58	VAL	CA-C-N	6.30	127.72	119.84
16	Q	58	VAL	C-N-CA	6.30	127.72	119.84
9	J	82	THR	N-CA-C	6.28	124.17	110.80
21	V	2	LYS	CA-C-N	-6.27	112.45	118.97
21	V	2	LYS	C-N-CA	-6.27	112.45	118.97
1	A	17	THR	CA-C-N	6.26	133.50	121.54
1	A	17	THR	C-N-CA	6.26	133.50	121.54
1	A	248	THR	CA-C-N	-6.25	115.33	121.65
1	A	248	THR	C-N-CA	-6.25	115.33	121.65
17	R	28	LYS	N-CA-C	-6.24	100.26	109.81
9	J	101	GLY	N-CA-C	-6.23	107.66	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	1975	G	C2'-C3'-O3'	6.23	118.84	109.50
1	A	57	GLY	N-CA-C	6.18	117.82	111.95
2	B	92	ASN	N-CA-C	6.13	118.76	111.71
1	A	31	LYS	N-CA-C	6.11	118.60	109.25
12	M	30	GLY	N-CA-C	-6.10	102.58	110.38
6	G	104	THR	N-CA-C	6.08	117.73	110.19
23	Z	56	GLN	N-CA-C	6.08	120.26	111.02
9	J	81	GLU	CA-C-N	6.07	133.13	121.54
9	J	81	GLU	C-N-CA	6.07	133.13	121.54
26	3	15	LYS	N-CA-C	6.06	118.78	110.24
3	C	66	ASN	N-CA-C	6.04	120.22	112.86
8	I	47	ALA	N-CA-C	6.01	120.32	112.92
25	2	6	GLN	CA-C-N	6.01	126.37	119.93
25	2	6	GLN	C-N-CA	6.01	126.37	119.93
7	H	85	ASP	N-CA-C	-5.96	105.50	112.89
16	Q	56	MET	N-CA-C	5.96	116.97	108.74
5	E	28	GLY	CA-C-N	5.96	125.58	119.56
5	E	28	GLY	C-N-CA	5.96	125.58	119.56
1	A	16	MET	N-CA-C	-5.96	98.94	109.06
23	Z	55	ARG	N-CA-C	5.93	119.19	108.69
27	X	1141	U	C2'-C3'-O3'	5.88	118.31	109.50
25	2	26	SER	N-CA-C	-5.86	105.02	111.82
22	W	12	ARG	CA-C-N	5.83	126.16	119.92
22	W	12	ARG	C-N-CA	5.83	126.16	119.92
25	2	5	TYR	N-CA-C	5.83	118.31	107.99
17	R	76	LEU	N-CA-C	5.79	118.22	109.41
17	R	26	SER	CB-CA-C	-5.79	108.23	116.34
15	P	98	ASP	N-CA-C	5.78	120.03	112.92
10	K	93	GLY	CA-C-N	-5.78	114.82	122.85
10	K	93	GLY	C-N-CA	-5.78	114.82	122.85
9	J	126	LEU	N-CA-C	5.78	118.00	109.62
3	C	145	THR	N-CA-C	-5.78	106.23	113.28
9	J	135	ARG	N-CA-C	5.77	118.36	109.07
24	1	41	ASP	CA-C-N	5.77	127.05	119.84
24	1	41	ASP	C-N-CA	5.77	127.05	119.84
1	A	215	LEU	N-CA-C	5.74	120.56	113.50
14	O	11	GLN	CB-CA-C	-5.72	108.33	116.34
9	J	15	ARG	N-CA-C	5.67	116.04	108.38
25	2	3	ARG	N-CA-C	5.67	118.21	110.55
2	B	17	ASN	CB-CA-C	-5.67	110.02	116.54
24	1	37	LEU	N-CA-C	5.63	118.49	110.10
3	C	167	VAL	N-CA-C	5.61	115.66	108.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	3	40	GLU	N-CA-C	-5.60	104.80	111.69
9	J	126	LEU	CA-C-N	5.60	125.30	119.82
9	J	126	LEU	C-N-CA	5.60	125.30	119.82
1	A	261	ARG	N-CA-C	5.58	116.73	108.86
9	J	39	GLU	CA-C-N	5.58	125.76	119.90
9	J	39	GLU	C-N-CA	5.58	125.76	119.90
8	I	84	GLU	CB-CA-C	-5.57	108.53	115.89
9	J	88	LYS	N-CA-C	5.57	117.97	109.95
1	A	44	ASN	N-CA-C	5.56	116.72	108.60
3	C	115	GLY	N-CA-C	5.51	118.75	111.03
15	P	22	LYS	CA-C-N	5.49	125.66	119.90
15	P	22	LYS	C-N-CA	5.49	125.66	119.90
17	R	103	LYS	N-CA-C	5.49	117.41	109.07
17	R	110	SER	N-CA-C	5.48	119.50	111.34
9	J	78	LYS	CA-C-N	-5.47	113.00	119.84
9	J	78	LYS	C-N-CA	-5.47	113.00	119.84
19	T	17	ASN	N-CA-C	5.47	117.09	108.23
1	A	120	GLY	CA-C-N	5.45	124.79	118.85
1	A	120	GLY	C-N-CA	5.45	124.79	118.85
8	I	61	PRO	CA-C-N	-5.44	114.26	122.81
8	I	61	PRO	C-N-CA	-5.44	114.26	122.81
14	O	50	ASP	N-CA-C	-5.43	106.33	113.17
21	V	39	GLN	CA-C-N	5.43	125.25	119.28
21	V	39	GLN	C-N-CA	5.43	125.25	119.28
26	3	14	ILE	N-CA-C	-5.41	107.21	112.29
17	R	106	VAL	N-CA-C	5.39	116.13	108.42
27	X	2705	A	C4'-C3'-O3'	5.39	117.48	109.40
3	C	178	TYR	N-CA-C	-5.38	105.11	110.97
7	H	116	ARG	N-CA-C	-5.34	106.76	113.28
20	U	51	ILE	N-CA-C	5.34	116.21	107.24
18	S	46	GLN	N-CA-C	5.34	118.25	111.69
15	P	41	VAL	CB-CA-C	-5.32	105.16	111.81
18	S	40	ASP	N-CA-C	-5.29	106.78	113.18
12	M	28	ARG	CA-C-N	-5.29	113.23	119.84
12	M	28	ARG	C-N-CA	-5.29	113.23	119.84
20	U	12	ASN	CB-CA-C	-5.29	110.50	116.63
19	T	74	LYS	CB-CA-C	-5.29	109.50	115.79
12	M	17	GLU	N-CA-C	-5.27	99.57	110.80
15	P	134	LYS	N-CA-C	5.26	117.70	111.33
15	P	66	GLU	CA-C-N	-5.26	114.40	119.87
15	P	66	GLU	C-N-CA	-5.26	114.40	119.87
26	3	36	LYS	N-CA-C	5.26	116.97	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	44	TYR	N-CA-C	5.26	117.81	109.50
3	C	67	ALA	N-CA-C	5.24	121.96	110.80
1	A	28	ARG	CA-C-N	5.22	125.69	120.52
1	A	28	ARG	C-N-CA	5.22	125.69	120.52
26	3	42	ARG	N-CA-C	-5.22	106.88	113.20
19	T	21	LEU	CB-CA-C	-5.22	109.58	115.79
11	L	53	ALA	N-CA-C	5.21	117.00	110.91
12	M	6	LYS	N-CA-C	-5.19	101.30	109.25
26	3	61	MET	N-CA-C	5.19	117.36	111.02
17	R	46	VAL	CB-CA-C	-5.19	102.95	110.63
16	Q	60	GLY	N-CA-C	5.18	125.46	113.18
1	A	136	VAL	CA-C-N	5.15	125.08	119.78
1	A	136	VAL	C-N-CA	5.15	125.08	119.78
12	M	42	GLY	N-CA-C	-5.15	105.11	111.70
27	X	1975	G	P-O3'-C3'	5.14	127.92	120.20
3	C	58	MET	N-CA-C	5.13	121.74	110.80
17	R	70	GLU	N-CA-C	5.13	117.68	110.14
16	Q	5	ASP	N-CA-C	-5.12	101.87	109.96
14	O	36	LYS	N-CA-C	5.09	117.86	110.17
19	T	24	LYS	N-CA-C	5.09	117.72	111.82
27	X	1141	U	P-O3'-C3'	5.09	127.83	120.20
17	R	13	LYS	N-CA-C	-5.07	103.98	110.53
13	N	23	GLY	N-CA-C	-5.07	107.40	115.66
19	T	72	LYS	N-CA-C	5.03	119.10	112.92
9	J	92	GLU	N-CA-C	-5.00	103.42	111.02

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	3	27	SER	Peptide
1	A	18	THR	Peptide
2	B	122	PHE	Peptide
2	B	146	THR	Peptide
6	G	108	GLY	Peptide
6	G	111	LYS	Peptide
6	G	120	SER	Peptide
6	G	34	PRO	Peptide
7	H	26	ASN	Peptide
8	I	35	LYS	Peptide
8	I	40	ARG	Peptide
10	K	93	GLY	Peptide

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Mol	Chain	Res	Type	Group
17	R	60	PRO	Peptide
17	R	65	PRO	Peptide
20	U	30	VAL	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	130	0
2	B	1539	0	1600	107	0
3	C	1481	0	1504	102	0
4	D	1400	0	1481	61	0
5	E	1286	0	1336	36	0
6	G	1114	0	1144	66	0
7	H	997	0	1046	64	0
8	I	1011	0	1047	55	0
9	J	1090	0	1125	57	0
10	K	878	0	930	40	0
11	L	779	0	820	40	0
12	M	871	0	894	50	0
13	N	978	0	1020	71	0
14	O	741	0	756	47	0
15	P	1038	0	1125	81	0
16	Q	726	0	753	37	0
17	R	825	0	881	52	0
18	S	1345	0	1372	44	0
19	T	556	0	579	28	0
20	U	552	0	604	30	0
21	V	525	0	546	16	0
22	W	424	0	470	16	0
23	Z	443	0	444	28	0
24	1	431	0	456	30	0
25	2	383	0	414	28	0
26	3	462	0	506	49	0
27	X	57254	0	28850	1335	0
28	Y	2601	0	1327	54	0
29	K	1	0	0	0	0
29	X	50	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	83768	0	55086	2395	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 18.

All (2395) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLY:H	1:A:217:ARG:HB2	1.20	1.04
2:B:136:ARG:HB3	27:X:1673:C:H5'	1.36	1.04
27:X:571:U:HO2'	27:X:581:A:H8	1.12	0.98
27:X:517:A:H5''	27:X:518:A:H5'	1.45	0.95
2:B:116:VAL:HG22	2:B:136:ARG:HG3	1.49	0.95
3:C:163:ASN:HD21	3:C:167:VAL:H	1.15	0.93
23:Z:19:ARG:NH2	27:X:1277:G:OP1	2.02	0.91
27:X:1542:G:H22	27:X:1562:G:H1	1.12	0.91
1:A:252:LYS:H	1:A:252:LYS:HZ2	1.17	0.90
2:B:133:LYS:HB2	2:B:137:ARG:HG2	1.55	0.89
7:H:25:LEU:HD11	7:H:52:VAL:HG23	1.53	0.89
27:X:833:A:N3	27:X:954:U:O2'	2.05	0.89
25:2:12:ARG:HG2	27:X:699:G:H1	1.40	0.85
13:N:5:LYS:HG3	13:N:7:GLY:H	1.39	0.84
8:I:62:LYS:HB3	26:3:12:ARG:HA	1.57	0.84
1:A:250:TRP:O	1:A:255:LYS:NZ	2.09	0.84
27:X:2757:G:H5''	27:X:2758:A:H5'	1.58	0.82
27:X:2510:A:H61	27:X:2641:A:H61	1.28	0.82
1:A:43:ARG:NH1	27:X:705:C:OP1	2.13	0.82
3:C:46:ARG:NH1	27:X:463:C:OP1	2.13	0.82
27:X:854:G:H1	27:X:948:C:H42	1.26	0.81
27:X:1850:G:O2'	27:X:1867:A:N6	2.14	0.81
6:G:74:MET:HA	6:G:140:GLN:HE22	1.45	0.81
8:I:38:LYS:NZ	27:X:954:U:OP2	2.10	0.81
27:X:1202:U:H2'	27:X:1203:A:H8	1.45	0.81
14:O:57:GLN:H	14:O:97:GLY:HA3	1.44	0.80
27:X:320:A:N3	27:X:340:G:O2'	2.13	0.80
27:X:1562:G:H5'	27:X:1563:U:H5'	1.62	0.80
27:X:123:A:O2'	27:X:124:A:OP1	1.99	0.80
25:2:19:ARG:HG2	27:X:123:A:H5''	1.63	0.80
6:G:34:PRO:HB3	6:G:69:ASP:HB3	1.64	0.79
20:U:8:THR:HA	20:U:14:VAL:HG21	1.61	0.79
27:X:538:A:O2'	27:X:539:A:O5'	1.99	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:41:GLU:HG3	12:M:46:ARG:HD2	1.63	0.79
15:P:122:LYS:NZ	27:X:1279:G:O6	2.13	0.79
20:U:50:ALA:HB3	20:U:62:LEU:HB2	1.65	0.79
27:X:1030:U:H3	27:X:1153:A:H62	1.27	0.79
2:B:118:LYS:NZ	27:X:2704:U:OP1	2.14	0.79
22:W:5:LEU:HB2	22:W:25:LEU:HD13	1.63	0.79
27:X:841:G:H2'	27:X:842:A:C8	2.18	0.79
1:A:28:ARG:HD3	27:X:1583:A:H62	1.46	0.79
3:C:161:ALA:HB1	3:C:167:VAL:HG21	1.63	0.78
27:X:1963:G:O2'	27:X:1965:U:OP2	2.00	0.78
27:X:2551:A:H5'	27:X:2553:G:H4'	1.64	0.78
2:B:189:PRO:HA	27:X:2659:C:H5'	1.63	0.78
13:N:66:ASN:HB3	13:N:76:TYR:HB2	1.65	0.78
2:B:174:GLU:HB3	2:B:183:LEU:HD12	1.66	0.78
15:P:97:VAL:HG13	15:P:125:SER:HB2	1.65	0.78
22:W:8:SER:HB2	27:X:999:A:H5''	1.65	0.78
26:3:52:LYS:NZ	27:X:2338:C:O2'	2.17	0.77
2:B:137:ARG:NH2	27:X:2034:A:OP1	2.17	0.77
7:H:40:GLY:HA3	27:X:2545:A:H61	1.47	0.77
27:X:2016:A:O2'	27:X:2018:G:OP2	2.01	0.77
2:B:10:GLY:HA3	12:M:13:LEU:HD21	1.66	0.77
1:A:79:VAL:HB	1:A:114:GLY:H	1.48	0.77
25:2:34:ARG:HD2	25:2:40:HIS:HB3	1.65	0.77
12:M:51:GLU:H	12:M:70:LYS:HZ1	1.32	0.77
17:R:56:LYS:HB3	17:R:69:GLN:HG2	1.66	0.77
3:C:5:ASN:N	3:C:5:ASN:OD1	2.18	0.77
27:X:864:C:O2	27:X:940:G:N2	2.18	0.77
1:A:17:THR:O	1:A:19:ALA:HA	1.83	0.77
27:X:2447:G:HO2'	27:X:2448:A:H8	1.33	0.77
7:H:3:MET:HE1	27:X:1683:G:H21	1.51	0.76
1:A:244:ARG:HH12	27:X:1834:G:H1'	1.50	0.76
27:X:2557:G:OP1	27:X:2593:A:N6	2.19	0.76
1:A:13:ARG:HE	1:A:27:LYS:HB3	1.49	0.75
7:H:62:GLY:O	7:H:65:LYS:NZ	2.12	0.75
27:X:2327:U:O4	27:X:2361:G:N2	2.19	0.75
23:Z:4:HIS:O	27:X:2039:G:N2	2.18	0.75
7:H:123:PHE:HB3	7:H:126:ILE:HG13	1.68	0.74
12:M:34:ARG:NH2	12:M:90:GLN:O	2.16	0.74
27:X:1856:U:OP1	27:X:2389:G:O2'	2.05	0.74
27:X:2818:G:H1	27:X:2849:C:H42	1.35	0.74
1:A:218:LYS:NZ	1:A:219:PRO:O	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:62:LEU:O	4:D:95:ARG:NH1	2.20	0.74
3:C:74:VAL:HG23	3:C:76:THR:H	1.50	0.74
4:D:75:SER:H	4:D:79:LEU:HD13	1.50	0.74
15:P:124:THR:HG21	15:P:126:HIS:CD2	2.23	0.74
3:C:162:ARG:NH1	3:C:162:ARG:O	2.19	0.74
15:P:34:SER:OG	15:P:122:LYS:NZ	2.20	0.74
27:X:793:G:H21	27:X:796:A:H62	1.34	0.74
4:D:116:GLY:HA2	4:D:176:PRO:HB2	1.70	0.74
18:S:47:SER:OG	18:S:48:THR:N	2.17	0.74
27:X:421:G:H22	27:X:433:G:H1'	1.51	0.74
3:C:68:ARG:HH12	27:X:2043:A:H62	1.33	0.74
8:I:41:SER:HB2	27:X:844:G:H5''	1.69	0.74
23:Z:9:LYS:NZ	27:X:2001:G:OP1	2.19	0.74
27:X:872:G:O2'	27:X:928:G:O6	2.06	0.74
5:E:160:LYS:HZ1	27:X:2637:C:H5'	1.53	0.73
26:3:42:ARG:NE	27:X:2328:G:OP1	2.21	0.73
26:3:32:GLN:NE2	27:X:2371:A:OP2	2.16	0.73
27:X:1465:G:H22	27:X:1476:G:H1	1.37	0.73
6:G:157:PRO:O	6:G:161:GLN:NE2	2.20	0.73
27:X:304:A:N7	27:X:356:A:N6	2.36	0.73
6:G:140:GLN:HG3	27:X:567:G:H5'	1.71	0.72
27:X:2451:G:O2'	27:X:2457:A:N6	2.22	0.72
24:1:30:ASN:ND2	27:X:2264:C:OP2	2.22	0.72
27:X:649:G:H22	27:X:661:C:H1'	1.53	0.72
4:D:115:ARG:HD2	4:D:178:ARG:HH22	1.53	0.72
27:X:412:U:H2'	27:X:413:G:H5'	1.69	0.72
27:X:1466:C:H2'	27:X:1467:U:O4'	1.89	0.72
27:X:200:A:HO2'	27:X:433:G:HO2'	1.36	0.72
3:C:136:TRP:O	3:C:140:ASN:ND2	2.23	0.72
27:X:203:G:O2'	27:X:205:A:N1	2.22	0.72
18:S:1:MET:HE2	18:S:52:PHE:HB3	1.72	0.72
27:X:168:A:H2'	27:X:169:C:C6	2.25	0.72
27:X:2811:G:H2'	27:X:2812:A:C8	2.25	0.72
3:C:162:ARG:HE	27:X:333:A:H5''	1.54	0.71
26:3:13:ARG:HE	26:3:25:PHE:H	1.37	0.71
27:X:2543:A:OP1	27:X:2627:G:O2'	2.04	0.71
28:Y:7:C:O2'	28:Y:29:C:O2	2.07	0.71
4:D:123:ASP:HB3	4:D:127:ASN:H	1.55	0.71
2:B:50:GLY:HA3	2:B:75:THR:HG21	1.72	0.71
3:C:83:ALA:HB3	27:X:595:A:H5'	1.72	0.71
27:X:1223:G:H5'	27:X:1225:G:O4'	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:215:G:H21	27:X:632:A:H8	1.37	0.71
1:A:233:HIS:NE2	1:A:245:VAL:O	2.24	0.71
24:1:28:ARG:NH1	27:X:2264:C:OP2	2.24	0.71
27:X:1412:C:O2'	27:X:1413:U:O5'	2.07	0.71
12:M:100:ARG:HD2	27:X:1744:G:OP1	1.90	0.71
27:X:1073:G:H22	27:X:1087:C:H42	1.39	0.71
27:X:2081:U:H3	27:X:2174:G:H1	1.39	0.71
27:X:552:C:H2'	27:X:553:C:H5''	1.71	0.70
15:P:35:PRO:HA	15:P:125:SER:HB3	1.73	0.70
1:A:89:SER:O	1:A:198:ASN:ND2	2.22	0.70
4:D:78:LYS:HG2	4:D:80:ARG:HH11	1.57	0.70
13:N:84:LYS:HB2	13:N:92:ARG:HH22	1.56	0.70
16:Q:31:PRO:HA	16:Q:76:LYS:HD3	1.73	0.70
27:X:825:C:HO2'	27:X:1239:A:HO2'	1.38	0.70
27:X:689:A:H8	27:X:2052:G:H21	1.40	0.70
16:Q:56:MET:HE3	16:Q:57:ASN:H	1.56	0.70
19:T:51:VAL:HG21	19:T:79:ILE:HG22	1.74	0.70
1:A:252:LYS:HZ2	1:A:252:LYS:N	1.90	0.70
1:A:24:LEU:HB2	1:A:205:VAL:HG22	1.74	0.70
1:A:52:ARG:HD3	27:X:1816:G:OP1	1.91	0.70
1:A:143:HIS:ND1	1:A:194:GLY:O	2.22	0.70
27:X:1109:A:H3'	27:X:1110:G:H8	1.55	0.70
27:X:1398:G:O2'	27:X:1399:C:O4'	2.10	0.70
8:I:40:ARG:NH2	27:X:820:U:OP1	2.25	0.70
6:G:103:TYR:CG	6:G:111:LYS:HB2	2.27	0.69
8:I:56:LEU:HD13	26:3:52:LYS:HZ2	1.57	0.69
11:L:38:ILE:HD11	11:L:40:ALA:HB2	1.74	0.69
18:S:93:GLU:HG2	18:S:123:VAL:HG13	1.74	0.69
3:C:54:THR:HG21	3:C:72:ARG:HB3	1.74	0.69
15:P:27:VAL:HG13	27:X:504:G:H4'	1.74	0.69
27:X:2371:A:H2	27:X:2403:C:H42	1.39	0.69
1:A:244:ARG:O	1:A:252:LYS:NZ	2.23	0.69
27:X:2757:G:OP2	27:X:2761:A:O2'	2.07	0.69
16:Q:43:GLN:HE21	16:Q:50:VAL:H	1.38	0.69
24:1:42:PRO:O	24:1:46:LYS:NZ	2.25	0.69
1:A:158:SER:HB2	27:X:1810:U:H5''	1.73	0.69
12:M:104:LEU:HA	12:M:106:TYR:CE2	2.27	0.69
27:X:2605:C:H2'	27:X:2606:G:H8	1.58	0.69
27:X:2796:A:H2'	27:X:2797:G:H8	1.56	0.69
1:A:157:ARG:NH1	27:X:1810:U:OP2	2.25	0.69
3:C:45:THR:OG1	3:C:86:PRO:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:176:ASN:HB3	3:C:179:ASP:HB2	1.73	0.69
8:I:65:PHE:HB2	27:X:2394:G:H4'	1.72	0.69
8:I:94:GLU:OE1	8:I:97:ARG:NH1	2.25	0.69
4:D:133:LYS:HD3	27:X:2284:U:H4'	1.74	0.69
18:S:125:PRO:O	18:S:129:ARG:NH1	2.25	0.69
3:C:144:GLY:HA3	3:C:166:TRP:CD1	2.27	0.69
27:X:1336:G:H2'	27:X:1337:G:H5'	1.74	0.69
27:X:1769:U:H2'	27:X:1775:A:H62	1.57	0.69
27:X:1975:G:H22	27:X:1979:C:H6	1.40	0.69
27:X:2378:G:H1	27:X:2396:C:H42	1.40	0.69
15:P:104:LYS:HZ2	15:P:104:LYS:HA	1.58	0.68
25:2:39:ARG:O	25:2:41:GLN:NE2	2.26	0.68
26:3:46:LYS:HD2	27:X:659:G:H1'	1.75	0.68
17:R:105:ARG:NH2	17:R:106:VAL:O	2.26	0.68
25:2:7:PRO:HB2	27:X:1322:G:H4'	1.76	0.68
27:X:1533:G:H2'	27:X:1534:A:H8	1.56	0.68
27:X:1733:U:OP2	27:X:1735:G:N2	2.25	0.68
2:B:26:VAL:HG11	2:B:198:LEU:HD21	1.76	0.68
2:B:140:SER:HB3	27:X:2554:C:O2'	1.93	0.68
27:X:2199:C:H2'	27:X:2200:G:H8	1.58	0.68
28:Y:26:G:N2	28:Y:30:C:N3	2.42	0.68
12:M:32:THR:O	12:M:51:GLU:HA	1.94	0.68
17:R:61:SER:HA	17:R:65:PRO:HB3	1.75	0.68
27:X:588:G:O2'	27:X:2002:A:OP1	2.12	0.68
27:X:2298:U:O2	27:X:2299:A:N6	2.26	0.68
2:B:34:VAL:HG12	2:B:72:VAL:HG21	1.76	0.68
27:X:661:C:H2'	27:X:662:G:H8	1.58	0.68
1:A:48:ARG:H	1:A:48:ARG:HD2	1.58	0.68
3:C:48:ARG:HB2	3:C:51:VAL:HG22	1.75	0.68
27:X:1065:A:H2'	27:X:1066:G:H8	1.58	0.68
13:N:13:ARG:NH2	27:X:1264:C:OP1	2.27	0.68
22:W:3:ILE:HD11	22:W:44:VAL:HG11	1.76	0.68
27:X:812:G:H3'	27:X:813:A:H2'	1.75	0.68
1:A:28:ARG:HD3	27:X:1583:A:N6	2.09	0.67
5:E:150:LYS:HZ3	27:X:2741:G:H21	1.41	0.67
27:X:537:C:H1'	27:X:538:A:C6	2.28	0.67
2:B:48:GLN:NE2	27:X:2614:A:O2'	2.27	0.67
6:G:132:PHE:CZ	6:G:145:HIS:HB2	2.30	0.67
8:I:53:ARG:HD2	8:I:54:SER:HB3	1.75	0.67
10:K:79:VAL:HA	10:K:83:VAL:HB	1.76	0.67
6:G:58:ILE:HG12	6:G:80:VAL:HG11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:137:ALA:HB1	3:C:142:LEU:HB2	1.76	0.67
6:G:43:VAL:HG21	6:G:158:HIS:HE1	1.59	0.67
14:O:38:LEU:HD23	14:O:47:PHE:HA	1.77	0.67
27:X:2546:G:H2'	27:X:2547:C:C6	2.30	0.67
1:A:68:LYS:HD3	1:A:68:LYS:H	1.60	0.67
4:D:16:LEU:O	4:D:20:PHE:N	2.28	0.67
3:C:45:THR:HG21	3:C:85:GLY:HA3	1.77	0.67
3:C:59:TYR:OH	3:C:67:ALA:HB3	1.95	0.67
4:D:64:LYS:O	28:Y:44:C:O2'	2.12	0.67
15:P:71:VAL:HG12	15:P:129:ILE:HD12	1.76	0.67
27:X:1561:A:O2'	27:X:1562:G:O4'	2.13	0.67
1:A:158:SER:O	1:A:196:VAL:HG21	1.95	0.67
24:1:27:ASN:ND2	24:1:36:GLU:OE2	2.28	0.66
28:Y:64:C:H2'	28:Y:65:A:H8	1.58	0.66
4:D:60:ILE:HG13	4:D:61:THR:HG23	1.78	0.66
20:U:31:GLY:H	20:U:32:ARG:NH1	1.93	0.66
27:X:712:A:H2'	27:X:713:G:O4'	1.96	0.66
27:X:1882:G:H21	27:X:1885:C:N4	1.94	0.66
19:T:23:VAL:HG13	19:T:38:VAL:HG22	1.78	0.66
13:N:37:GLN:HG3	27:X:1265:G:H1	1.58	0.66
16:Q:2:SER:N	16:Q:5:ASP:OD2	2.28	0.66
16:Q:60:GLY:HA3	16:Q:72:ARG:HA	1.77	0.66
27:X:820:U:H2'	27:X:821:A:H8	1.59	0.66
2:B:108:SER:HB3	2:B:163:GLU:H	1.61	0.66
6:G:34:PRO:HB3	6:G:69:ASP:CB	2.26	0.66
18:S:19:ILE:HD11	18:S:36:ARG:HD3	1.78	0.66
27:X:1350:G:H2'	27:X:1351:G:H8	1.60	0.66
23:Z:31:THR:OG1	27:X:2861:A:O2'	2.11	0.66
27:X:1059:A:O2'	27:X:1060:C:OP1	2.12	0.66
27:X:1573:G:O6	27:X:1574:A:N6	2.29	0.66
24:1:41:ASP:HB2	24:1:46:LYS:HD3	1.77	0.65
25:2:34:ARG:NH2	27:X:477:A:OP1	2.29	0.65
1:A:229:VAL:HG21	27:X:797:A:C5	2.31	0.65
2:B:5:LEU:HD23	2:B:195:LEU:HD11	1.77	0.65
13:N:95:LEU:HD12	13:N:98:ILE:HD12	1.77	0.65
15:P:57:LEU:HD13	15:P:69:ALA:HA	1.78	0.65
27:X:832:A:OP2	27:X:1201:G:N2	2.25	0.65
27:X:1678:G:H1	27:X:1982:C:H42	1.43	0.65
8:I:53:ARG:HH21	8:I:54:SER:HB3	1.60	0.65
17:R:59:LYS:HD2	17:R:62:MET:HB2	1.78	0.65
3:C:119:ALA:HB3	3:C:189:ASP:HA	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:55:THR:HG23	17:R:72:ARG:HD3	1.78	0.65
27:X:318:G:N2	27:X:321:A:OP2	2.29	0.65
27:X:800:U:H5''	27:X:801:A:H5'	1.78	0.65
20:U:38:THR:HB	27:X:2063:A:H5'	1.77	0.65
21:V:32:ALA:HA	21:V:37:LEU:HD22	1.78	0.65
2:B:152:LYS:HB2	6:G:106:TYR:HB2	1.79	0.65
4:D:117:ILE:HG13	4:D:176:PRO:HG2	1.77	0.65
4:D:132:ILE:HG13	4:D:154:ILE:HD13	1.79	0.65
7:H:113:PRO:HD3	12:M:73:PHE:HB2	1.77	0.65
27:X:664:C:H5'	27:X:666:U:H5''	1.79	0.65
1:A:172:TYR:HA	1:A:186:HIS:HA	1.78	0.65
1:A:88:ARG:NH2	27:X:1809:G:OP1	2.30	0.65
27:X:1919:A:H62	27:X:1946:U:H3	1.45	0.65
1:A:251:GLY:HA3	1:A:255:LYS:NZ	2.12	0.65
13:N:66:ASN:O	13:N:70:ARG:NH1	2.29	0.65
24:1:41:ASP:HB2	24:1:46:LYS:HB3	1.78	0.65
27:X:2237:C:O2'	27:X:2406:C:OP2	2.15	0.65
2:B:9:ILE:HD11	2:B:27:LEU:HB2	1.79	0.64
27:X:2492:G:H2'	27:X:2493:U:C6	2.32	0.64
2:B:128:SER:HB3	27:X:1976:U:H4'	1.77	0.64
27:X:1033:G:H22	27:X:1153:A:H2	1.45	0.64
27:X:1919:A:H2	27:X:1926:U:N3	1.95	0.64
10:K:6:ALA:HB1	27:X:2848:A:H2	1.62	0.64
11:L:88:VAL:HG11	27:X:2357:A:H1'	1.79	0.64
12:M:51:GLU:H	12:M:70:LYS:NZ	1.94	0.64
27:X:573:C:O2'	27:X:1266:G:O6	2.14	0.64
27:X:1283:C:H5''	27:X:1284:G:H5'	1.79	0.64
8:I:90:ARG:HA	8:I:121:HIS:HB2	1.80	0.64
15:P:36:ARG:HG2	27:X:1279:G:N7	2.12	0.64
27:X:145:C:O2	27:X:152:G:N2	2.28	0.64
27:X:1079:G:N2	27:X:1106:A:O2'	2.29	0.64
1:A:159:ALA:HA	1:A:198:ASN:CG	2.23	0.64
1:A:258:LYS:HD3	1:A:264:LYS:HZ1	1.60	0.64
10:K:10:LEU:HD11	10:K:17:ARG:HD3	1.80	0.64
27:X:218:A:H5'	27:X:220:U:H1'	1.79	0.64
27:X:1329:U:H2'	27:X:1330:G:H8	1.61	0.64
27:X:1843:U:H3	27:X:1874:G:H1	1.45	0.64
17:R:23:ILE:HG22	17:R:33:THR:HB	1.80	0.64
19:T:70:ILE:HB	19:T:78:PHE:HB2	1.80	0.64
27:X:1465:G:N2	27:X:1466:C:N3	2.45	0.64
4:D:51:ASP:HB3	4:D:55:LYS:HE2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:492:G:H1'	27:X:516:G:N2	2.13	0.63
27:X:590:C:H2'	27:X:591:G:H8	1.63	0.63
6:G:70:PHE:HB3	13:N:64:ARG:HG2	1.79	0.63
23:Z:41:LEU:HD12	23:Z:42:SER:H	1.63	0.63
27:X:82:G:H1	27:X:100:G:HO2'	1.46	0.63
27:X:748:A:H5'	27:X:749:C:OP2	1.99	0.63
27:X:2605:C:H2'	27:X:2606:G:C8	2.33	0.63
28:Y:40:C:O2	28:Y:50:U:O2'	2.16	0.63
18:S:154:LEU:HD11	18:S:160:LEU:HG	1.79	0.63
27:X:759:C:H5''	27:X:761:G:H1'	1.79	0.63
27:X:1089:C:O2'	27:X:1099:A:OP1	2.17	0.63
27:X:2672:U:H2'	27:X:2673:G:H8	1.62	0.63
28:Y:27:A:O2'	28:Y:28:A:O5'	2.14	0.63
6:G:100:TYR:HB2	6:G:116:ARG:NH1	2.14	0.63
13:N:31:GLN:NE2	27:X:589:C:H4'	2.12	0.63
3:C:117:LEU:HD22	3:C:187:VAL:HG13	1.81	0.63
18:S:71:MET:SD	18:S:71:MET:N	2.66	0.63
27:X:617:U:H5	27:X:632:A:C2	2.16	0.63
27:X:661:C:H2'	27:X:662:G:C8	2.33	0.63
27:X:1468:A:P	27:X:1468:A:H8	2.21	0.63
27:X:1923:U:OP1	27:X:2582:G:N2	2.31	0.63
18:S:51:LEU:HB2	18:S:64:ALA:O	1.99	0.63
27:X:2336:G:N2	27:X:2339:A:OP2	2.31	0.63
15:P:118:ASN:HD21	15:P:120:ILE:HB	1.64	0.63
27:X:1058:G:H2'	27:X:1121:G:H22	1.64	0.63
6:G:106:TYR:CD2	6:G:108:GLY:HA2	2.33	0.63
27:X:313:U:H2'	27:X:314:G:H8	1.64	0.63
2:B:110:GLY:O	10:K:3:HIS:HD2	1.81	0.62
15:P:11:LYS:HG2	15:P:14:ARG:HH12	1.62	0.62
16:Q:63:LYS:HE2	16:Q:69:ILE:HA	1.79	0.62
23:Z:31:THR:HG1	27:X:2861:A:HO2'	1.47	0.62
26:3:32:GLN:HB3	27:X:2400:G:N7	2.14	0.62
27:X:1017:C:H2'	27:X:1018:C:H6	1.64	0.62
26:3:25:PHE:CD2	26:3:46:LYS:HA	2.34	0.62
10:K:36:THR:OG1	27:X:1291:G:OP1	2.13	0.62
2:B:176:ARG:NH2	12:M:16:ILE:HG23	2.14	0.62
27:X:1769:U:H2'	27:X:1775:A:N6	2.15	0.62
7:H:89:ILE:HG23	12:M:79:ARG:HD3	1.80	0.62
27:X:590:C:H2'	27:X:591:G:C8	2.34	0.62
3:C:53:LYS:H	3:C:53:LYS:HE2	1.62	0.62
3:C:106:MET:O	3:C:110:SER:OG	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:403:A:H4'	27:X:404:A:H5'	1.81	0.62
27:X:469:G:N2	27:X:480:G:H2'	2.14	0.62
27:X:619:A:N6	27:X:630:G:O2'	2.33	0.62
27:X:754:G:H2'	27:X:755:C:H6	1.63	0.62
27:X:1349:A:H2'	27:X:1350:G:C8	2.35	0.62
27:X:222:G:O2'	27:X:397:U:O2	2.16	0.62
27:X:1007:A:H2'	27:X:1008:G:H8	1.64	0.62
1:A:48:ARG:HD3	27:X:1797:C:H4'	1.81	0.62
1:A:145:LEU:HB3	1:A:155:LEU:HB2	1.80	0.62
27:X:854:G:H1	27:X:948:C:N4	1.95	0.62
27:X:2020:G:H2'	27:X:2021:G:C8	2.34	0.62
27:X:2085:G:N2	27:X:2171:U:O2'	2.32	0.62
8:I:42:GLY:HA2	8:I:45:LYS:HE3	1.82	0.62
18:S:162:ALA:HB1	18:S:166:LEU:HD13	1.82	0.62
19:T:74:LYS:C	19:T:76:ALA:H	2.07	0.62
26:3:39:ASP:OD1	27:X:2329:C:N4	2.33	0.62
27:X:1373:G:H22	27:X:2192:U:H3	1.47	0.62
1:A:164:GLN:HG3	1:A:176:ARG:HB3	1.82	0.62
2:B:117:MET:HA	2:B:121:ASN:O	2.00	0.62
3:C:112:GLN:HA	3:C:116:LYS:HE2	1.82	0.62
27:X:437:G:H2'	27:X:438:G:H8	1.63	0.62
27:X:1065:A:H2'	27:X:1066:G:C8	2.35	0.62
27:X:1235:C:H42	27:X:1240:G:H1	1.46	0.62
27:X:1937:G:O2'	27:X:1939:U:O4	2.13	0.62
1:A:43:ARG:HD3	1:A:55:GLY:HA2	1.81	0.61
7:H:47:VAL:HG11	7:H:115:ALA:HB3	1.81	0.61
15:P:97:VAL:CG1	15:P:125:SER:HB2	2.30	0.61
27:X:2447:G:O2'	27:X:2448:A:H8	1.82	0.61
2:B:9:ILE:HD13	12:M:12:LEU:HD13	1.82	0.61
6:G:132:PHE:CE2	6:G:145:HIS:HB2	2.35	0.61
24:1:30:ASN:N	24:1:30:ASN:OD1	2.32	0.61
27:X:1991:C:H2'	27:X:1992:G:H8	1.66	0.61
3:C:42:THR:HG21	27:X:38:G:H21	1.63	0.61
15:P:17:GLN:HG3	15:P:18:VAL:HG23	1.82	0.61
17:R:54:ILE:HD13	17:R:71:GLN:HA	1.81	0.61
27:X:2174:G:H2'	27:X:2175:A:H8	1.63	0.61
27:X:2796:A:H2'	27:X:2797:G:C8	2.35	0.61
8:I:18:ARG:HH12	27:X:609:U:H4'	1.65	0.61
11:L:16:LYS:HE3	11:L:28:ARG:HH12	1.66	0.61
27:X:469:G:H22	27:X:480:G:H2'	1.65	0.61
27:X:2174:G:H2'	27:X:2175:A:C8	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:SER:OG	1:A:159:ALA:N	2.26	0.61
3:C:6:VAL:HG12	3:C:7:ILE:HG12	1.83	0.61
27:X:1399:C:H2'	27:X:1400:A:H8	1.66	0.61
27:X:1448:A:H61	27:X:1574:A:H61	1.47	0.61
3:C:111:ARG:NH1	3:C:180:ILE:O	2.33	0.61
7:H:6:SER:HB2	27:X:1683:G:O3'	2.00	0.61
27:X:587:A:OP1	27:X:1268:U:O2'	2.13	0.61
27:X:953:G:O2'	27:X:1203:A:N3	2.34	0.61
27:X:2286:G:O6	27:X:2287:G:N2	2.33	0.61
8:I:53:ARG:HD2	8:I:54:SER:H	1.65	0.61
15:P:39:ARG:HH11	15:P:39:ARG:HB2	1.66	0.61
19:T:40:GLN:HE22	19:T:43:THR:HA	1.65	0.61
27:X:1222:G:O2'	27:X:1250:A:N6	2.34	0.61
3:C:53:LYS:NZ	27:X:463:C:O3'	2.33	0.61
9:J:83:ARG:HH22	27:X:971:A:H61	1.47	0.61
27:X:1030:U:H2'	27:X:1032:A:H2	1.65	0.61
2:B:146:THR:HG1	27:X:2550:C:HO2'	1.48	0.61
27:X:825:C:O2'	27:X:1239:A:O2'	2.13	0.61
27:X:2546:G:H2'	27:X:2547:C:H6	1.64	0.61
3:C:33:TRP:NE1	3:C:95:LEU:HB2	2.16	0.60
9:J:67:ILE:HG12	9:J:105:PHE:HD1	1.66	0.60
17:R:13:LYS:NZ	27:X:349:G:OP1	2.22	0.60
20:U:51:ILE:HG23	20:U:59:THR:HA	1.82	0.60
5:E:154:PRO:HA	5:E:160:LYS:O	2.00	0.60
6:G:67:ARG:HH21	6:G:72:PRO:HA	1.65	0.60
15:P:33:MET:SD	15:P:37:LYS:NZ	2.74	0.60
23:Z:55:ARG:HH21	23:Z:58:LEU:HA	1.66	0.60
27:X:163:A:H2'	27:X:164:G:C8	2.36	0.60
12:M:29:PRO:HB2	12:M:99:VAL:HG11	1.82	0.60
1:A:96:HIS:CE1	27:X:1517:C:H4'	2.36	0.60
2:B:35:GLN:HG3	2:B:66:HIS:HE1	1.66	0.60
3:C:152:THR:OG1	3:C:153:ASP:O	2.19	0.60
17:R:38:LEU:H	17:R:47:VAL:HB	1.65	0.60
25:2:33:ARG:NE	27:X:478:G:OP1	2.31	0.60
26:3:14:ILE:HD11	26:3:56:ALA:HB1	1.83	0.60
27:X:2516:U:H2'	27:X:2517:C:C6	2.36	0.60
27:X:2660:C:H42	27:X:2705:A:H2	1.48	0.60
1:A:91:ARG:HB2	1:A:107:ALA:HB3	1.82	0.60
2:B:143:GLN:O	27:X:2035:G:H4'	2.00	0.60
3:C:173:ALA:HB1	3:C:193:LEU:HD13	1.83	0.60
7:H:23:ARG:NH1	27:X:2526:U:O2	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:29:VAL:HG21	16:Q:38:ILE:HD11	1.82	0.60
27:X:1117:G:H2'	27:X:1118:G:H8	1.65	0.60
27:X:1542:G:N2	27:X:1562:G:H1	1.91	0.60
27:X:1859:A:H2'	27:X:1860:A:H8	1.67	0.60
27:X:1988:A:H5'	27:X:1989:C:OP2	2.01	0.60
3:C:33:TRP:CD1	3:C:95:LEU:HB2	2.36	0.60
18:S:28:ASN:OD1	18:S:28:ASN:N	2.29	0.60
24:1:2:ALA:N	27:X:2369:U:OP2	2.34	0.60
25:2:12:ARG:HG2	27:X:699:G:N1	2.14	0.60
27:X:582:G:O2'	27:X:583:C:H3'	2.01	0.60
26:3:25:PHE:HA	26:3:47:GLY:H	1.67	0.60
27:X:116:A:N3	27:X:155:G:H1'	2.17	0.60
27:X:2417:U:O2'	27:X:2419:C:OP1	2.19	0.60
27:X:2634:G:O2'	27:X:2635:U:OP2	2.20	0.60
14:O:22:VAL:HG13	27:X:1173:G:H4'	1.84	0.60
27:X:1643:A:H61	27:X:1656:U:H3	1.50	0.60
27:X:2234:G:H2'	27:X:2235:G:O4'	2.01	0.60
27:X:2311:U:O2'	27:X:2315:A:N7	2.34	0.60
6:G:84:ASN:O	6:G:152:ALA:HA	2.00	0.60
6:G:107:GLN:HB3	27:X:1142:G:H5'	1.83	0.60
8:I:56:LEU:HD23	8:I:59:ARG:HH21	1.65	0.60
19:T:23:VAL:HA	19:T:38:VAL:HG13	1.84	0.60
27:X:1455:C:H2'	27:X:1456:C:H6	1.67	0.60
27:X:1699:A:H61	27:X:1723:U:H3	1.48	0.60
1:A:161:THR:H	1:A:196:VAL:HG22	1.66	0.59
27:X:836:G:H2'	27:X:837:U:H6	1.67	0.59
27:X:1836:C:H42	27:X:1879:G:H1	1.48	0.59
8:I:59:ARG:HB2	27:X:2371:A:H8	1.67	0.59
9:J:44:LYS:HB2	9:J:47:GLN:HG3	1.84	0.59
15:P:59:PHE:HE1	23:Z:40:LYS:HA	1.66	0.59
20:U:39:LYS:HA	27:X:2063:A:H4'	1.84	0.59
1:A:37:LEU:HD12	27:X:1808:C:H41	1.67	0.59
1:A:108:PRO:HB3	1:A:143:HIS:CE1	2.37	0.59
27:X:627:A:H2'	27:X:628:A:C8	2.37	0.59
27:X:1371:G:O2'	27:X:1386:A:N6	2.35	0.59
27:X:2845:C:H2'	27:X:2846:G:H5'	1.85	0.59
15:P:118:ASN:ND2	27:X:1996:A:OP1	2.35	0.59
26:3:13:ARG:HE	26:3:25:PHE:N	2.00	0.59
27:X:82:G:O2'	27:X:100:G:N2	2.34	0.59
27:X:2270:U:O2'	27:X:2353:G:N3	2.35	0.59
1:A:108:PRO:HB3	1:A:143:HIS:HE1	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:4:LEU:HG	4:D:5:LYS:H	1.67	0.59
15:P:87:GLU:HA	15:P:90:LEU:HG	1.84	0.59
1:A:88:ARG:HD2	1:A:92:ILE:HD11	1.84	0.59
3:C:53:LYS:HE3	27:X:464:G:H8	1.67	0.59
6:G:93:LYS:HD2	6:G:96:ASP:HB2	1.85	0.59
7:H:99:ILE:HD12	7:H:103:GLY:HA2	1.85	0.59
21:V:15:ALA:HA	21:V:18:ILE:HD12	1.84	0.59
27:X:752:G:N2	27:X:753:U:O4	2.31	0.59
27:X:1845:A:N3	27:X:2212:U:O2'	2.30	0.59
27:X:2708:U:H2'	27:X:2709:C:C6	2.38	0.59
10:K:3:HIS:NE2	27:X:2797:G:OP2	2.35	0.59
27:X:90:G:H3'	27:X:91:A:H8	1.68	0.59
27:X:2014:A:C6	27:X:2477:C:H1'	2.38	0.59
9:J:70:PHE:CE2	27:X:884:C:H4'	2.38	0.59
13:N:66:ASN:CB	13:N:76:TYR:HB2	2.32	0.59
17:R:37:LEU:HD11	17:R:49:GLU:HG3	1.84	0.59
20:U:17:SER:HB2	20:U:44:ALA:HA	1.84	0.59
22:W:37:THR:HG22	22:W:38:PRO:HD2	1.84	0.59
27:X:670:U:H2'	27:X:671:A:C8	2.38	0.59
27:X:1383:C:H3'	27:X:1384:G:H8	1.68	0.59
27:X:2329:C:H2'	27:X:2330:G:O4'	2.03	0.59
27:X:540:G:C5	27:X:2005:U:H5''	2.37	0.58
14:O:10:LYS:NZ	14:O:13:ARG:HH12	2.01	0.58
21:V:26:MET:HA	21:V:29:ARG:HE	1.66	0.58
27:X:1554:G:H2'	27:X:1555:A:H8	1.68	0.58
1:A:37:LEU:HD22	1:A:38:PRO:HD2	1.84	0.58
1:A:231:HIS:CD2	1:A:232:PRO:HD2	2.38	0.58
6:G:116:ARG:HE	6:G:126:VAL:HG22	1.68	0.58
22:W:23:LEU:HD11	22:W:44:VAL:HG22	1.83	0.58
27:X:163:A:H2'	27:X:164:G:H8	1.67	0.58
27:X:2431:C:H2'	27:X:2432:A:C8	2.37	0.58
1:A:46:ARG:NE	27:X:1383:C:OP1	2.36	0.58
6:G:124:GLU:OE1	6:G:124:GLU:N	2.36	0.58
15:P:35:PRO:HG3	15:P:123:ARG:HD3	1.84	0.58
25:2:28:ARG:HH11	25:2:31:LEU:HG	1.68	0.58
27:X:874:A:H2'	27:X:875:G:O4'	2.03	0.58
27:X:1811:A:H4'	27:X:1812:U:O5'	2.03	0.58
27:X:2691:C:O2'	27:X:2693:U:H5'	2.04	0.58
9:J:39:GLU:HG2	28:Y:92:G:H22	1.68	0.58
10:K:24:GLN:HB3	10:K:44:LEU:HD22	1.86	0.58
15:P:89:ARG:HE	15:P:137:LYS:HE3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1223:G:H4'	27:X:1224:A:H5''	1.85	0.58
1:A:252:LYS:HD2	1:A:253:PRO:HD3	1.86	0.58
27:X:2560:G:OP2	27:X:2560:G:N2	2.34	0.58
6:G:56:THR:HG21	27:X:1016:C:O2'	2.04	0.58
17:R:22:VAL:HG11	17:R:80:LYS:HE3	1.85	0.58
17:R:84:VAL:HG21	17:R:89:GLY:HA2	1.85	0.58
18:S:41:ARG:NH1	27:X:1052:C:OP1	2.36	0.58
27:X:26:G:H1'	27:X:525:A:H61	1.68	0.58
27:X:421:G:N2	27:X:433:G:H1'	2.19	0.58
27:X:571:U:O2'	27:X:581:A:H8	1.82	0.58
27:X:840:U:H4'	27:X:841:G:C2	2.38	0.58
27:X:1437:A:H2'	27:X:1438:G:C8	2.39	0.58
2:B:116:VAL:H	2:B:136:ARG:HG3	1.68	0.58
6:G:109:GLY:H	6:G:111:LYS:HG3	1.68	0.58
10:K:5:LYS:HD2	27:X:2795:A:H4'	1.85	0.58
28:Y:96:C:H2'	28:Y:97:C:H6	1.69	0.58
14:O:78:VAL:HG22	27:X:1202:U:H5'	1.86	0.58
27:X:1329:U:H2'	27:X:1330:G:C8	2.37	0.58
27:X:2494:C:H42	27:X:2548:G:H1	1.50	0.58
27:X:784:U:H2'	27:X:785:U:C6	2.39	0.58
27:X:1698:C:O2'	27:X:1753:A:N3	2.31	0.58
27:X:2284:U:H2'	27:X:2285:U:H5''	1.85	0.58
27:X:2772:U:H1'	27:X:2781:G:N2	2.19	0.58
5:E:150:LYS:NZ	27:X:2741:G:H21	2.01	0.57
11:L:48:GLY:O	28:Y:115:G:N2	2.31	0.57
25:2:27:GLY:HA2	25:2:30:ILE:HD12	1.86	0.57
27:X:160:C:O2'	27:X:445:A:N3	2.32	0.57
27:X:2807:U:H6	27:X:2807:U:H5''	1.69	0.57
2:B:203:LYS:NZ	2:B:204:ALA:H	2.02	0.57
3:C:163:ASN:ND2	3:C:167:VAL:H	1.94	0.57
15:P:29:LYS:HA	15:P:126:HIS:CD2	2.39	0.57
4:D:60:ILE:HG22	4:D:140:GLU:HB2	1.84	0.57
27:X:2318:U:H4'	28:Y:43:G:N2	2.19	0.57
3:C:89:ARG:HD2	27:X:599:A:OP1	2.05	0.57
9:J:100:PRO:HB2	18:S:74:ARG:HG2	1.84	0.57
27:X:1103:C:H42	27:X:1110:G:H1	1.51	0.57
5:E:157:TYR:CZ	27:X:2510:A:H5''	2.39	0.57
7:H:124:MET:O	7:H:127:VAL:HG12	2.05	0.57
9:J:78:LYS:HA	9:J:88:LYS:HZ1	1.69	0.57
26:3:25:PHE:CG	26:3:46:LYS:HA	2.39	0.57
27:X:28:A:H1'	27:X:523:A:C2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1141:U:O2'	27:X:1142:G:O5'	2.15	0.57
27:X:1479:G:H2'	27:X:1480:G:C8	2.39	0.57
27:X:1727:C:H2'	27:X:1728:A:C8	2.40	0.57
1:A:99:ASP:OD1	27:X:1506:C:H2'	2.04	0.57
2:B:119:ARG:HG2	2:B:120:TRP:CD1	2.40	0.57
15:P:36:ARG:NH2	27:X:1279:G:O5'	2.38	0.57
16:Q:35:LYS:HE2	16:Q:55:THR:HG22	1.87	0.57
26:3:34:THR:OG1	26:3:35:GLY:N	2.36	0.57
27:X:474:G:N2	27:X:477:A:OP2	2.32	0.57
27:X:558:G:H4'	27:X:559:C:C4	2.39	0.57
2:B:146:THR:OG1	27:X:2550:C:O2'	2.19	0.57
6:G:31:THR:OG1	27:X:1006:C:O2	2.18	0.57
9:J:73:LYS:H	9:J:94:TRP:HD1	1.53	0.57
15:P:27:VAL:HA	15:P:128:THR:HA	1.86	0.57
27:X:90:G:H3'	27:X:91:A:C8	2.40	0.57
27:X:1399:C:H2'	27:X:1400:A:C8	2.40	0.57
27:X:2262:C:H2'	27:X:2263:C:O4'	2.05	0.57
27:X:2263:C:O2'	27:X:2267:A:N6	2.37	0.57
27:X:48:A:H4'	27:X:49:U:O5'	2.05	0.57
27:X:1468:A:H8	27:X:1468:A:O5'	1.87	0.57
27:X:2201:G:H2'	27:X:2202:G:H8	1.70	0.57
27:X:2212:U:H2'	27:X:2213:G:C8	2.40	0.57
2:B:14:ILE:HG12	12:M:20:HIS:CD2	2.39	0.57
4:D:92:ARG:NH2	28:Y:45:C:O2	2.38	0.57
6:G:67:ARG:HD3	6:G:70:PHE:HA	1.86	0.57
20:U:48:LYS:HG3	20:U:49:LYS:N	2.18	0.57
27:X:774:A:H8	27:X:774:A:O5'	1.88	0.57
27:X:1223:G:H5''	27:X:1224:A:H3'	1.85	0.57
9:J:131:LYS:HD2	18:S:76:ARG:HH21	1.70	0.57
27:X:138:G:H2'	27:X:139:A:H8	1.70	0.57
27:X:1348:C:H2'	27:X:1349:A:C8	2.40	0.57
27:X:2283:G:H22	27:X:2291:U:H3	1.53	0.57
3:C:162:ARG:HE	27:X:333:A:C5'	2.18	0.56
11:L:8:ARG:HG3	11:L:9:ARG:H	1.70	0.56
24:1:41:ASP:OD1	24:1:41:ASP:N	2.38	0.56
26:3:19:THR:OG1	27:X:661:C:OP1	2.22	0.56
27:X:500:G:C2	27:X:501:G:H1'	2.40	0.56
27:X:1539:U:H2'	27:X:1540:C:C6	2.39	0.56
27:X:2442:C:H2'	27:X:2443:C:H6	1.70	0.56
20:U:52:ARG:HB3	20:U:79:GLU:HA	1.87	0.56
27:X:555:U:OP2	27:X:556:A:O2'	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1039:A:N6	27:X:1136:G:H2'	2.20	0.56
27:X:1782:A:N6	27:X:1820:G:O2'	2.38	0.56
2:B:4:ILE:HD13	2:B:28:ALA:HB1	1.87	0.56
2:B:35:GLN:HG3	2:B:66:HIS:CE1	2.41	0.56
3:C:34:GLN:O	3:C:37:SER:OG	2.14	0.56
6:G:170:PRO:O	6:G:171:LEU:HB2	2.05	0.56
13:N:66:ASN:HB2	13:N:70:ARG:HH12	1.70	0.56
17:R:15:HIS:CE1	17:R:16:PHE:HD2	2.23	0.56
27:X:1286:U:O2	27:X:1985:G:O2'	2.23	0.56
1:A:13:ARG:CZ	1:A:27:LYS:HD3	2.35	0.56
2:B:154:LYS:HG3	2:B:155:ARG:N	2.19	0.56
4:D:13:ARG:NH1	4:D:14:PRO:HG3	2.21	0.56
4:D:66:ILE:HD12	28:Y:43:G:H5''	1.86	0.56
7:H:76:ARG:NH1	7:H:113:PRO:O	2.38	0.56
26:3:30:ARG:HB2	27:X:2372:A:OP1	2.05	0.56
27:X:135:U:H2'	27:X:136:A:C8	2.41	0.56
1:A:42:GLY:C	1:A:43:ARG:HE	2.13	0.56
9:J:21:ASP:C	9:J:99:LYS:HG2	2.31	0.56
15:P:59:PHE:CE1	23:Z:40:LYS:HA	2.40	0.56
20:U:17:SER:OG	20:U:45:ASN:N	2.39	0.56
24:1:16:ALA:HB2	24:1:50:PHE:CE1	2.40	0.56
27:X:197:G:N3	27:X:210:A:H2	2.03	0.56
27:X:2484:G:HO2'	27:X:2485:U:H6	1.52	0.56
27:X:2555:G:H5'	27:X:2558:C:H41	1.70	0.56
28:Y:58:G:H4'	28:Y:59:A:O5'	2.03	0.56
13:N:93:LYS:HB3	27:X:1007:A:O3'	2.05	0.56
14:O:15:SER:HA	14:O:95:ILE:O	2.06	0.56
27:X:2557:G:H2'	27:X:2558:C:C6	2.40	0.56
27:X:2818:G:H1	27:X:2849:C:N4	2.02	0.56
3:C:19:LEU:HA	3:C:20:PRO:C	2.30	0.56
27:X:1645:U:H2'	27:X:1646:G:C8	2.41	0.56
27:X:1725:C:H42	27:X:1741:G:H1	1.52	0.56
27:X:2297:G:O2'	27:X:2300:G:O6	2.23	0.56
1:A:60:ARG:HD3	1:A:86:PRO:HB2	1.87	0.56
1:A:252:LYS:H	1:A:252:LYS:NZ	1.96	0.56
3:C:163:ASN:HD22	3:C:165:SER:N	2.04	0.56
9:J:83:ARG:NH2	27:X:970:A:H62	2.03	0.56
17:R:17:LYS:HG3	27:X:83:A:H5''	1.87	0.56
25:2:22:MET:HA	25:2:28:ARG:HG2	1.86	0.56
27:X:89:A:O2'	27:X:91:A:N6	2.39	0.56
27:X:398:C:H42	27:X:424:G:H1	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:939:C:H3'	27:X:940:G:O4'	2.06	0.56
27:X:1272:G:H2'	27:X:1273:G:C8	2.41	0.56
27:X:1451:C:H1'	27:X:1532:A:H2	1.70	0.56
27:X:1554:G:H2'	27:X:1555:A:C8	2.41	0.56
27:X:1982:C:H5''	27:X:2703:C:O2'	2.05	0.56
9:J:17:ARG:HB2	27:X:969:U:C4	2.41	0.56
27:X:224:G:H4'	27:X:399:G:C5	2.40	0.56
27:X:796:A:H8	27:X:797:A:H4'	1.70	0.56
1:A:88:ARG:HG2	1:A:90:ALA:HB3	1.88	0.56
2:B:165:VAL:HG12	2:B:189:PRO:HG3	1.87	0.56
26:3:6:THR:N	26:3:59:LYS:O	2.39	0.56
27:X:89:A:H4'	27:X:90:G:H5'	1.88	0.56
27:X:492:G:H1'	27:X:516:G:H21	1.71	0.56
27:X:1348:C:H2'	27:X:1349:A:H8	1.71	0.56
27:X:1827:G:H1'	27:X:1914:U:C2	2.41	0.56
27:X:2772:U:H2'	27:X:2773:G:C8	2.41	0.56
1:A:246:PRO:HD2	1:A:251:GLY:HA2	1.86	0.55
3:C:71:ASP:OD1	3:C:72:ARG:N	2.35	0.55
24:1:27:ASN:HD21	24:1:33:ALA:HB1	1.70	0.55
26:3:15:LYS:O	26:3:23:MET:N	2.31	0.55
27:X:616:U:O2'	27:X:671:A:H4'	2.06	0.55
28:Y:64:C:H2'	28:Y:65:A:C8	2.41	0.55
2:B:31:CYS:HB3	2:B:49:ILE:HD12	1.88	0.55
3:C:129:LYS:C	3:C:131:LYS:H	2.14	0.55
27:X:69:G:H1'	27:X:72:A:H1'	1.88	0.55
1:A:183:ARG:NH2	27:X:1791:C:OP2	2.39	0.55
6:G:43:VAL:HG21	6:G:158:HIS:CE1	2.39	0.55
16:Q:49:ARG:NH2	27:X:1612:U:OP1	2.38	0.55
20:U:13:LEU:HD11	20:U:16:ASN:HD22	1.71	0.55
27:X:1705:U:O2	27:X:1717:A:H5'	2.07	0.55
5:E:104:GLU:HG2	5:E:114:ILE:HG22	1.87	0.55
16:Q:56:MET:HG2	27:X:1354:A:H4'	1.88	0.55
1:A:210:GLY:HA2	1:A:213:ARG:HG2	1.89	0.55
1:A:231:HIS:CD2	1:A:247:VAL:HA	2.41	0.55
3:C:34:GLN:NE2	27:X:627:A:OP1	2.36	0.55
12:M:27:PHE:HA	12:M:96:ARG:NH2	2.22	0.55
27:X:75:C:H2'	27:X:76:C:C6	2.41	0.55
27:X:649:G:H2'	27:X:650:U:H6	1.71	0.55
27:X:1762:C:H2'	27:X:1763:G:C8	2.42	0.55
27:X:2672:U:H2'	27:X:2673:G:C8	2.39	0.55
13:N:58:ARG:NH1	27:X:1166:A:OP2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:93:LYS:HE3	14:O:6:GLN:HG3	1.88	0.55
15:P:41:VAL:HG11	15:P:65:SER:HA	1.89	0.55
19:T:21:LEU:HD11	19:T:41:ARG:HD2	1.89	0.55
27:X:758:G:H2'	27:X:759:C:H5'	1.88	0.55
27:X:826:U:H2'	27:X:827:C:C6	2.41	0.55
27:X:876:A:H2	27:X:926:C:H41	1.53	0.55
27:X:938:G:O2'	27:X:939:C:H5''	2.07	0.55
19:T:40:GLN:NE2	19:T:42:GLY:O	2.40	0.55
27:X:2245:A:H4'	27:X:2246:A:N3	2.22	0.55
6:G:95:LEU:HD23	6:G:95:LEU:H	1.72	0.55
27:X:1140:A:O2'	27:X:2494:C:O2'	2.19	0.55
28:Y:22:U:H2'	28:Y:23:G:C8	2.42	0.55
3:C:59:TYR:CD1	3:C:64:THR:HG21	2.42	0.55
4:D:65:PRO:HA	4:D:89:VAL:HG13	1.89	0.55
17:R:105:ARG:HH12	17:R:113:THR:H	1.55	0.55
27:X:718:A:H2'	27:X:719:A:H8	1.71	0.55
27:X:2081:U:O2	27:X:2174:G:N2	2.36	0.55
27:X:2241:U:H2'	27:X:2242:C:C6	2.42	0.55
2:B:141:ILE:HD11	27:X:2034:A:O4'	2.07	0.55
6:G:126:VAL:HG12	6:G:127:ILE:HD12	1.88	0.55
15:P:11:LYS:NZ	27:X:1247:U:OP2	2.23	0.55
15:P:27:VAL:HB	15:P:128:THR:HG22	1.89	0.55
3:C:133:PHE:CE1	3:C:161:ALA:HB2	2.42	0.54
8:I:26:THR:OG1	27:X:676:G:OP1	2.16	0.54
10:K:39:THR:HG21	27:X:1668:G:H5'	1.88	0.54
12:M:109:GLU:N	12:M:109:GLU:OE2	2.40	0.54
15:P:35:PRO:HG3	15:P:123:ARG:HH11	1.72	0.54
18:S:3:LEU:HD13	18:S:33:ALA:H	1.70	0.54
27:X:1296:G:N2	27:X:1299:A:H5'	2.23	0.54
27:X:1479:G:H2'	27:X:1480:G:H8	1.72	0.54
27:X:1654:A:H4'	27:X:2690:A:O2'	2.07	0.54
27:X:1714:A:OP2	27:X:1715:A:O2'	2.25	0.54
27:X:2191:A:OP1	27:X:2193:C:N4	2.39	0.54
27:X:2335:U:H2'	27:X:2336:G:C8	2.42	0.54
2:B:162:MET:SD	27:X:2796:A:H4'	2.47	0.54
3:C:128:ALA:C	3:C:130:THR:H	2.15	0.54
6:G:109:GLY:HA2	6:G:111:LYS:HE3	1.89	0.54
24:1:42:PRO:HG3	24:1:50:PHE:HE1	1.73	0.54
27:X:580:A:H4'	27:X:581:A:OP1	2.07	0.54
27:X:2345:A:H2'	27:X:2346:G:O4'	2.08	0.54
6:G:109:GLY:HA2	6:G:111:LYS:CE	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:14:SER:HB3	27:X:2693:U:OP1	2.07	0.54
21:V:26:MET:HA	21:V:29:ARG:NE	2.23	0.54
27:X:138:G:H2'	27:X:139:A:C8	2.42	0.54
27:X:781:G:N2	27:X:1392:U:O2'	2.39	0.54
27:X:833:A:H1'	27:X:954:U:H1'	1.90	0.54
27:X:1174:G:H2'	27:X:1175:A:H8	1.73	0.54
2:B:143:GLN:NE2	2:B:143:GLN:H	2.05	0.54
13:N:10:ARG:HG3	27:X:1264:C:OP1	2.06	0.54
23:Z:16:ARG:HD3	23:Z:20:ARG:NH1	2.22	0.54
27:X:652:C:O2'	27:X:2329:C:OP1	2.17	0.54
27:X:718:A:H2'	27:X:719:A:C8	2.42	0.54
27:X:2281:C:H42	27:X:2293:G:H1	1.55	0.54
3:C:46:ARG:HD2	3:C:51:VAL:HB	1.90	0.54
7:H:27:SER:HA	7:H:50:ILE:HD12	1.89	0.54
9:J:17:ARG:NH1	27:X:969:U:O4'	2.41	0.54
16:Q:28:TRP:CE3	16:Q:75:ARG:HD2	2.42	0.54
27:X:1086:C:H3'	27:X:1087:C:H5''	1.89	0.54
27:X:1793:A:H2'	27:X:1794:A:C8	2.43	0.54
27:X:1974:U:H2'	27:X:1975:G:H5''	1.89	0.54
27:X:2053:G:H2'	27:X:2054:A:C8	2.43	0.54
27:X:2663:U:H3	27:X:2705:A:H62	1.55	0.54
3:C:6:VAL:H	3:C:119:ALA:HA	1.72	0.54
4:D:134:GLU:HG2	4:D:136:LEU:H	1.73	0.54
17:R:51:VAL:HG12	17:R:74:LEU:HD23	1.89	0.54
26:3:13:ARG:NH2	26:3:25:PHE:HB2	2.23	0.54
27:X:26:G:C6	27:X:27:G:N1	2.76	0.54
27:X:1859:A:H2'	27:X:1860:A:C8	2.42	0.54
27:X:2781:G:H2'	27:X:2782:G:H5''	1.90	0.54
2:B:136:ARG:HB3	27:X:1673:C:C5'	2.26	0.54
6:G:120:SER:HA	6:G:123:PRO:HG3	1.90	0.54
11:L:104:ALA:O	11:L:108:ARG:HB2	2.07	0.54
16:Q:28:TRP:CZ3	16:Q:77:LYS:HB2	2.43	0.54
20:U:78:ILE:HG12	20:U:79:GLU:H	1.71	0.54
27:X:646:C:O2'	27:X:650:U:OP1	2.26	0.54
28:Y:5:C:H2'	28:Y:6:C:O4'	2.07	0.54
4:D:78:LYS:HG2	4:D:80:ARG:NH1	2.22	0.54
27:X:754:G:H2'	27:X:755:C:C6	2.41	0.54
27:X:1973:C:H2'	27:X:1974:U:C6	2.43	0.54
3:C:128:ALA:HB1	3:C:160:ALA:HA	1.90	0.54
6:G:71:THR:O	6:G:71:THR:OG1	2.23	0.54
9:J:12:LYS:HD3	27:X:923:A:N7	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:68:LYS:HA	14:O:87:ARG:HG2	1.89	0.54
27:X:2199:C:O2'	27:X:2200:G:H5'	2.08	0.54
3:C:148:VAL:HB	3:C:167:VAL:HG12	1.90	0.54
4:D:51:ASP:O	4:D:55:LYS:HG2	2.08	0.54
10:K:10:LEU:HG	10:K:17:ARG:HB3	1.90	0.54
13:N:39:LEU:HA	13:N:42:ALA:HB3	1.90	0.54
16:Q:15:LYS:NZ	16:Q:19:ALA:HB2	2.23	0.54
18:S:3:LEU:HB2	18:S:33:ALA:O	2.07	0.54
27:X:1204:G:H2'	27:X:1205:G:H8	1.72	0.54
27:X:1816:G:H2'	27:X:1817:U:H6	1.73	0.54
3:C:163:ASN:HD21	3:C:167:VAL:N	1.95	0.53
7:H:34:LEU:HD13	7:H:50:ILE:HD13	1.90	0.53
7:H:42:LYS:HD2	27:X:2653:A:H4'	1.90	0.53
7:H:131:PRO:HB3	12:M:73:PHE:CE2	2.43	0.53
10:K:81:ASP:O	10:K:85:PRO:HG2	2.08	0.53
13:N:49:ASP:HA	13:N:52:ASN:HB2	1.90	0.53
19:T:21:LEU:HD21	19:T:41:ARG:NH1	2.23	0.53
27:X:788:G:H4'	27:X:789:G:O5'	2.08	0.53
27:X:2235:G:N2	27:X:2254:C:C4	2.76	0.53
17:R:95:ARG:HH21	27:X:308:C:H4'	1.72	0.53
2:B:78:LEU:O	2:B:79:ARG:NE	2.36	0.53
3:C:10:ASN:HD21	3:C:13:ARG:NH1	2.06	0.53
9:J:83:ARG:HH12	27:X:971:A:H61	1.56	0.53
18:S:122:ILE:HG22	18:S:160:LEU:HA	1.90	0.53
9:J:76:THR:HA	9:J:89:GLY:O	2.07	0.53
15:P:40:LEU:HD13	23:Z:25:LEU:HD13	1.91	0.53
19:T:64:ASP:OD1	19:T:64:ASP:N	2.41	0.53
21:V:26:MET:HB2	21:V:29:ARG:HH21	1.74	0.53
27:X:684:C:H2'	27:X:685:U:C6	2.42	0.53
27:X:859:U:O2'	27:X:860:U:O5'	2.27	0.53
27:X:2200:G:H2'	27:X:2201:G:C8	2.44	0.53
1:A:26:LYS:HE3	1:A:28:ARG:HH21	1.73	0.53
6:G:102:ARG:HH21	27:X:2620:G:P	2.31	0.53
7:H:123:PHE:HB3	7:H:126:ILE:CG1	2.36	0.53
17:R:22:VAL:HG11	17:R:80:LYS:HB2	1.91	0.53
27:X:2040:A:H2'	27:X:2041:A:C8	2.43	0.53
27:X:2598:C:O2'	27:X:2599:U:H5'	2.08	0.53
4:D:39:GLY:O	4:D:150:ARG:NH2	2.38	0.53
6:G:61:ARG:HA	6:G:61:ARG:HE	1.74	0.53
6:G:162:LYS:HE3	27:X:5:A:H1'	1.90	0.53
10:K:43:GLU:O	10:K:46:PRO:HD2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:978:U:H2'	27:X:979:A:C8	2.44	0.53
27:X:998:C:O2'	27:X:1011:A:N3	2.35	0.53
27:X:1349:A:H2'	27:X:1350:G:H8	1.72	0.53
27:X:2054:A:H2'	27:X:2055:G:H8	1.74	0.53
27:X:330:C:H2'	27:X:331:U:O4'	2.08	0.53
27:X:2351:G:H1	27:X:2360:C:H42	1.57	0.53
27:X:2604:G:H2'	27:X:2605:C:C6	2.43	0.53
4:D:74:ILE:HG23	4:D:79:LEU:HB2	1.91	0.53
27:X:578:U:O2'	27:X:994:A:N1	2.38	0.53
27:X:1422:C:H2'	27:X:1423:A:C8	2.44	0.53
27:X:2041:A:H8	27:X:2041:A:O5'	1.92	0.53
5:E:139:GLN:NE2	27:X:2726:U:O2'	2.40	0.53
13:N:93:LYS:HE2	14:O:10:LYS:HD3	1.90	0.53
27:X:1140:A:HO2'	27:X:2494:C:HO2'	1.55	0.53
27:X:2581:A:H2'	27:X:2582:G:H4'	1.91	0.53
8:I:28:LYS:NZ	27:X:596:C:O2'	2.39	0.53
18:S:6:LYS:HD2	18:S:32:PHE:HA	1.91	0.53
27:X:305:A:H5'	27:X:306:G:OP2	2.09	0.53
27:X:1454:U:H2'	27:X:1455:C:C6	2.44	0.53
27:X:2860:C:H2'	27:X:2861:A:O4'	2.08	0.53
1:A:108:PRO:HG2	1:A:111:LEU:HD12	1.91	0.52
27:X:1149:G:O2'	27:X:1154:A:N1	2.41	0.52
27:X:1872:A:H2'	27:X:1873:A:C8	2.44	0.52
3:C:2:ALA:HA	3:C:13:ARG:HD2	1.91	0.52
11:L:33:ARG:HH21	11:L:103:LEU:HD12	1.72	0.52
27:X:116:A:OP2	27:X:117:A:H2'	2.10	0.52
27:X:1840:A:H2'	27:X:1841:G:O4'	2.09	0.52
27:X:2198:U:C2	27:X:2199:C:H1'	2.44	0.52
4:D:79:LEU:HD11	27:X:2289:A:C2	2.44	0.52
11:L:15:ARG:HA	11:L:15:ARG:HH11	1.74	0.52
23:Z:4:HIS:HB3	23:Z:5:PRO:HD3	1.91	0.52
27:X:1030:U:H3	27:X:1153:A:N6	2.04	0.52
27:X:2222:U:H2'	27:X:2223:U:C6	2.44	0.52
27:X:2873:G:H2'	27:X:2874:A:C8	2.44	0.52
2:B:121:ASN:O	2:B:122:PHE:HB2	2.09	0.52
5:E:94:PHE:HB3	5:E:107:ILE:HG22	1.91	0.52
9:J:78:LYS:HA	9:J:88:LYS:NZ	2.25	0.52
12:M:27:PHE:HA	12:M:96:ARG:HH22	1.74	0.52
22:W:47:VAL:HG23	22:W:51:LEU:HD11	1.91	0.52
27:X:346:C:H6	27:X:347:C:H5	1.56	0.52
27:X:1212:U:H2'	27:X:1213:U:C6	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1675:C:H2'	27:X:1676:U:C6	2.43	0.52
27:X:2056:C:HO2'	27:X:2577:A:HO2'	1.55	0.52
2:B:115:GLY:HA2	2:B:136:ARG:HD2	1.92	0.52
3:C:45:THR:HG22	3:C:82:VAL:HG21	1.91	0.52
9:J:72:ASP:OD2	9:J:72:ASP:N	2.42	0.52
9:J:78:LYS:NZ	27:X:2438:A:N3	2.57	0.52
11:L:65:THR:OG1	28:Y:52:G:OP1	2.28	0.52
18:S:10:PRO:HB2	18:S:13:LYS:HD2	1.92	0.52
27:X:1835:C:H2'	27:X:1836:C:C6	2.45	0.52
27:X:1943:A:H5'	27:X:1944:C:OP2	2.09	0.52
27:X:2557:G:H2'	27:X:2558:C:H6	1.73	0.52
3:C:109:ALA:HA	3:C:112:GLN:HG2	1.91	0.52
6:G:160:ALA:HB3	6:G:161:GLN:HE21	1.75	0.52
27:X:242:A:N6	27:X:440:U:O2'	2.42	0.52
27:X:717:G:H1'	27:X:739:G:N2	2.25	0.52
27:X:1429:A:H1'	27:X:1603:A:C6	2.45	0.52
27:X:1481:U:O2'	27:X:1562:G:O2'	2.17	0.52
25:2:19:ARG:HG3	25:2:23:LYS:HE3	1.92	0.52
27:X:537:C:C5	27:X:2759:U:H2'	2.44	0.52
27:X:1211:G:N2	27:X:1262:U:O2	2.33	0.52
27:X:1342:U:H5''	27:X:1343:C:H5	1.74	0.52
3:C:2:ALA:N	3:C:12:GLY:O	2.42	0.52
3:C:54:THR:HG22	3:C:55:GLY:O	2.10	0.52
8:I:35:LYS:NZ	27:X:575:U:H5''	2.25	0.52
10:K:12:ARG:NH2	10:K:20:LEU:HD13	2.24	0.52
17:R:84:VAL:CG1	17:R:90:LYS:H	2.23	0.52
27:X:692:C:H2'	27:X:693:A:C8	2.45	0.52
27:X:1816:G:H2'	27:X:1817:U:C6	2.45	0.52
1:A:13:ARG:NE	1:A:27:LYS:HD3	2.24	0.52
1:A:66:ASP:OD2	1:A:103:ARG:NH1	2.43	0.52
8:I:53:ARG:HD2	8:I:54:SER:N	2.25	0.52
9:J:99:LYS:HG3	9:J:100:PRO:HD2	1.92	0.52
25:2:8:ASN:HB3	25:2:11:LYS:HB3	1.91	0.52
27:X:2543:A:H5'	27:X:2627:G:H4'	1.92	0.52
3:C:56:ARG:NE	27:X:814:G:OP2	2.43	0.52
3:C:163:ASN:HA	27:X:334:G:O2'	2.10	0.52
4:D:111:ILE:HB	4:D:114:PHE:HB2	1.92	0.52
14:O:22:VAL:HA	14:O:91:THR:HG23	1.92	0.52
18:S:140:LYS:HE3	18:S:147:ILE:HD11	1.91	0.52
27:X:125:A:H5''	27:X:126:C:O4'	2.10	0.52
27:X:624:A:O5'	27:X:626:A:N6	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1674:C:H2'	27:X:1675:C:C6	2.45	0.52
27:X:2241:U:H2'	27:X:2242:C:H6	1.75	0.52
6:G:103:TYR:HB3	6:G:107:GLN:HE21	1.75	0.51
8:I:30:ALA:N	27:X:824:U:H2'	2.25	0.51
24:1:14:SER:OG	24:1:52:GLU:HG2	2.10	0.51
27:X:2640:G:H2'	27:X:2641:A:C8	2.44	0.51
7:H:100:ASN:HD21	7:H:104:GLU:HG3	1.74	0.51
9:J:24:GLY:HA3	27:X:920:G:P	2.50	0.51
13:N:24:PHE:O	13:N:29:SER:HB3	2.11	0.51
15:P:66:GLU:HB3	15:P:67:PRO:HD3	1.92	0.51
19:T:60:PHE:CZ	27:X:2344:G:H4'	2.45	0.51
24:1:38:LYS:HD2	27:X:2265:A:C6	2.44	0.51
27:X:227:G:C6	27:X:228:A:C6	2.98	0.51
27:X:455:A:H2	27:X:1258:G:N3	2.09	0.51
27:X:518:A:H4'	27:X:519:C:OP2	2.10	0.51
27:X:746:G:N7	27:X:774:A:C6	2.78	0.51
27:X:1751:A:H2'	27:X:1752:U:C6	2.46	0.51
27:X:1865:C:H2'	27:X:1866:G:H8	1.75	0.51
27:X:1991:C:H2'	27:X:1992:G:C8	2.45	0.51
27:X:2167:A:H2'	27:X:2168:A:C8	2.45	0.51
12:M:100:ARG:NH1	27:X:2824:C:OP2	2.44	0.51
22:W:3:ILE:HG21	22:W:23:LEU:HD13	1.92	0.51
27:X:165:G:H1	27:X:185:C:H42	1.57	0.51
27:X:650:U:H2'	27:X:651:C:C6	2.45	0.51
27:X:1301:U:O2'	27:X:1664:G:N2	2.43	0.51
27:X:2039:G:C2	27:X:2040:A:C8	2.98	0.51
27:X:2484:G:O2'	27:X:2485:U:H6	1.93	0.51
27:X:2621:G:H1	27:X:2752:C:H42	1.58	0.51
1:A:61:LEU:HG	27:X:1584:G:H5''	1.93	0.51
1:A:243:GLY:C	1:A:244:ARG:HE	2.19	0.51
6:G:139:ARG:HG2	6:G:142:ARG:HH12	1.75	0.51
15:P:14:ARG:HA	15:P:17:GLN:HG2	1.92	0.51
27:X:542:A:OP1	27:X:570:G:N2	2.38	0.51
3:C:176:ASN:ND2	3:C:178:TYR:HB3	2.26	0.51
7:H:17:ARG:H	7:H:58:ALA:HA	1.76	0.51
9:J:137:VAL:HG21	18:S:71:MET:HG3	1.93	0.51
16:Q:62:ARG:O	16:Q:70:GLY:HA2	2.11	0.51
27:X:930:A:C2	28:Y:82:U:H4'	2.46	0.51
27:X:2284:U:H5''	27:X:2286:G:H22	1.75	0.51
2:B:54:LYS:HD3	2:B:59:VAL:HG22	1.92	0.51
11:L:79:ALA:HB1	11:L:84:ILE:HB	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:58:ARG:O	13:N:62:ILE:HG13	2.10	0.51
17:R:97:GLN:HB2	17:R:100:ASP:O	2.10	0.51
27:X:828:C:H42	27:X:1206:G:H1	1.57	0.51
27:X:1656:U:C2'	27:X:1657:A:H5''	2.41	0.51
27:X:1777:A:H1'	27:X:1921:A:N6	2.25	0.51
27:X:1831:G:H2'	27:X:1832:G:H8	1.76	0.51
27:X:2516:U:H2'	27:X:2517:C:H6	1.74	0.51
1:A:133:LEU:HB2	1:A:187:SER:HA	1.93	0.51
6:G:132:PHE:HZ	6:G:142:ARG:HA	1.75	0.51
18:S:20:ALA:O	18:S:80:HIS:ND1	2.43	0.51
24:1:40:TYR:HB2	24:1:50:PHE:HB2	1.92	0.51
27:X:77:C:H42	27:X:106:G:H1	1.59	0.51
27:X:746:G:N7	27:X:774:A:C5	2.79	0.51
1:A:250:TRP:HA	1:A:250:TRP:CE3	2.46	0.51
3:C:163:ASN:HD22	3:C:165:SER:H	1.58	0.51
8:I:101:ARG:HG3	27:X:637:G:N1	2.26	0.51
11:L:16:LYS:HE2	28:Y:10:U:H5''	1.92	0.51
15:P:108:PRO:HD3	15:P:119:ILE:HG21	1.92	0.51
20:U:47:HIS:HE1	27:X:409:G:H4'	1.74	0.51
27:X:451:A:H2'	27:X:452:G:C8	2.46	0.51
27:X:768:U:H2'	27:X:769:C:O4'	2.11	0.51
27:X:1678:G:H1	27:X:1982:C:N4	2.09	0.51
4:D:56:GLU:HA	4:D:59:LEU:HD12	1.93	0.51
27:X:218:A:H61	27:X:232:A:H5''	1.76	0.51
27:X:1313:U:H4'	27:X:1314:A:H5'	1.93	0.51
27:X:1692:C:H5	27:X:1693:A:C5	2.28	0.51
2:B:136:ARG:HH12	27:X:2033:C:H5''	1.75	0.51
5:E:57:ASP:HB3	5:E:62:ARG:HE	1.76	0.51
10:K:82:GLU:O	10:K:85:PRO:HD2	2.11	0.51
13:N:3:ARG:HB2	27:X:1261:G:C5	2.46	0.51
18:S:104:SER:HA	18:S:139:THR:HA	1.92	0.51
18:S:168:VAL:HG12	18:S:169:VAL:HG12	1.93	0.51
20:U:20:ARG:O	20:U:43:ARG:NH2	2.44	0.51
27:X:2372:A:H62	27:X:2401:A:N6	2.09	0.51
27:X:2751:C:H2'	27:X:2752:C:C6	2.46	0.51
28:Y:17:A:H1'	28:Y:112:A:N7	2.26	0.51
2:B:136:ARG:HG2	2:B:137:ARG:N	2.25	0.50
22:W:3:ILE:HG12	22:W:44:VAL:HG21	1.93	0.50
27:X:87:G:H2'	27:X:88:G:H5''	1.93	0.50
27:X:876:A:H2'	27:X:877:G:C8	2.45	0.50
9:J:75:VAL:O	9:J:92:GLU:HB3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:63:ARG:HA	10:K:80:MET:HE3	1.92	0.50
13:N:22:LYS:C	13:N:24:PHE:H	2.18	0.50
15:P:29:LYS:HA	15:P:126:HIS:HD2	1.75	0.50
25:2:12:ARG:HG2	27:X:699:G:H22	1.75	0.50
27:X:537:C:O2'	27:X:538:A:O5'	2.29	0.50
27:X:674:U:H2'	27:X:675:C:O4'	2.11	0.50
27:X:1672:A:C6	27:X:1673:C:C2	3.00	0.50
1:A:246:PRO:HD3	1:A:252:LYS:HE3	1.94	0.50
2:B:116:VAL:HG22	2:B:136:ARG:CG	2.31	0.50
2:B:189:PRO:HA	27:X:2659:C:C5'	2.38	0.50
2:B:193:GLY:O	12:M:2:GLN:N	2.44	0.50
27:X:1501:C:H2'	27:X:1502:G:O4'	2.11	0.50
27:X:1532:A:O2'	27:X:1572:C:O2'	2.25	0.50
27:X:1923:U:P	27:X:2582:G:H21	2.33	0.50
27:X:2500:C:H42	27:X:2523:G:H1	1.58	0.50
28:Y:16:U:O2'	28:Y:110:U:O2	2.30	0.50
2:B:203:LYS:HE3	27:X:2713:A:H61	1.77	0.50
8:I:62:LYS:NZ	26:3:13:ARG:HH11	2.09	0.50
11:L:8:ARG:CG	11:L:9:ARG:H	2.24	0.50
16:Q:54:SER:HB2	27:X:1354:A:H1'	1.92	0.50
16:Q:73:ASN:N	16:Q:73:ASN:OD1	2.44	0.50
27:X:1422:C:H2'	27:X:1423:A:H8	1.76	0.50
27:X:2655:C:O2	27:X:2712:G:N2	2.41	0.50
27:X:2761:A:H5''	27:X:2762:G:H5'	1.92	0.50
7:H:28:GLY:HA3	7:H:35:THR:OG1	2.10	0.50
9:J:6:LYS:HG3	9:J:45:SER:HB2	1.93	0.50
14:O:36:LYS:HE3	14:O:56:VAL:HG22	1.93	0.50
14:O:36:LYS:NZ	14:O:54:TYR:HB3	2.27	0.50
18:S:117:VAL:HG22	18:S:168:VAL:HA	1.93	0.50
25:2:4:THR:O	27:X:700:C:H5'	2.12	0.50
27:X:591:G:H1	27:X:1271:C:H42	1.57	0.50
27:X:1949:A:O2'	27:X:2572:U:H5'	2.11	0.50
27:X:2309:G:H2'	27:X:2310:G:O4'	2.11	0.50
1:A:171:ASP:O	1:A:186:HIS:HB2	2.12	0.50
2:B:133:LYS:C	2:B:134:TRP:CD1	2.90	0.50
3:C:111:ARG:NH1	3:C:183:HIS:O	2.45	0.50
4:D:53:ALA:HB3	4:D:87:ILE:HD12	1.93	0.50
9:J:26:ASP:OD1	9:J:27:TYR:N	2.42	0.50
12:M:9:ARG:HA	12:M:12:LEU:HB2	1.94	0.50
27:X:114:C:O2'	27:X:124:A:N3	2.38	0.50
27:X:2528:G:H2'	27:X:2529:G:H8	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2645:C:H3'	27:X:2646:C:H6	1.76	0.50
28:Y:17:A:H1'	28:Y:112:A:C5	2.47	0.50
7:H:64:VAL:HG22	7:H:106:ARG:NH2	2.27	0.50
8:I:41:SER:O	8:I:41:SER:OG	2.25	0.50
11:L:8:ARG:HE	11:L:9:ARG:HG3	1.77	0.50
14:O:17:GLY:HA2	14:O:94:LYS:HA	1.92	0.50
24:1:21:TYR:HB3	24:1:50:PHE:HZ	1.75	0.50
27:X:393:U:H2'	27:X:394:U:C6	2.46	0.50
27:X:1141:U:HO2'	27:X:1142:G:P	2.34	0.50
27:X:1806:G:H5''	27:X:1807:A:H2'	1.94	0.50
27:X:1846:A:H62	27:X:1871:G:H8	1.60	0.50
27:X:2328:G:O6	27:X:2361:G:N2	2.37	0.50
2:B:122:PHE:CE1	2:B:138:PRO:HB3	2.47	0.50
4:D:74:ILE:HA	4:D:79:LEU:HB2	1.93	0.50
5:E:9:ILE:HA	5:E:69:ARG:HH11	1.77	0.50
5:E:76:VAL:HA	5:E:79:VAL:HG22	1.93	0.50
17:R:42:ARG:NH2	27:X:86:U:OP2	2.45	0.50
27:X:577:U:O2'	27:X:579:G:N7	2.40	0.50
27:X:1050:G:N2	27:X:1051:U:O4	2.44	0.50
27:X:1103:C:H2'	27:X:1104:G:H8	1.77	0.50
27:X:1103:C:N4	27:X:1110:G:H1	2.10	0.50
27:X:1202:U:H2'	27:X:1203:A:C8	2.35	0.50
27:X:1656:U:H2'	27:X:1657:A:H5''	1.94	0.50
17:R:74:LEU:HG	17:R:76:LEU:HD21	1.94	0.50
26:3:17:THR:OG1	26:3:18:GLY:N	2.45	0.50
27:X:1070:G:H5''	27:X:1071:U:H2'	1.94	0.50
27:X:1098:G:C5	27:X:1100:G:H1'	2.46	0.50
27:X:1982:C:H4'	27:X:2703:C:O2	2.12	0.50
27:X:2318:U:H4'	28:Y:43:G:H22	1.75	0.50
27:X:2820:C:H2'	27:X:2821:G:H8	1.77	0.50
1:A:28:ARG:NH1	27:X:1583:A:N7	2.59	0.49
11:L:61:SER:O	11:L:61:SER:OG	2.25	0.49
15:P:37:LYS:CE	15:P:64:ALA:HB2	2.42	0.49
18:S:1:MET:HE3	18:S:54:ILE:HG12	1.94	0.49
20:U:20:ARG:HB3	20:U:43:ARG:NH2	2.27	0.49
27:X:4:C:H42	27:X:2873:G:H1	1.60	0.49
27:X:2581:A:H8	27:X:2582:G:O4'	1.95	0.49
27:X:2617:G:H1	27:X:2755:A:H2'	1.77	0.49
1:A:182:LEU:HD12	1:A:269:PHE:HB2	1.93	0.49
1:A:207:GLY:O	27:X:1782:A:O2'	2.25	0.49
5:E:136:ILE:HD12	5:E:137:ASP:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:109:ARG:HA	7:H:129:LEU:HD22	1.94	0.49
9:J:48:ILE:HD12	9:J:71:PRO:HD3	1.95	0.49
16:Q:48:VAL:HG11	16:Q:82:LEU:HD13	1.93	0.49
17:R:22:VAL:HG13	17:R:81:VAL:H	1.77	0.49
23:Z:7:PRO:HA	27:X:2594:U:C6	2.47	0.49
27:X:113:C:HO2'	27:X:125:A:HO2'	1.59	0.49
27:X:659:G:H2'	27:X:660:G:C8	2.46	0.49
27:X:854:G:H2'	27:X:855:G:C8	2.47	0.49
27:X:1107:A:H3'	27:X:1108:U:H5''	1.94	0.49
27:X:1159:U:H2'	27:X:1160:C:H6	1.77	0.49
27:X:1235:C:N4	27:X:1240:G:H1	2.10	0.49
27:X:2422:C:H2'	27:X:2423:G:H8	1.77	0.49
28:Y:58:G:O2'	28:Y:59:A:H5''	2.12	0.49
9:J:21:ASP:OD1	9:J:21:ASP:N	2.45	0.49
9:J:77:LYS:HD3	9:J:92:GLU:OE2	2.12	0.49
10:K:87:TYR:OH	10:K:115:LEU:HD22	2.12	0.49
15:P:124:THR:OG1	15:P:126:HIS:N	2.29	0.49
17:R:84:VAL:HG11	17:R:90:LYS:H	1.77	0.49
27:X:854:G:H2'	27:X:855:G:H8	1.77	0.49
27:X:2006:G:H5'	27:X:2596:C:H4'	1.94	0.49
27:X:2513:A:C2	27:X:2514:G:H1'	2.46	0.49
27:X:2757:G:H1'	27:X:2759:U:H5	1.77	0.49
28:Y:27:A:HO2'	28:Y:28:A:P	2.36	0.49
1:A:160:GLY:HA3	27:X:1812:U:N3	2.27	0.49
1:A:203:ASN:N	1:A:203:ASN:OD1	2.45	0.49
12:M:50:PHE:CE1	12:M:79:ARG:HG3	2.47	0.49
15:P:80:LEU:HD11	15:P:87:GLU:HB3	1.94	0.49
17:R:55:THR:OG1	17:R:72:ARG:NH1	2.46	0.49
26:3:62:LEU:HD23	27:X:219:G:H5'	1.95	0.49
27:X:1431:U:H4'	27:X:1604:A:H4'	1.95	0.49
27:X:1818:G:H2'	27:X:1819:U:H6	1.78	0.49
10:K:72:ASP:HB3	10:K:75:VAL:HG23	1.94	0.49
11:L:85:LYS:HE3	11:L:86:GLN:NE2	2.27	0.49
16:Q:46:PHE:CD2	16:Q:88:ILE:HB	2.47	0.49
18:S:151:ASP:OD2	18:S:151:ASP:N	2.44	0.49
27:X:217:U:H3'	27:X:218:A:H2'	1.93	0.49
27:X:218:A:N6	27:X:232:A:H5''	2.28	0.49
27:X:321:A:C6	27:X:323:G:C4	3.01	0.49
27:X:1310:C:H2'	27:X:1311:C:H6	1.77	0.49
27:X:1412:C:HO2'	27:X:1413:U:P	2.35	0.49
27:X:1449:C:N4	27:X:1450:G:O6	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2085:G:N1	27:X:2171:U:O2	2.45	0.49
27:X:2549:G:H2'	27:X:2550:C:O4'	2.12	0.49
27:X:2594:U:H2'	27:X:2595:C:H6	1.77	0.49
3:C:24:SER:HA	3:C:27:LEU:HD22	1.94	0.49
3:C:77:PHE:CD2	27:X:1270:C:H4'	2.48	0.49
3:C:158:ARG:CZ	3:C:171:PRO:HB3	2.43	0.49
5:E:9:ILE:O	5:E:49:GLN:HB3	2.12	0.49
27:X:693:A:H2'	27:X:694:G:C8	2.47	0.49
27:X:1854:G:H2'	27:X:1855:G:H8	1.78	0.49
27:X:2856:U:H2'	27:X:2857:C:H6	1.78	0.49
1:A:100:GLY:O	27:X:1516:A:O2'	2.26	0.49
1:A:156:ALA:HB2	1:A:163:VAL:HG23	1.93	0.49
2:B:62:PRO:HG3	27:X:2767:C:H1'	1.93	0.49
6:G:103:TYR:CD1	6:G:111:LYS:HB2	2.47	0.49
10:K:6:ALA:HB1	27:X:2848:A:C2	2.46	0.49
11:L:15:ARG:O	11:L:18:ARG:HB3	2.13	0.49
13:N:4:ALA:HB2	27:X:1213:U:H1'	1.95	0.49
13:N:7:GLY:O	13:N:8:ILE:HG12	2.12	0.49
27:X:930:A:N3	28:Y:82:U:H4'	2.27	0.49
28:Y:73:C:H2'	28:Y:74:A:O4'	2.12	0.49
3:C:17:LEU:HD23	3:C:112:GLN:HG3	1.94	0.49
4:D:65:PRO:HB3	4:D:89:VAL:HG22	1.94	0.49
4:D:122:PHE:HA	27:X:2282:G:H4'	1.95	0.49
6:G:36:ASN:OD1	6:G:36:ASN:N	2.42	0.49
9:J:26:ASP:H	9:J:103:VAL:HG12	1.78	0.49
9:J:77:LYS:HD3	9:J:92:GLU:CD	2.38	0.49
10:K:53:THR:OG1	27:X:2815:C:OP1	2.28	0.49
17:R:95:ARG:HE	27:X:308:C:H5''	1.78	0.49
27:X:540:G:C6	27:X:2005:U:H5''	2.48	0.49
27:X:635:C:O2'	27:X:670:U:OP1	2.27	0.49
27:X:946:U:H2'	27:X:947:C:H6	1.78	0.49
27:X:966:A:H5''	27:X:967:G:OP2	2.13	0.49
27:X:1183:C:H2'	27:X:1184:G:H8	1.78	0.49
27:X:1451:C:H2'	27:X:1452:U:C6	2.48	0.49
27:X:2705:A:C8	27:X:2706:U:H2'	2.48	0.49
1:A:43:ARG:HE	1:A:43:ARG:N	2.11	0.49
10:K:76:VAL:HA	10:K:79:VAL:HG12	1.95	0.49
18:S:69:VAL:HG22	18:S:81:VAL:HG22	1.94	0.49
27:X:57:G:H1	27:X:68:C:H42	1.59	0.49
27:X:399:G:H5'	27:X:401:G:H22	1.78	0.49
27:X:649:G:C8	27:X:650:U:H5	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1484:G:O6	27:X:1538:A:N6	2.46	0.49
27:X:1660:G:H2'	27:X:1661:C:O4'	2.12	0.49
27:X:1766:U:H2'	27:X:1767:G:O4'	2.13	0.49
27:X:2519:C:O2'	27:X:2720:A:N3	2.40	0.49
27:X:2677:U:H2'	27:X:2678:C:C6	2.48	0.49
27:X:2758:A:O2'	27:X:2760:G:O2'	2.31	0.49
2:B:154:LYS:HG3	2:B:155:ARG:H	1.77	0.49
7:H:47:VAL:HA	7:H:74:VAL:HG12	1.95	0.49
14:O:35:LEU:HA	14:O:55:THR:HG22	1.95	0.49
17:R:56:LYS:HD2	27:X:494:A:C8	2.47	0.49
26:3:26:LYS:HB2	26:3:45:GLY:H	1.78	0.49
27:X:303:C:H2'	27:X:304:A:H5''	1.95	0.49
27:X:1987:G:C5	27:X:1988:A:C8	3.01	0.49
27:X:1988:A:H5''	27:X:1989:C:H5	1.77	0.49
27:X:2007:G:C2	27:X:2023:C:C2	3.00	0.49
27:X:2837:G:H2'	27:X:2838:U:H6	1.76	0.49
1:A:159:ALA:HA	1:A:198:ASN:OD1	2.13	0.48
2:B:144:ARG:HD3	27:X:2551:A:C8	2.48	0.48
7:H:21:CYS:SG	7:H:22:ILE:N	2.86	0.48
13:N:86:ALA:C	13:N:88:ILE:N	2.71	0.48
15:P:118:ASN:ND2	15:P:120:ILE:HB	2.28	0.48
27:X:388:G:H2'	27:X:389:G:H8	1.78	0.48
27:X:1787:U:H2'	27:X:1788:C:C6	2.47	0.48
27:X:2167:A:H2'	27:X:2168:A:H8	1.78	0.48
1:A:159:ALA:HB3	27:X:1813:A:OP1	2.13	0.48
2:B:87:ASP:OD2	2:B:87:ASP:N	2.45	0.48
4:D:71:LYS:N	27:X:2291:U:OP1	2.47	0.48
11:L:16:LYS:NZ	11:L:90:ASP:OD2	2.26	0.48
14:O:24:SER:OG	14:O:25:LEU:N	2.45	0.48
27:X:405:C:H2'	27:X:406:G:C8	2.48	0.48
27:X:1586:A:H2'	27:X:1587:A:C8	2.48	0.48
27:X:2663:U:H3	27:X:2705:A:N6	2.11	0.48
27:X:2827:G:H2'	27:X:2828:C:O4'	2.13	0.48
27:X:2837:G:H2'	27:X:2838:U:C6	2.48	0.48
7:H:76:ARG:O	7:H:94:ASN:HA	2.13	0.48
16:Q:10:PRO:HA	16:Q:27:PHE:HB3	1.95	0.48
25:2:33:ARG:HH21	27:X:478:G:P	2.36	0.48
25:2:43:THR:HA	25:2:46:ASP:HB2	1.96	0.48
27:X:29:U:O5'	27:X:29:U:H6	1.97	0.48
27:X:810:U:H2'	27:X:811:G:O4'	2.13	0.48
27:X:838:A:H4'	27:X:2407:G:C5	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1326:U:H4'	27:X:1345:G:H4'	1.96	0.48
27:X:1350:G:H2'	27:X:1351:G:C8	2.45	0.48
27:X:1563:U:H2'	27:X:1564:U:C6	2.47	0.48
27:X:1655:C:H5''	27:X:2689:C:O2'	2.13	0.48
27:X:2284:U:H5''	27:X:2286:G:N2	2.28	0.48
27:X:2811:G:H2'	27:X:2812:A:H8	1.74	0.48
2:B:35:GLN:HB2	2:B:48:GLN:OE1	2.13	0.48
8:I:101:ARG:HG3	27:X:637:G:H1	1.78	0.48
25:2:21:ARG:NH2	27:X:476:G:O3'	2.46	0.48
27:X:1008:G:H1	27:X:1169:C:H42	1.61	0.48
27:X:2058:U:C4	27:X:2217:G:C6	3.02	0.48
9:J:83:ARG:HH12	27:X:971:A:N6	2.12	0.48
12:M:34:ARG:NH2	12:M:35:VAL:O	2.26	0.48
23:Z:10:LYS:HE2	27:X:1275:A:N3	2.29	0.48
26:3:16:ILE:HD12	26:3:64:ARG:HE	1.78	0.48
27:X:231:G:H4'	27:X:397:U:H5''	1.95	0.48
27:X:540:G:N1	27:X:2005:U:OP1	2.46	0.48
27:X:838:A:H2'	27:X:839:U:O4'	2.14	0.48
27:X:1031:C:H5''	27:X:1032:A:N3	2.29	0.48
27:X:1135:C:H2'	27:X:1136:G:O4'	2.12	0.48
27:X:1441:A:H4'	27:X:1442:C:O5'	2.13	0.48
27:X:1514:C:H4'	27:X:1592:U:O2'	2.13	0.48
27:X:2185:U:H2'	27:X:2186:G:C8	2.49	0.48
1:A:55:GLY:N	1:A:217:ARG:HB2	2.05	0.48
1:A:143:HIS:HB2	1:A:156:ALA:O	2.14	0.48
2:B:5:LEU:HD12	2:B:49:ILE:HD11	1.96	0.48
6:G:62:ILE:O	6:G:77:GLY:HA3	2.13	0.48
7:H:40:GLY:HA3	27:X:2545:A:N6	2.23	0.48
11:L:8:ARG:HH21	11:L:9:ARG:NE	2.12	0.48
15:P:106:LEU:O	15:P:109:ARG:HD2	2.14	0.48
17:R:45:LYS:HA	17:R:76:LEU:O	2.13	0.48
17:R:59:LYS:HD2	17:R:62:MET:CB	2.41	0.48
18:S:46:GLN:HE22	18:S:52:PHE:HB2	1.78	0.48
27:X:48:A:H4'	27:X:49:U:C5'	2.43	0.48
27:X:1072:U:H4'	27:X:1081:A:O2'	2.13	0.48
27:X:1316:G:H5'	27:X:1659:G:H21	1.78	0.48
27:X:1342:U:H5''	27:X:1343:C:C5	2.48	0.48
7:H:90:ARG:HH12	12:M:108:ARG:NH2	2.11	0.48
12:M:2:GLN:HG3	12:M:3:THR:N	2.29	0.48
13:N:47:TYR:CE2	14:O:73:LYS:HE2	2.47	0.48
24:1:9:ILE:O	24:1:10:VAL:HB	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:29:LYS:HD2	26:3:33:ASN:O	2.13	0.48
27:X:1060:C:H1'	27:X:1124:U:O2'	2.13	0.48
27:X:1495:G:H5'	27:X:1574:A:H2	1.77	0.48
27:X:1794:A:N1	27:X:1814:G:O2'	2.40	0.48
28:Y:46:G:N3	28:Y:49:C:N4	2.62	0.48
4:D:57:LEU:O	4:D:61:THR:OG1	2.30	0.48
5:E:160:LYS:NZ	27:X:2636:A:O3'	2.47	0.48
6:G:101:THR:HG23	6:G:103:TYR:CE1	2.49	0.48
7:H:28:GLY:O	7:H:35:THR:HG23	2.13	0.48
14:O:48:GLY:C	14:O:50:ASP:H	2.22	0.48
19:T:74:LYS:O	19:T:76:ALA:N	2.42	0.48
23:Z:8:LYS:HE2	27:X:2039:G:O2'	2.14	0.48
27:X:246:C:H1'	27:X:437:G:N2	2.28	0.48
27:X:492:G:HO2'	27:X:493:A:P	2.37	0.48
27:X:1935:A:C6	27:X:1936:A:N1	2.82	0.48
3:C:70:GLY:H	27:X:687:G:H5''	1.78	0.48
4:D:35:VAL:HG11	27:X:2293:G:H5'	1.95	0.48
7:H:75:VAL:HG22	7:H:96:ALA:HA	1.96	0.48
8:I:62:LYS:HZ1	26:3:13:ARG:HH11	1.61	0.48
8:I:75:VAL:O	8:I:108:LEU:HD12	2.14	0.48
9:J:15:ARG:HG2	9:J:73:LYS:HZ2	1.79	0.48
11:L:65:THR:HG21	28:Y:52:G:OP2	2.13	0.48
12:M:103:LYS:HD2	12:M:103:LYS:N	2.28	0.48
13:N:37:GLN:NE2	27:X:1265:G:H22	2.12	0.48
27:X:2437:G:H21	27:X:2438:A:H61	1.62	0.48
28:Y:80:A:H2'	28:Y:81:C:O4'	2.14	0.48
2:B:165:VAL:HG11	27:X:2658:A:H4'	1.95	0.48
9:J:83:ARG:NH2	27:X:971:A:H61	2.11	0.48
13:N:13:ARG:NH1	27:X:1264:C:H5''	2.29	0.48
15:P:78:ASN:HD21	27:X:504:G:H21	1.61	0.48
20:U:63:SER:O	20:U:67:LEU:N	2.47	0.48
27:X:73:A:H5''	27:X:74:G:O4'	2.13	0.48
27:X:587:A:OP2	27:X:587:A:H8	1.97	0.48
27:X:1098:G:N2	27:X:1114:A:H1'	2.29	0.48
27:X:1919:A:N6	27:X:1946:U:H3	2.10	0.48
27:X:1924:C:C4	27:X:1925:C:C4	3.02	0.48
27:X:1947:G:O2'	27:X:1950:C:OP1	2.28	0.48
27:X:2437:G:H21	27:X:2438:A:N6	2.12	0.48
2:B:116:VAL:HG13	2:B:136:ARG:HE	1.78	0.47
4:D:106:ILE:HG21	4:D:139:PRO:HB3	1.95	0.47
6:G:75:ILE:HB	6:G:147:ARG:HH12	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:83:ARG:HH22	27:X:971:A:N6	2.11	0.47
13:N:7:GLY:O	13:N:9:VAL:HG23	2.14	0.47
14:O:75:LYS:HB2	14:O:80:TYR:HD1	1.79	0.47
21:V:47:ARG:HH22	27:X:59:G:P	2.37	0.47
27:X:820:U:H2'	27:X:821:A:C8	2.45	0.47
27:X:1332:G:C6	27:X:1333:G:N1	2.82	0.47
27:X:1686:A:H5''	27:X:1687:C:OP2	2.13	0.47
27:X:2498:U:C5	27:X:2520:A:C6	3.02	0.47
2:B:14:ILE:HG12	12:M:20:HIS:HD2	1.77	0.47
5:E:88:GLU:HB3	5:E:163:ARG:HG3	1.96	0.47
7:H:64:VAL:HG22	7:H:106:ARG:HH21	1.80	0.47
9:J:6:LYS:O	9:J:71:PRO:HG2	2.14	0.47
9:J:70:PHE:CD2	27:X:884:C:H4'	2.49	0.47
15:P:95:ALA:HB2	15:P:129:ILE:HG23	1.95	0.47
18:S:71:MET:HA	18:S:78:PRO:HA	1.96	0.47
20:U:48:LYS:HD2	27:X:2074:U:H1'	1.96	0.47
21:V:23:LYS:O	21:V:27:GLU:HG2	2.14	0.47
22:W:22:ALA:HA	27:X:942:U:O2'	2.13	0.47
27:X:1141:U:H6	27:X:1141:U:O5'	1.97	0.47
27:X:1573:G:H3'	27:X:1574:A:H5''	1.95	0.47
27:X:2442:C:H2'	27:X:2443:C:C6	2.48	0.47
27:X:2625:U:O5'	27:X:2625:U:H6	1.97	0.47
9:J:73:LYS:H	9:J:94:TRP:CD1	2.32	0.47
10:K:29:LEU:HD13	10:K:79:VAL:HB	1.96	0.47
12:M:27:PHE:HB3	12:M:93:ILE:HD12	1.95	0.47
14:O:36:LYS:HZ2	14:O:54:TYR:HB3	1.79	0.47
15:P:80:LEU:HD21	15:P:87:GLU:HB3	1.97	0.47
26:3:19:THR:HB	26:3:21:LYS:HG3	1.96	0.47
27:X:219:G:N2	27:X:231:G:H2'	2.29	0.47
27:X:692:C:H2'	27:X:693:A:H8	1.79	0.47
27:X:725:C:H2'	27:X:726:G:C8	2.50	0.47
27:X:841:G:H2'	27:X:842:A:N7	2.28	0.47
27:X:1204:G:H2'	27:X:1205:G:C8	2.48	0.47
27:X:2487:G:C2	27:X:2561:G:C6	3.02	0.47
8:I:62:LYS:HG3	26:3:13:ARG:HG2	1.95	0.47
28:Y:32:C:H1'	28:Y:59:A:H61	1.79	0.47
1:A:38:PRO:HB3	27:X:1586:A:H5'	1.96	0.47
1:A:142:VAL:HA	1:A:194:GLY:H	1.78	0.47
3:C:27:LEU:O	3:C:31:VAL:HG22	2.13	0.47
27:X:203:G:H2'	27:X:204:A:C8	2.49	0.47
27:X:502:A:H2'	27:X:503:G:O4'	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1021:A:N3	27:X:1164:C:H1'	2.29	0.47
27:X:1316:G:N2	27:X:1317:G:H1'	2.30	0.47
27:X:1774:A:H5'	27:X:2587:G:H4'	1.95	0.47
28:Y:53:G:H2'	28:Y:54:U:H5''	1.97	0.47
2:B:110:GLY:O	10:K:3:HIS:CD2	2.65	0.47
20:U:20:ARG:HB3	20:U:43:ARG:CZ	2.44	0.47
24:1:9:ILE:HA	24:1:28:ARG:HA	1.96	0.47
27:X:82:G:N2	27:X:100:G:H1'	2.29	0.47
27:X:126:C:N4	27:X:127:C:H41	2.12	0.47
27:X:346:C:H2'	27:X:347:C:C5	2.49	0.47
27:X:1495:G:H5'	27:X:1574:A:C2	2.48	0.47
27:X:2662:C:H2'	27:X:2663:U:H6	1.79	0.47
1:A:209:ALA:HB2	27:X:1781:C:O2'	2.15	0.47
2:B:14:ILE:HA	12:M:20:HIS:HD2	1.79	0.47
2:B:38:THR:HG22	2:B:40:GLN:H	1.78	0.47
4:D:55:LYS:O	4:D:59:LEU:HG	2.14	0.47
5:E:17:VAL:HG22	5:E:26:VAL:HG13	1.96	0.47
7:H:13:ASN:HD21	7:H:109:ARG:H	1.63	0.47
7:H:47:VAL:HG11	7:H:115:ALA:CB	2.44	0.47
9:J:53:ILE:O	9:J:57:ARG:HG2	2.14	0.47
10:K:92:GLY:O	27:X:2855:C:H1'	2.14	0.47
13:N:54:LYS:NZ	27:X:1006:C:OP2	2.47	0.47
14:O:39:PHE:HE2	14:O:46:VAL:HB	1.79	0.47
16:Q:20:MET:HG3	16:Q:25:TYR:HE1	1.80	0.47
16:Q:35:LYS:HB2	27:X:1614:C:H5''	1.97	0.47
17:R:26:SER:OG	17:R:27:GLY:N	2.45	0.47
27:X:302:U:O4	27:X:360:A:N6	2.48	0.47
27:X:398:C:N4	27:X:424:G:H1	2.12	0.47
27:X:498:C:N4	27:X:499:G:O6	2.48	0.47
27:X:557:U:H1'	27:X:558:G:C5	2.49	0.47
27:X:774:A:O5'	27:X:774:A:C8	2.68	0.47
27:X:824:U:O2	27:X:1263:G:H3'	2.15	0.47
27:X:936:A:H2'	27:X:937:C:O4'	2.14	0.47
27:X:1193:G:H2'	27:X:1194:U:C6	2.49	0.47
27:X:1211:G:H2'	27:X:1212:U:H6	1.80	0.47
27:X:1376:C:O2'	27:X:1800:A:H1'	2.15	0.47
27:X:1436:G:N2	27:X:1514:C:H1'	2.30	0.47
27:X:1478:U:H2'	27:X:1479:G:C8	2.50	0.47
27:X:1621:C:H2'	27:X:1622:G:O4'	2.14	0.47
27:X:1785:A:H2'	27:X:1786:C:C6	2.50	0.47
27:X:2298:U:H1'	27:X:2299:A:C6	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2579:A:H2'	27:X:2580:C:C6	2.50	0.47
28:Y:96:C:H2'	28:Y:97:C:C6	2.48	0.47
1:A:13:ARG:NE	1:A:27:LYS:HB3	2.24	0.47
2:B:203:LYS:HD2	2:B:203:LYS:HA	1.49	0.47
3:C:77:PHE:CE2	27:X:1270:C:H4'	2.49	0.47
6:G:70:PHE:O	13:N:64:ARG:NE	2.41	0.47
12:M:101:ARG:HG2	12:M:101:ARG:HH21	1.80	0.47
24:1:51:ARG:NH1	24:1:53:LYS:HB3	2.29	0.47
26:3:16:ILE:HD12	26:3:64:ARG:HG2	1.97	0.47
26:3:34:THR:HG23	27:X:2399:C:OP2	2.15	0.47
27:X:554:U:H5''	27:X:556:A:C2	2.50	0.47
27:X:2194:A:H2'	27:X:2195:C:O4'	2.14	0.47
4:D:148:LYS:H	4:D:148:LYS:HD3	1.80	0.47
5:E:56:SER:OG	5:E:61:HIS:NE2	2.48	0.47
7:H:11:ALA:N	7:H:96:ALA:O	2.39	0.47
8:I:35:LYS:HZ2	27:X:575:U:H5''	1.79	0.47
8:I:51:GLY:HA3	26:3:59:LYS:HE3	1.97	0.47
10:K:49:GLU:O	10:K:52:ILE:HG12	2.15	0.47
14:O:71:ILE:HD13	27:X:1003:C:H4'	1.96	0.47
20:U:15:VAL:HA	20:U:45:ASN:O	2.14	0.47
27:X:105:G:H21	27:X:357:A:H61	1.63	0.47
27:X:228:A:C5	27:X:229:G:H1'	2.50	0.47
27:X:437:G:H2'	27:X:438:G:C8	2.47	0.47
27:X:793:G:N2	27:X:796:A:H62	2.09	0.47
27:X:825:C:H5''	27:X:1263:G:O2'	2.14	0.47
27:X:1726:C:O2'	27:X:2834:A:N3	2.42	0.47
27:X:1770:U:H5	27:X:1775:A:N7	2.13	0.47
27:X:2707:G:H2'	27:X:2708:U:C6	2.50	0.47
2:B:52:ALA:O	2:B:76:ARG:N	2.31	0.47
2:B:124:GLY:HA2	2:B:135:HIS:O	2.15	0.47
4:D:37:ASN:ND2	4:D:87:ILE:O	2.48	0.47
5:E:67:LEU:O	5:E:71:LEU:HG	2.15	0.47
8:I:32:ARG:HH12	14:O:82:ARG:HH21	1.63	0.47
10:K:73:LYS:HA	10:K:76:VAL:HG12	1.97	0.47
17:R:48:VAL:HG13	17:R:50:GLY:H	1.79	0.47
18:S:141:MET:SD	18:S:147:ILE:HG12	2.55	0.47
23:Z:10:LYS:HG3	27:X:1276:U:H1'	1.96	0.47
27:X:5:A:H2'	27:X:6:A:C8	2.49	0.47
27:X:732:G:H2'	27:X:733:G:C8	2.49	0.47
27:X:773:G:H2'	27:X:774:A:H5'	1.97	0.47
27:X:1174:G:C2	27:X:1175:A:C5	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2010:G:C6	27:X:2011:U:C4	3.03	0.47
1:A:27:LYS:HE2	1:A:29:PRO:HD3	1.97	0.46
4:D:4:LEU:C	4:D:6:THR:H	2.24	0.46
8:I:58:ALA:O	8:I:59:ARG:HG2	2.15	0.46
13:N:8:ILE:O	13:N:12:ARG:HG3	2.15	0.46
27:X:346:C:H2'	27:X:347:C:C6	2.50	0.46
27:X:476:G:H2'	27:X:477:A:C8	2.49	0.46
27:X:552:C:C2'	27:X:553:C:H5''	2.43	0.46
27:X:992:A:N1	27:X:2010:G:O2'	2.37	0.46
27:X:2200:G:H2'	27:X:2201:G:H8	1.79	0.46
27:X:2494:C:O2	27:X:2549:G:C2	2.68	0.46
27:X:2645:C:H3'	27:X:2646:C:C6	2.50	0.46
1:A:118:ASN:HD22	1:A:119:ALA:H	1.63	0.46
1:A:157:ARG:HB2	1:A:157:ARG:HH11	1.80	0.46
1:A:182:LEU:HB2	1:A:268:ARG:O	2.14	0.46
1:A:218:LYS:HE2	1:A:218:LYS:HB2	1.44	0.46
2:B:133:LYS:O	2:B:134:TRP:HD1	1.98	0.46
4:D:135:GLN:N	4:D:150:ARG:O	2.48	0.46
9:J:77:LYS:H	9:J:89:GLY:HA3	1.79	0.46
12:M:55:ILE:O	12:M:103:LYS:O	2.33	0.46
14:O:72:ARG:HA	14:O:82:ARG:O	2.15	0.46
27:X:170:U:O3'	27:X:816:U:H4'	2.15	0.46
27:X:1256:C:H2'	27:X:1257:U:C6	2.50	0.46
27:X:2691:C:H2'	27:X:2694:G:H5''	1.97	0.46
27:X:2844:G:H2'	27:X:2845:C:O4'	2.15	0.46
2:B:9:ILE:CD1	2:B:27:LEU:HB2	2.44	0.46
2:B:21:ILE:HD12	2:B:185:LYS:HD2	1.96	0.46
3:C:15:ILE:HD11	3:C:195:ILE:HA	1.98	0.46
7:H:7:ARG:HA	7:H:20:MET:HA	1.97	0.46
10:K:87:TYR:HE1	10:K:94:TYR:HD1	1.63	0.46
12:M:103:LYS:HG2	27:X:2698:G:H4'	1.95	0.46
15:P:26:ALA:O	15:P:128:THR:HA	2.15	0.46
16:Q:15:LYS:HD2	16:Q:15:LYS:HA	1.62	0.46
17:R:14:LEU:HA	17:R:14:LEU:HD23	1.62	0.46
27:X:26:G:H1'	27:X:525:A:N6	2.30	0.46
27:X:1018:C:C5	27:X:1019:U:H5	2.33	0.46
27:X:1156:U:H2'	27:X:1157:G:H8	1.81	0.46
27:X:1427:G:O6	27:X:1428:G:N2	2.36	0.46
27:X:2223:U:H2'	27:X:2224:U:O4'	2.15	0.46
27:X:2732:C:H2'	27:X:2733:A:O4'	2.15	0.46
27:X:2825:A:C2	27:X:2826:C:C2	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:72:LYS:HA	4:D:81:GLN:HA	1.97	0.46
6:G:65:LYS:HE3	6:G:66:HIS:CE1	2.49	0.46
8:I:73:GLU:OE2	8:I:101:ARG:HB2	2.16	0.46
17:R:105:ARG:NH1	17:R:113:THR:H	2.14	0.46
23:Z:51:TYR:CE2	23:Z:55:ARG:HB2	2.50	0.46
27:X:78:C:O2'	27:X:357:A:N3	2.45	0.46
27:X:555:U:O2'	27:X:1234:C:H5'	2.16	0.46
27:X:1398:G:O2'	27:X:1399:C:O5'	2.33	0.46
27:X:1418:C:H2'	27:X:1419:G:C8	2.49	0.46
27:X:1777:A:C4	27:X:1921:A:C6	3.04	0.46
27:X:2230:G:OP2	27:X:2230:G:H8	1.98	0.46
27:X:2478:C:N4	27:X:2479:U:C4	2.84	0.46
27:X:2555:G:OP1	27:X:2555:G:H3'	2.16	0.46
2:B:34:VAL:HG21	2:B:78:LEU:HD22	1.97	0.46
9:J:68:ARG:CZ	9:J:103:VAL:HG11	2.46	0.46
10:K:3:HIS:CD2	10:K:5:LYS:NZ	2.83	0.46
12:M:13:LEU:HD12	12:M:13:LEU:HA	1.60	0.46
14:O:73:LYS:HB2	14:O:82:ARG:HB2	1.98	0.46
21:V:6:MET:HE1	21:V:52:GLN:HB3	1.96	0.46
21:V:25:LEU:HD12	21:V:25:LEU:HA	1.63	0.46
25:2:13:ALA:HB1	27:X:123:A:H1'	1.97	0.46
27:X:192:G:H4'	27:X:193:A:H4'	1.98	0.46
27:X:624:A:H4'	27:X:626:A:N7	2.30	0.46
27:X:1212:U:H2'	27:X:1213:U:H6	1.80	0.46
27:X:1355:A:N1	27:X:1358:C:C2	2.83	0.46
27:X:1451:C:H2'	27:X:1452:U:H6	1.80	0.46
5:E:86:ASN:HB2	5:E:165:VAL:HG22	1.98	0.46
6:G:103:TYR:CD2	27:X:1142:G:N3	2.83	0.46
7:H:55:VAL:HG23	7:H:68:ASP:O	2.16	0.46
24:1:3:LYS:NZ	24:1:7:ARG:HH11	2.14	0.46
27:X:721:C:H42	27:X:736:G:H1	1.64	0.46
27:X:1467:U:H3'	27:X:1467:U:H6	1.80	0.46
27:X:2199:C:H2'	27:X:2200:G:C8	2.46	0.46
27:X:2299:A:H5''	27:X:2300:G:OP1	2.16	0.46
27:X:2522:G:H2'	27:X:2523:G:C8	2.51	0.46
1:A:251:GLY:HA3	1:A:255:LYS:HZ1	1.79	0.46
2:B:5:LEU:HD11	2:B:79:ARG:HB3	1.97	0.46
3:C:40:ARG:NH2	27:X:39:C:O2	2.49	0.46
5:E:163:ARG:NH2	5:E:169:ILE:HB	2.31	0.46
14:O:10:LYS:NZ	14:O:13:ARG:HH22	2.12	0.46
27:X:591:G:H1	27:X:1271:C:N4	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:597:U:O4	27:X:683:A:H1'	2.16	0.46
27:X:618:A:H2'	27:X:619:A:C8	2.50	0.46
27:X:650:U:H2'	27:X:651:C:H6	1.80	0.46
27:X:2453:C:H5''	27:X:2454:C:OP2	2.16	0.46
2:B:136:ARG:HH22	27:X:2033:C:H4'	1.81	0.46
4:D:22:TYR:OH	4:D:165:GLU:OE1	2.30	0.46
9:J:82:THR:HG22	27:X:2475:C:OP2	2.15	0.46
11:L:91:ARG:NH2	27:X:2355:A:H61	2.14	0.46
13:N:2:PRO:HA	27:X:457:C:OP1	2.15	0.46
14:O:86:HIS:NE2	14:O:88:GLN:HB2	2.31	0.46
15:P:21:ARG:NH2	27:X:507:A:OP1	2.49	0.46
15:P:78:ASN:HD21	27:X:504:G:N2	2.14	0.46
16:Q:55:THR:OG1	16:Q:76:LYS:HE3	2.15	0.46
17:R:16:PHE:CZ	17:R:46:VAL:HG22	2.51	0.46
17:R:103:LYS:HB3	17:R:103:LYS:HE2	1.76	0.46
23:Z:15:LYS:HA	23:Z:15:LYS:HD2	1.64	0.46
27:X:627:A:H2'	27:X:628:A:H8	1.78	0.46
27:X:1081:A:N7	27:X:1108:U:H4'	2.31	0.46
27:X:1455:C:H2'	27:X:1456:C:C6	2.49	0.46
27:X:1834:G:H2'	27:X:1835:C:C6	2.50	0.46
27:X:1872:A:N1	27:X:2213:G:H1'	2.30	0.46
27:X:2372:A:H62	27:X:2401:A:H61	1.64	0.46
27:X:2656:G:H1	27:X:2710:C:H42	1.64	0.46
1:A:39:LYS:HB2	1:A:62:TYR:HB2	1.98	0.46
2:B:114:GLN:HG3	2:B:160:MET:SD	2.55	0.46
2:B:203:LYS:HZ3	2:B:204:ALA:H	1.63	0.46
3:C:162:ARG:HG3	27:X:333:A:OP1	2.16	0.46
9:J:117:GLU:HA	9:J:120:ARG:HB2	1.97	0.46
15:P:30:TYR:CE1	15:P:101:PRO:HG3	2.51	0.46
15:P:31:VAL:O	15:P:124:THR:HA	2.15	0.46
15:P:114:ARG:HD2	27:X:760:U:O2	2.16	0.46
16:Q:20:MET:HG3	16:Q:25:TYR:CE1	2.51	0.46
18:S:134:LEU:HD12	18:S:134:LEU:HA	1.81	0.46
19:T:37:LEU:HD23	19:T:79:ILE:HG21	1.98	0.46
27:X:105:G:N2	27:X:357:A:H61	2.14	0.46
27:X:2245:A:H4'	27:X:2246:A:C2	2.51	0.46
6:G:69:ASP:C	6:G:71:THR:HG22	2.41	0.46
14:O:40:VAL:HA	14:O:45:THR:HG22	1.97	0.46
27:X:27:G:O2'	27:X:28:A:OP2	2.28	0.46
27:X:179:U:H2'	27:X:180:C:O4'	2.16	0.46
27:X:408:U:H2'	27:X:409:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:485:G:C6	27:X:520:C:N4	2.83	0.46
27:X:788:G:H5'	27:X:790:A:H1'	1.98	0.46
27:X:788:G:H5'	27:X:790:A:C1'	2.45	0.46
27:X:1073:G:H1	27:X:1087:C:H42	1.64	0.46
27:X:1174:G:H2'	27:X:1175:A:C8	2.49	0.46
27:X:1795:C:H2'	27:X:1796:A:C8	2.51	0.46
27:X:2427:A:H3'	27:X:2428:U:H2'	1.97	0.46
28:Y:39:C:H5'	28:Y:40:C:OP2	2.16	0.46
7:H:80:ALA:HB2	7:H:90:ARG:HD3	1.98	0.45
8:I:31:GLY:O	8:I:32:ARG:HG3	2.16	0.45
18:S:147:ILE:HB	18:S:169:VAL:HG13	1.97	0.45
27:X:12:U:H5	27:X:536:A:H62	1.64	0.45
27:X:849:G:C5	27:X:850:C:C4	3.04	0.45
27:X:1468:A:C8	27:X:1468:A:OP2	2.69	0.45
27:X:2055:G:C6	27:X:2056:C:C4	3.04	0.45
1:A:208:LYS:HD3	1:A:208:LYS:HA	1.60	0.45
4:D:46:ASP:HB2	4:D:49:ALA:H	1.81	0.45
6:G:67:ARG:CG	6:G:70:PHE:HA	2.47	0.45
12:M:50:PHE:CE2	12:M:70:LYS:HB3	2.50	0.45
14:O:20:ILE:HG12	14:O:21:ARG:N	2.31	0.45
15:P:104:LYS:NZ	15:P:119:ILE:HG22	2.31	0.45
19:T:74:LYS:C	19:T:76:ALA:N	2.74	0.45
27:X:540:G:H21	27:X:2004:U:H1'	1.81	0.45
27:X:877:G:H1	27:X:924:C:H42	1.62	0.45
27:X:1283:C:H5''	27:X:1284:G:C5'	2.46	0.45
27:X:1793:A:OP2	27:X:1806:G:N1	2.49	0.45
27:X:1802:A:H2'	27:X:1803:G:O4'	2.16	0.45
1:A:210:GLY:HA2	1:A:213:ARG:CG	2.46	0.45
1:A:218:LYS:HA	1:A:219:PRO:HD3	1.58	0.45
3:C:128:ALA:O	3:C:130:THR:N	2.49	0.45
7:H:17:ARG:HG3	7:H:58:ALA:HA	1.98	0.45
10:K:66:VAL:HG12	10:K:76:VAL:HG23	1.98	0.45
10:K:88:ALA:C	10:K:90:ARG:H	2.24	0.45
12:M:69:ARG:HG3	12:M:78:GLU:HG2	1.98	0.45
15:P:33:MET:O	15:P:123:ARG:O	2.34	0.45
15:P:100:GLY:C	15:P:123:ARG:HB2	2.42	0.45
27:X:706:A:H2'	27:X:707:U:O4'	2.16	0.45
27:X:824:U:H1'	27:X:1264:C:O4'	2.16	0.45
27:X:825:C:H5''	27:X:1263:G:HO2'	1.80	0.45
27:X:1433:A:OP2	27:X:1593:C:N4	2.45	0.45
27:X:2178:U:H2'	27:X:2179:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:155:ASP:OD2	5:E:158:HIS:N	2.33	0.45
10:K:102:THR:HA	10:K:109:THR:HA	1.99	0.45
20:U:49:LYS:HB2	20:U:61:TRP:NE1	2.31	0.45
24:1:36:GLU:HB3	24:1:52:GLU:HB2	1.97	0.45
26:3:29:LYS:HE3	26:3:34:THR:HB	1.98	0.45
27:X:490:A:H1'	27:X:491:A:H5''	1.98	0.45
27:X:1925:C:OP2	27:X:1926:U:O2'	2.29	0.45
27:X:2268:G:H5'	27:X:2363:G:O2'	2.16	0.45
27:X:2572:U:H2'	27:X:2573:C:C6	2.51	0.45
1:A:223:GLY:O	1:A:226:MET:N	2.37	0.45
6:G:100:TYR:HB2	6:G:116:ARG:CZ	2.46	0.45
18:S:74:ARG:HH22	28:Y:94:G:H5''	1.81	0.45
18:S:88:TYR:C	18:S:127:PRO:HG2	2.41	0.45
23:Z:6:VAL:HG22	23:Z:7:PRO:HD2	1.97	0.45
23:Z:12:SER:OG	27:X:2004:U:OP1	2.23	0.45
26:3:23:MET:HG2	26:3:48:PHE:CE2	2.51	0.45
27:X:224:G:H4'	27:X:399:G:C6	2.51	0.45
27:X:225:G:N7	27:X:227:G:H1'	2.30	0.45
2:B:133:LYS:C	2:B:134:TRP:HD1	2.24	0.45
3:C:42:THR:HG21	27:X:38:G:N2	2.30	0.45
12:M:37:THR:HG22	12:M:87:LEU:HD22	1.99	0.45
13:N:91:ASN:HB3	13:N:95:LEU:HD13	1.99	0.45
27:X:2053:G:C2	27:X:2054:A:C4	3.05	0.45
27:X:2170:C:H3'	27:X:2171:U:H5''	1.98	0.45
2:B:39:ALA:HA	2:B:43:GLY:H	1.82	0.45
8:I:94:GLU:CD	8:I:97:ARG:HH11	2.23	0.45
15:P:32:ARG:CZ	15:P:32:ARG:HB3	2.47	0.45
18:S:22:VAL:HG21	28:Y:77:G:H1'	1.99	0.45
27:X:836:G:H2'	27:X:837:U:C6	2.51	0.45
27:X:1407:G:O6	27:X:1408:A:N6	2.50	0.45
27:X:1750:A:H4'	27:X:2695:C:O4'	2.17	0.45
27:X:1781:C:H2'	27:X:1782:A:C5	2.51	0.45
3:C:18:PRO:HD2	3:C:109:ALA:HB2	1.99	0.45
3:C:74:VAL:HG22	3:C:77:PHE:HD1	1.81	0.45
3:C:97:ARG:O	3:C:101:GLN:HG2	2.17	0.45
10:K:49:GLU:OE1	10:K:95:THR:HG22	2.16	0.45
12:M:16:ILE:H	12:M:16:ILE:HD12	1.81	0.45
15:P:98:ASP:CG	27:X:23:G:H21	2.25	0.45
16:Q:56:MET:HE1	27:X:1617:G:OP2	2.17	0.45
24:1:42:PRO:O	24:1:46:LYS:HG2	2.16	0.45
24:1:46:LYS:O	24:1:48:VAL:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:597:U:H5''	27:X:598:U:OP2	2.17	0.45
27:X:2191:A:H5''	27:X:2192:U:H5	1.82	0.45
1:A:15:GLN:CD	1:A:17:THR:HG1	2.25	0.45
1:A:163:VAL:HG22	1:A:177:LEU:HA	1.99	0.45
13:N:66:ASN:HD22	13:N:70:ARG:NH2	2.14	0.45
17:R:23:ILE:HD12	17:R:31:GLY:HA2	1.97	0.45
20:U:49:LYS:HB2	20:U:61:TRP:CD1	2.52	0.45
27:X:588:G:N2	27:X:1275:A:C4	2.84	0.45
27:X:1142:G:O6	27:X:2023:C:H1'	2.17	0.45
27:X:1561:A:O2'	27:X:1562:G:OP2	2.34	0.45
27:X:2791:C:O2	27:X:2858:A:O2'	2.30	0.45
1:A:76:ASN:ND2	1:A:118:ASN:OD1	2.43	0.45
2:B:133:LYS:HB2	2:B:137:ARG:CG	2.38	0.45
5:E:110:SER:HB2	27:X:2646:C:O2	2.17	0.45
9:J:64:LYS:HD2	9:J:108:ALA:O	2.16	0.45
13:N:89:ASP:HB3	13:N:91:ASN:HB2	1.99	0.45
13:N:93:LYS:HB3	27:X:1007:A:H4'	1.99	0.45
27:X:564:U:H2'	27:X:565:A:C8	2.51	0.45
27:X:584:A:OP2	27:X:2038:C:N4	2.50	0.45
27:X:828:C:N4	27:X:1206:G:H1	2.15	0.45
27:X:873:U:H1'	27:X:2247:A:H5''	1.99	0.45
27:X:1011:A:N7	27:X:1165:G:N2	2.65	0.45
27:X:1468:A:P	27:X:1468:A:C8	3.05	0.45
27:X:1725:C:N4	27:X:1741:G:H1	2.15	0.45
27:X:2056:C:O2'	27:X:2577:A:O2'	2.32	0.45
27:X:2433:G:C4	27:X:2434:G:C8	3.05	0.45
27:X:2494:C:N4	27:X:2548:G:H1	2.12	0.45
27:X:2674:C:H2'	27:X:2675:U:C6	2.52	0.45
1:A:43:ARG:HD2	27:X:704:G:O3'	2.17	0.44
3:C:30:VAL:HG11	3:C:177:VAL:HG21	1.99	0.44
4:D:46:ASP:HB2	4:D:49:ALA:HB3	1.99	0.44
7:H:82:LYS:HB2	7:H:82:LYS:HE3	1.87	0.44
9:J:37:ALA:O	9:J:100:PRO:HA	2.17	0.44
12:M:34:ARG:HH12	12:M:91:VAL:CA	2.30	0.44
13:N:47:TYR:CE1	13:N:51:ARG:HD3	2.52	0.44
17:R:92:THR:HA	17:R:108:VAL:HG22	1.98	0.44
23:Z:18:MET:O	23:Z:21:SER:HB3	2.16	0.44
24:1:41:ASP:HB2	24:1:46:LYS:CB	2.46	0.44
27:X:91:A:H2'	27:X:92:U:C6	2.52	0.44
27:X:760:U:H4'	27:X:761:G:H5''	1.99	0.44
27:X:837:U:H2'	27:X:838:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1124:U:H2'	27:X:1125:G:C8	2.52	0.44
27:X:1141:U:O2	27:X:2008:C:H5''	2.16	0.44
27:X:1671:A:H1'	27:X:2798:A:OP2	2.17	0.44
27:X:2312:A:H4'	27:X:2313:G:O5'	2.16	0.44
27:X:2424:G:O2'	27:X:2425:G:H5'	2.17	0.44
3:C:53:LYS:HZ1	27:X:464:G:P	2.40	0.44
3:C:111:ARG:O	3:C:116:LYS:HG3	2.17	0.44
7:H:28:GLY:C	7:H:35:THR:H	2.25	0.44
13:N:32:TYR:O	13:N:35:ALA:N	2.50	0.44
19:T:36:ILE:HD12	19:T:58:THR:HG21	1.99	0.44
27:X:577:U:H2'	27:X:579:G:OP2	2.16	0.44
27:X:794:A:H2	27:X:1767:G:N3	2.15	0.44
27:X:923:A:N3	27:X:2243:C:H1'	2.31	0.44
27:X:1174:G:N2	27:X:1175:A:C4	2.85	0.44
27:X:2477:C:O2'	27:X:2478:C:H5'	2.18	0.44
27:X:2696:A:H2'	27:X:2697:G:H8	1.82	0.44
28:Y:39:C:N4	28:Y:51:G:O4'	2.51	0.44
1:A:26:LYS:HE3	1:A:28:ARG:NH2	2.31	0.44
1:A:32:ALA:HB3	1:A:83:GLU:CD	2.42	0.44
1:A:164:GLN:HE21	1:A:164:GLN:HB2	1.57	0.44
2:B:67:PHE:HE1	2:B:78:LEU:HD21	1.81	0.44
11:L:72:GLY:HA2	11:L:107:ALA:HB2	1.98	0.44
16:Q:46:PHE:HD2	16:Q:88:ILE:HB	1.83	0.44
19:T:40:GLN:NE2	19:T:57:HIS:O	2.47	0.44
22:W:46:THR:HG22	22:W:47:VAL:HG13	1.99	0.44
25:2:24:THR:HG23	25:2:27:GLY:H	1.81	0.44
27:X:313:U:H2'	27:X:314:G:C8	2.48	0.44
27:X:517:A:H1'	27:X:519:C:N3	2.31	0.44
27:X:1250:A:OP1	27:X:1250:A:H4'	2.18	0.44
27:X:2495:G:C5	27:X:2496:C:C4	3.06	0.44
27:X:2495:G:N2	27:X:2548:G:H1'	2.33	0.44
1:A:36:ALA:HB1	1:A:63:ARG:HA	2.00	0.44
1:A:161:THR:H	1:A:196:VAL:CG2	2.30	0.44
5:E:6:LYS:HE2	5:E:6:LYS:HB2	1.84	0.44
7:H:2:ILE:HG12	7:H:45:ALA:O	2.17	0.44
7:H:75:VAL:HG12	7:H:118:LEU:HD11	1.99	0.44
10:K:17:ARG:HE	10:K:18:VAL:HG23	1.82	0.44
15:P:62:ARG:HD3	27:X:1993:G:OP1	2.18	0.44
19:T:45:PHE:CE2	19:T:77:ARG:HD3	2.53	0.44
27:X:200:A:N1	27:X:420:C:O2'	2.50	0.44
27:X:571:U:C2	27:X:581:A:C8	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1332:G:O2'	27:X:1333:G:H5'	2.17	0.44
28:Y:63:A:H2'	28:Y:64:C:C6	2.53	0.44
1:A:151:LYS:N	27:X:2186:G:O2'	2.50	0.44
1:A:254:THR:O	27:X:1836:C:H5'	2.16	0.44
5:E:165:VAL:HB	5:E:166:GLY:H	1.55	0.44
7:H:38:GLY:HA2	27:X:2627:G:O2'	2.18	0.44
8:I:95:ALA:HA	8:I:100:ARG:HB3	2.00	0.44
11:L:15:ARG:HA	11:L:15:ARG:HD3	1.63	0.44
11:L:60:LYS:H	11:L:60:LYS:HD3	1.83	0.44
13:N:66:ASN:HB2	13:N:70:ARG:NH1	2.33	0.44
14:O:63:HIS:CD2	14:O:91:THR:HB	2.52	0.44
15:P:81:HIS:C	15:P:81:HIS:CD2	2.95	0.44
22:W:12:ARG:HG2	22:W:12:ARG:HH11	1.83	0.44
27:X:799:C:H2'	27:X:800:U:O4'	2.18	0.44
27:X:831:G:H5'	27:X:852:U:OP1	2.17	0.44
27:X:1351:G:C2	27:X:1352:G:C4	3.06	0.44
27:X:1779:C:O5'	27:X:1779:C:H6	2.01	0.44
27:X:2432:A:O2'	27:X:2551:A:H1'	2.16	0.44
6:G:84:ASN:C	6:G:86:ALA:H	2.26	0.44
7:H:9:ASP:HB2	7:H:95:ALA:HB2	1.99	0.44
15:P:34:SER:HG	15:P:122:LYS:NZ	2.16	0.44
27:X:172:A:H5''	27:X:173:A:OP2	2.18	0.44
27:X:461:A:C4	27:X:462:G:C8	3.06	0.44
27:X:683:A:H4'	27:X:684:C:H5''	2.00	0.44
27:X:876:A:H2	27:X:926:C:N4	2.16	0.44
27:X:1333:G:N7	27:X:1342:U:H5'	2.32	0.44
27:X:1357:U:H4'	27:X:1397:A:C6	2.52	0.44
27:X:1430:G:H2'	27:X:1431:U:C6	2.52	0.44
27:X:1551:U:OP2	27:X:1553:G:N2	2.50	0.44
27:X:1573:G:O5'	27:X:1574:A:H5''	2.18	0.44
27:X:1856:U:H2'	27:X:1857:G:C8	2.53	0.44
27:X:2168:A:H2'	27:X:2169:A:O4'	2.17	0.44
27:X:2756:A:H3'	27:X:2756:A:OP1	2.18	0.44
2:B:140:SER:HA	27:X:2035:G:OP1	2.18	0.44
5:E:6:LYS:O	5:E:69:ARG:HG3	2.17	0.44
5:E:11:VAL:HG21	5:E:50:LEU:HB2	1.99	0.44
13:N:20:ARG:HD2	13:N:39:LEU:HD22	1.99	0.44
15:P:116:SER:HB3	27:X:1997:A:H4'	1.99	0.44
17:R:29:HIS:CD2	17:R:51:VAL:HG13	2.52	0.44
17:R:40:LEU:HD23	17:R:40:LEU:HA	1.68	0.44
27:X:70:A:OP2	27:X:111:G:H4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1026:U:H2'	27:X:1027:C:C6	2.52	0.44
27:X:1724:C:C2	27:X:1747:G:C6	3.06	0.44
27:X:1939:U:H1'	27:X:2531:U:OP1	2.17	0.44
27:X:2031:A:H2'	27:X:2032:G:O4'	2.18	0.44
27:X:2260:C:O2'	27:X:2261:G:H5'	2.17	0.44
28:Y:39:C:H5''	28:Y:40:C:C5	2.52	0.44
2:B:9:ILE:HG23	12:M:9:ARG:HB2	1.99	0.44
2:B:95:ILE:HA	2:B:95:ILE:HD13	1.80	0.44
12:M:31:ASP:OD2	12:M:31:ASP:N	2.51	0.44
16:Q:51:ILE:HD11	16:Q:83:ALA:HA	1.99	0.44
27:X:148:C:H2'	27:X:149:A:O4'	2.18	0.44
27:X:334:G:OP1	27:X:349:G:N2	2.50	0.44
27:X:388:G:H2'	27:X:389:G:C8	2.53	0.44
27:X:433:G:N2	27:X:434:C:O2	2.50	0.44
27:X:1030:U:O2	27:X:1155:G:N2	2.51	0.44
27:X:1117:G:H2'	27:X:1118:G:C8	2.50	0.44
27:X:1608:U:H2'	27:X:1609:G:C8	2.53	0.44
27:X:1724:C:C2	27:X:1747:G:C5	3.06	0.44
27:X:1800:A:C6	27:X:1802:A:C6	3.06	0.44
27:X:2241:U:H4'	27:X:2307:A:H2	1.83	0.44
27:X:2261:G:H21	27:X:2369:U:H3	1.65	0.44
1:A:229:VAL:HG21	27:X:797:A:N7	2.33	0.44
1:A:244:ARG:HG2	27:X:1885:C:H5'	1.99	0.44
3:C:54:THR:HB	3:C:73:SER:HB3	2.00	0.44
3:C:147:LYS:HB2	3:C:184:ASP:HB2	2.00	0.44
13:N:2:PRO:HD3	27:X:456:C:P	2.58	0.44
15:P:45:ILE:HD11	15:P:57:LEU:CG	2.48	0.44
27:X:861:G:C4	27:X:862:A:C8	3.06	0.44
27:X:875:G:N2	27:X:928:G:H1'	2.33	0.44
27:X:1454:U:H3	27:X:1567:A:H61	1.66	0.44
27:X:1550:C:H4'	27:X:1551:U:H5	1.82	0.44
27:X:2551:A:H5'	27:X:2553:G:C4'	2.41	0.44
28:Y:63:A:H2'	28:Y:64:C:H6	1.82	0.44
4:D:122:PHE:HD1	4:D:129:ASN:H	1.64	0.43
15:P:118:ASN:ND2	27:X:1995:G:O3'	2.51	0.43
15:P:121:LYS:NZ	27:X:1336:G:OP1	2.47	0.43
17:R:80:LYS:HE3	17:R:80:LYS:HB2	1.79	0.43
24:1:9:ILE:HG13	24:1:10:VAL:N	2.33	0.43
27:X:543:G:C5	27:X:544:U:C4	3.05	0.43
27:X:957:G:H1	27:X:982:C:H42	1.65	0.43
27:X:991:A:H62	27:X:992:A:N6	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1303:U:H2'	27:X:1304:U:C6	2.52	0.43
27:X:1867:A:O2'	27:X:1868:A:H8	2.01	0.43
27:X:2301:A:H2'	27:X:2302:G:O4'	2.18	0.43
1:A:267:ASP:HB3	1:A:270:ILE:HG22	2.00	0.43
3:C:84:PHE:HB3	27:X:597:U:O2'	2.17	0.43
7:H:90:ARG:NH1	12:M:78:GLU:OE1	2.51	0.43
15:P:118:ASN:CG	15:P:120:ILE:H	2.26	0.43
16:Q:63:LYS:HG3	16:Q:64:ARG:N	2.31	0.43
17:R:20:ASP:HB3	17:R:83:LEU:HG	2.00	0.43
17:R:95:ARG:HB2	17:R:104:VAL:HB	2.00	0.43
20:U:22:GLY:N	20:U:39:LYS:HB2	2.33	0.43
27:X:98:U:H4'	27:X:99:U:H5''	2.01	0.43
27:X:346:C:C6	27:X:347:C:H5	2.35	0.43
27:X:500:G:H2'	27:X:501:G:O4'	2.18	0.43
27:X:640:C:H1'	27:X:650:U:H1'	2.00	0.43
27:X:944:A:H2'	27:X:945:G:H8	1.82	0.43
27:X:946:U:H2'	27:X:947:C:C6	2.52	0.43
27:X:1200:G:H2'	27:X:1201:G:O4'	2.17	0.43
27:X:1374:G:N2	27:X:1384:G:H1'	2.32	0.43
27:X:1684:G:H1	27:X:1974:U:H3'	1.83	0.43
27:X:2277:A:H2'	27:X:2278:A:O4'	2.18	0.43
27:X:2483:U:H2'	27:X:2484:G:H5'	2.00	0.43
27:X:2579:A:H2'	27:X:2580:C:H6	1.83	0.43
27:X:2811:G:C5	27:X:2858:A:C6	3.06	0.43
27:X:2869:U:H2'	27:X:2870:C:C6	2.53	0.43
1:A:20:ASP:HB3	1:A:21:PHE:CE2	2.53	0.43
5:E:67:LEU:HD21	27:X:2738:A:C4	2.53	0.43
8:I:59:ARG:CB	27:X:2371:A:H8	2.30	0.43
8:I:73:GLU:CD	8:I:101:ARG:HB2	2.44	0.43
9:J:17:ARG:HB2	27:X:969:U:C5	2.53	0.43
9:J:39:GLU:HB3	9:J:128:ILE:CG2	2.48	0.43
11:L:32:TYR:O	11:L:38:ILE:HA	2.17	0.43
17:R:35:LYS:HE3	17:R:37:LEU:HD21	2.00	0.43
20:U:10:LYS:NZ	20:U:11:LYS:HG3	2.33	0.43
20:U:46:LEU:C	20:U:47:HIS:CG	2.96	0.43
25:2:3:ARG:HD3	25:2:3:ARG:HA	1.49	0.43
27:X:324:C:H2'	27:X:325:U:O4'	2.18	0.43
27:X:439:C:H2'	27:X:440:U:O4'	2.18	0.43
27:X:494:A:C8	27:X:495:C:C5	3.07	0.43
27:X:624:A:H4'	27:X:626:A:H62	1.84	0.43
27:X:1001:A:H1'	27:X:1167:A:N3	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1039:A:H2'	27:X:1040:A:C8	2.53	0.43
27:X:1346:C:H6	27:X:1346:C:O5'	2.01	0.43
27:X:1552:C:O2	27:X:1553:G:N2	2.51	0.43
27:X:1679:U:O2	27:X:2666:U:H5''	2.18	0.43
27:X:1681:A:C2	27:X:2706:U:C2	3.06	0.43
27:X:1773:C:H1'	27:X:2588:U:H5'	2.01	0.43
27:X:2078:G:H1	27:X:2177:U:H3	1.66	0.43
27:X:2691:C:HO2'	27:X:2692:A:P	2.40	0.43
3:C:170:LEU:HD12	3:C:170:LEU:HA	1.84	0.43
5:E:91:GLY:HA3	5:E:94:PHE:CD2	2.53	0.43
6:G:70:PHE:HB3	13:N:64:ARG:CG	2.48	0.43
7:H:129:LEU:O	7:H:131:PRO:HD3	2.18	0.43
11:L:33:ARG:NH2	11:L:38:ILE:HG21	2.33	0.43
11:L:64:LYS:HG3	28:Y:53:G:H5''	1.99	0.43
12:M:28:ARG:H	12:M:28:ARG:HG2	1.61	0.43
13:N:95:LEU:HA	13:N:98:ILE:HD12	2.01	0.43
17:R:97:GLN:CD	17:R:101:GLY:HA2	2.43	0.43
18:S:19:ILE:HG12	18:S:36:ARG:HB2	2.01	0.43
27:X:339:U:O4	27:X:343:A:H8	2.01	0.43
27:X:682:G:H3'	27:X:683:A:C8	2.53	0.43
27:X:958:G:H2'	27:X:959:C:C6	2.54	0.43
27:X:987:G:C2	27:X:988:G:C8	3.07	0.43
27:X:1002:C:H2'	27:X:1003:C:H6	1.84	0.43
27:X:1040:A:C8	27:X:1041:G:C8	3.07	0.43
27:X:1333:G:N2	27:X:1344:C:N4	2.65	0.43
27:X:2015:G:N1	27:X:2551:A:C8	2.87	0.43
27:X:2324:G:N3	27:X:2360:C:H2'	2.34	0.43
27:X:2526:U:H2'	27:X:2527:G:H8	1.83	0.43
27:X:2571:G:H2'	27:X:2572:U:O4'	2.18	0.43
1:A:222:ARG:HE	1:A:222:ARG:HB2	1.61	0.43
3:C:94:THR:OG1	27:X:618:A:OP1	2.27	0.43
7:H:23:ARG:NH1	7:H:40:GLY:O	2.51	0.43
8:I:75:VAL:HG22	8:I:99:VAL:HG11	2.00	0.43
8:I:94:GLU:H	8:I:94:GLU:HG2	1.39	0.43
9:J:39:GLU:HA	9:J:40:PRO:HD3	1.75	0.43
9:J:137:VAL:HG11	18:S:71:MET:SD	2.58	0.43
13:N:3:ARG:HB2	27:X:1261:G:C8	2.53	0.43
14:O:10:LYS:HZ1	14:O:13:ARG:HH12	1.66	0.43
14:O:38:LEU:HD22	14:O:39:PHE:H	1.83	0.43
14:O:65:ARG:HE	14:O:87:ARG:HD3	1.84	0.43
15:P:19:LYS:NZ	27:X:507:A:OP2	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:14:GLU:OE2	27:X:1405:A:N6	2.45	0.43
17:R:17:LYS:HG2	17:R:18:LYS:HD3	1.99	0.43
21:V:42:ARG:HG3	21:V:46:LEU:HD12	2.01	0.43
27:X:50:G:H4'	27:X:51:A:O5'	2.18	0.43
27:X:411:C:OP1	27:X:2073:A:O2'	2.32	0.43
27:X:503:G:H2'	27:X:504:G:O4'	2.18	0.43
27:X:681:A:H2'	27:X:683:A:H62	1.82	0.43
27:X:770:U:C4	27:X:771:C:C5	3.06	0.43
27:X:933:G:H2'	27:X:934:G:H8	1.82	0.43
27:X:1066:G:H2'	27:X:1067:G:O4'	2.18	0.43
27:X:1179:A:H2'	27:X:1180:A:C8	2.53	0.43
27:X:1395:A:H2'	27:X:1396:C:H6	1.84	0.43
27:X:1429:A:N6	27:X:1600:U:H4'	2.33	0.43
27:X:2026:C:H2'	27:X:2027:C:H6	1.84	0.43
27:X:2796:A:O2'	27:X:2801:A:N1	2.41	0.43
2:B:136:ARG:O	2:B:137:ARG:C	2.61	0.43
2:B:144:ARG:HH11	27:X:2551:A:H2'	1.84	0.43
3:C:112:GLN:NE2	3:C:116:LYS:HG2	2.34	0.43
5:E:105:MET:HE2	5:E:105:MET:HB3	1.89	0.43
6:G:106:TYR:CE2	6:G:108:GLY:HA2	2.54	0.43
9:J:82:THR:HB	9:J:83:ARG:H	1.33	0.43
9:J:83:ARG:HD3	9:J:83:ARG:HA	1.66	0.43
17:R:18:LYS:HD2	27:X:83:A:H3'	2.00	0.43
17:R:90:LYS:HE3	17:R:108:VAL:HB	2.00	0.43
19:T:69:PHE:CZ	19:T:79:ILE:HD11	2.54	0.43
27:X:617:U:C5	27:X:632:A:N1	2.87	0.43
27:X:638:A:H4'	27:X:639:G:H5'	2.00	0.43
27:X:2065:A:H3'	27:X:2066:G:H8	1.84	0.43
27:X:2252:A:H2'	27:X:2253:A:C8	2.54	0.43
27:X:2354:G:N2	27:X:2357:A:OP2	2.52	0.43
27:X:2820:C:H2'	27:X:2821:G:C8	2.53	0.43
27:X:2838:U:H2'	27:X:2839:G:H8	1.83	0.43
3:C:16:GLU:H	3:C:16:GLU:HG3	1.59	0.43
3:C:68:ARG:NH1	27:X:2043:A:H62	2.08	0.43
11:L:28:ARG:O	11:L:43:ILE:HD12	2.19	0.43
12:M:17:GLU:HG3	12:M:62:SER:H	1.84	0.43
13:N:37:GLN:HE21	27:X:1265:G:H22	1.67	0.43
17:R:38:LEU:HD23	17:R:38:LEU:HA	1.74	0.43
19:T:40:GLN:NE2	19:T:43:THR:HA	2.32	0.43
20:U:78:ILE:HG12	20:U:79:GLU:N	2.33	0.43
27:X:796:A:C8	27:X:797:A:H4'	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1217:U:H2'	27:X:1218:C:C6	2.53	0.43
27:X:1336:G:C2'	27:X:1337:G:H5'	2.46	0.43
27:X:1674:C:H2'	27:X:1675:C:H6	1.83	0.43
27:X:1882:G:H21	27:X:1885:C:H41	1.63	0.43
27:X:2057:U:O3'	27:X:2576:G:O2'	2.36	0.43
27:X:2563:U:O2'	27:X:2564:U:H5'	2.18	0.43
9:J:40:PRO:HB3	9:J:99:LYS:HD2	1.99	0.43
9:J:88:LYS:NZ	27:X:968:C:OP2	2.51	0.43
11:L:32:TYR:CG	28:Y:9:G:H4'	2.54	0.43
12:M:34:ARG:HH22	12:M:90:GLN:C	2.17	0.43
21:V:26:MET:HA	21:V:29:ARG:HB2	2.01	0.43
27:X:45:C:OP2	27:X:192:G:H2'	2.18	0.43
27:X:318:G:N1	27:X:321:A:OP2	2.52	0.43
27:X:746:G:C8	27:X:774:A:C6	3.06	0.43
27:X:1361:G:H1	27:X:1614:C:H42	1.66	0.43
27:X:1663:C:H5''	27:X:1664:G:H5''	2.01	0.43
27:X:1987:G:C6	27:X:1988:A:C4	3.06	0.43
27:X:2434:G:C6	27:X:2435:C:N4	2.87	0.43
27:X:2492:G:C2	27:X:2493:U:C2	3.07	0.43
27:X:2519:C:O2	27:X:2720:A:H2	2.01	0.43
27:X:2768:C:O2'	27:X:2784:A:N3	2.44	0.43
27:X:2810:A:N6	27:X:2853:U:H2'	2.33	0.43
1:A:252:LYS:HG2	27:X:1816:G:O2'	2.18	0.43
2:B:14:ILE:O	2:B:21:ILE:N	2.46	0.43
3:C:48:ARG:C	3:C:50:GLN:N	2.76	0.43
4:D:130:LEU:O	27:X:2283:G:O2'	2.33	0.43
11:L:29:LEU:HA	11:L:42:ILE:HD13	2.01	0.43
11:L:32:TYR:CE2	28:Y:9:G:H5'	2.54	0.43
13:N:24:PHE:CE1	27:X:543:G:H5'	2.54	0.43
15:P:127:ILE:HG22	15:P:128:THR:N	2.34	0.43
19:T:34:GLY:HA3	27:X:2332:G:H1'	2.00	0.43
27:X:492:G:O2'	27:X:493:A:P	2.77	0.43
27:X:554:U:H5''	27:X:556:A:N3	2.34	0.43
27:X:1054:C:N4	27:X:1055:A:N1	2.67	0.43
27:X:2056:C:O2'	27:X:2057:U:H5'	2.19	0.43
27:X:2201:G:H2'	27:X:2202:G:C8	2.53	0.43
27:X:2266:A:H62	27:X:2323:U:H3	1.65	0.43
27:X:2668:U:OP2	27:X:2847:G:N2	2.43	0.43
6:G:132:PHE:CZ	6:G:142:ARG:HA	2.53	0.43
11:L:45:ASP:OD1	11:L:45:ASP:N	2.31	0.43
21:V:32:ALA:HB2	21:V:37:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:533:C:O2	27:X:563:U:O2'	2.36	0.43
27:X:938:G:C2'	27:X:939:C:H5''	2.48	0.43
27:X:1184:G:H3'	27:X:1185:C:H5''	2.00	0.43
27:X:1361:G:H1	27:X:1614:C:N4	2.17	0.43
1:A:173:VAL:HG12	1:A:175:VAL:HG13	2.01	0.42
1:A:214:TRP:CD1	27:X:1582:A:C8	3.07	0.42
1:A:226:MET:HB3	1:A:230:ASP:HB2	2.01	0.42
2:B:7:THR:O	2:B:9:ILE:HG13	2.18	0.42
3:C:74:VAL:HG23	3:C:76:THR:N	2.24	0.42
4:D:41:GLY:HA2	4:D:45:GLU:HB2	2.00	0.42
7:H:34:LEU:HG	7:H:101:ASN:O	2.19	0.42
10:K:10:LEU:HD21	10:K:17:ARG:HG2	2.01	0.42
12:M:98:LYS:HE3	12:M:99:VAL:N	2.34	0.42
15:P:31:VAL:N	15:P:124:THR:HB	2.34	0.42
15:P:100:GLY:HA2	27:X:25:U:H5'	2.00	0.42
18:S:104:SER:OG	18:S:113:VAL:HG21	2.18	0.42
23:Z:45:ILE:HG21	23:Z:57:VAL:HG23	2.01	0.42
27:X:306:G:N2	27:X:355:G:H1'	2.34	0.42
27:X:513:A:C6	27:X:515:A:C6	3.07	0.42
27:X:539:A:OP1	27:X:539:A:H4'	2.18	0.42
27:X:1693:A:H2'	27:X:1694:A:O4'	2.18	0.42
27:X:1715:A:C8	27:X:1717:A:O4'	2.72	0.42
27:X:2370:G:O6	27:X:2406:C:H1'	2.19	0.42
27:X:2394:G:C2	27:X:2395:C:C2	3.07	0.42
2:B:77:ILE:HD13	2:B:195:LEU:HD22	2.01	0.42
4:D:75:SER:OG	27:X:2289:A:H1'	2.20	0.42
5:E:60:LYS:H	5:E:60:LYS:HG2	1.68	0.42
6:G:153:GLY:C	6:G:157:PRO:HG2	2.44	0.42
11:L:16:LYS:HE3	11:L:28:ARG:NH1	2.32	0.42
13:N:13:ARG:CZ	27:X:1264:C:H5''	2.49	0.42
15:P:123:ARG:H	15:P:123:ARG:CD	2.32	0.42
16:Q:11:VAL:HG21	16:Q:77:LYS:HE3	2.00	0.42
16:Q:28:TRP:CD2	16:Q:75:ARG:HD2	2.53	0.42
20:U:21:ARG:NH2	20:U:23:LYS:HB3	2.34	0.42
27:X:563:U:H2'	27:X:564:U:O4'	2.19	0.42
27:X:1250:A:H2'	27:X:1251:G:O4'	2.18	0.42
27:X:1279:G:O2'	27:X:1995:G:O6	2.16	0.42
27:X:2228:U:H4'	27:X:2254:C:C5	2.54	0.42
27:X:2572:U:H2'	27:X:2573:C:H6	1.84	0.42
28:Y:71:G:C6	28:Y:72:C:C4	3.07	0.42
3:C:170:LEU:HA	3:C:171:PRO:HD3	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:46:HIS:CD2	7:H:49:ASP:OD2	2.72	0.42
11:L:13:THR:HG22	27:X:2313:G:C2	2.54	0.42
13:N:13:ARG:NH2	27:X:1264:C:H5''	2.34	0.42
13:N:17:VAL:HG21	13:N:32:TYR:HE1	1.84	0.42
13:N:62:ILE:HG23	13:N:76:TYR:CE1	2.55	0.42
18:S:101:THR:HG21	18:S:135:VAL:HG13	2.00	0.42
27:X:310:A:N1	27:X:333:A:O2'	2.45	0.42
27:X:742:G:H2'	27:X:1766:U:H1'	2.00	0.42
27:X:762:A:H2	27:X:766:A:HO2'	1.65	0.42
27:X:1703:C:H2'	27:X:1704:G:O4'	2.20	0.42
27:X:1724:C:N3	27:X:1747:G:C6	2.88	0.42
27:X:1780:A:H2'	27:X:1781:C:C6	2.54	0.42
27:X:2043:A:O4'	27:X:2481:G:H1'	2.18	0.42
27:X:2377:U:H3	27:X:2397:A:H61	1.68	0.42
1:A:69:ARG:CZ	1:A:130:ALA:HB2	2.49	0.42
2:B:39:ALA:HA	2:B:44:TYR:N	2.34	0.42
3:C:171:PRO:HB2	3:C:172:VAL:HG23	2.01	0.42
6:G:30:LYS:HB2	6:G:30:LYS:NZ	2.34	0.42
7:H:75:VAL:HG23	7:H:76:ARG:HG3	2.01	0.42
9:J:83:ARG:NH1	27:X:971:A:H61	2.17	0.42
15:P:39:ARG:CZ	15:P:97:VAL:HG12	2.49	0.42
15:P:122:LYS:H	15:P:122:LYS:HG3	1.39	0.42
16:Q:89:GLU:HB3	16:Q:90:ALA:H	1.57	0.42
25:2:33:ARG:O	25:2:37:LYS:HG3	2.19	0.42
26:3:12:ARG:HG2	26:3:13:ARG:N	2.35	0.42
26:3:15:LYS:HA	26:3:15:LYS:HD3	1.62	0.42
26:3:36:LYS:HD2	26:3:36:LYS:HA	1.80	0.42
27:X:29:U:H2'	27:X:30:G:H8	1.83	0.42
27:X:656:U:H4'	27:X:657:A:C8	2.54	0.42
27:X:661:C:C2	27:X:662:G:N7	2.88	0.42
27:X:1332:G:C2	27:X:1333:G:C2	3.07	0.42
27:X:1827:G:H1	27:X:1888:C:H42	1.67	0.42
27:X:2078:G:H2'	27:X:2079:A:C8	2.55	0.42
27:X:2792:C:H2'	27:X:2793:G:O4'	2.19	0.42
2:B:152:LYS:NZ	27:X:2598:C:OP1	2.34	0.42
3:C:163:ASN:ND2	3:C:166:TRP:N	2.66	0.42
5:E:121:VAL:HG11	5:E:144:VAL:HG21	2.02	0.42
8:I:38:LYS:HG2	27:X:954:U:OP2	2.19	0.42
13:N:2:PRO:HD3	27:X:456:C:O5'	2.19	0.42
13:N:51:ARG:H	13:N:51:ARG:HG2	1.73	0.42
14:O:64:GLY:HA3	14:O:90:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:28:ARG:HA	25:2:31:LEU:HB2	2.02	0.42
27:X:13:A:N3	27:X:15:G:C6	2.88	0.42
27:X:242:A:C8	27:X:441:A:N6	2.87	0.42
27:X:405:C:H2'	27:X:406:G:H8	1.84	0.42
27:X:947:C:H2'	27:X:948:C:C6	2.54	0.42
27:X:1469:U:H5'	27:X:1470:G:OP2	2.20	0.42
27:X:1692:C:C5	27:X:1693:A:C4	3.07	0.42
27:X:1774:A:C6	27:X:2566:A:C2	3.08	0.42
27:X:2528:G:H2'	27:X:2529:G:C8	2.53	0.42
27:X:2848:A:O2'	27:X:2849:C:H5'	2.18	0.42
1:A:107:ALA:HA	1:A:108:PRO:HD2	1.74	0.42
2:B:122:PHE:HB3	2:B:123:ALA:H	1.53	0.42
2:B:156:MET:HE1	27:X:2033:C:H1'	2.02	0.42
4:D:79:LEU:HD11	27:X:2289:A:H2	1.82	0.42
4:D:118:ASN:HB3	4:D:122:PHE:HZ	1.84	0.42
5:E:139:GLN:HG2	27:X:2726:U:H4'	2.02	0.42
9:J:17:ARG:HD3	27:X:969:U:C2	2.54	0.42
14:O:11:GLN:HE21	14:O:12:TYR:N	2.17	0.42
14:O:88:GLN:HE21	14:O:88:GLN:HB3	1.68	0.42
25:2:16:HIS:O	25:2:43:THR:OG1	2.24	0.42
27:X:21:A:C6	27:X:530:G:C6	3.08	0.42
27:X:167:A:C6	27:X:168:A:C6	3.08	0.42
27:X:171:G:H2'	27:X:172:A:O4'	2.20	0.42
27:X:343:A:H1'	27:X:346:C:N4	2.34	0.42
27:X:488:A:H8	27:X:488:A:OP1	2.02	0.42
27:X:1378:A:H5'	27:X:1379:A:OP2	2.19	0.42
27:X:1480:G:H2'	27:X:1481:U:O4'	2.19	0.42
27:X:2226:A:H2'	27:X:2227:C:C6	2.54	0.42
27:X:2721:A:H2'	27:X:2722:C:O4'	2.19	0.42
27:X:2746:G:H2'	27:X:2746:G:N3	2.35	0.42
1:A:261:ARG:NH2	27:X:1791:C:OP1	2.52	0.42
5:E:44:ARG:NH2	5:E:46:ASP:HB2	2.35	0.42
7:H:47:VAL:HB	7:H:117:GLU:OE1	2.19	0.42
10:K:18:VAL:HG12	10:K:19:ALA:N	2.35	0.42
15:P:45:ILE:HD11	15:P:57:LEU:HG	2.02	0.42
26:3:61:MET:O	26:3:64:ARG:HG3	2.20	0.42
27:X:514:G:H4'	27:X:515:A:OP2	2.20	0.42
27:X:1332:G:C5	27:X:1333:G:C6	3.07	0.42
27:X:1451:C:H1'	27:X:1532:A:C2	2.53	0.42
27:X:1574:A:H2'	27:X:1575:C:H5''	2.01	0.42
27:X:1964:A:H5''	27:X:1965:U:OP2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2441:U:H6	27:X:2441:U:O5'	2.02	0.42
1:A:18:THR:HG21	1:A:20:ASP:OD2	2.20	0.42
2:B:38:THR:O	2:B:42:ASP:HB2	2.19	0.42
3:C:164:VAL:HG13	27:X:335:A:OP1	2.19	0.42
3:C:191:ALA:HA	3:C:194:GLU:HB3	2.01	0.42
7:H:9:ASP:O	7:H:96:ALA:N	2.50	0.42
8:I:17:LYS:HE3	27:X:1257:U:OP1	2.20	0.42
9:J:120:ARG:NH2	27:X:2447:G:OP1	2.52	0.42
13:N:31:GLN:HB3	27:X:590:C:OP1	2.20	0.42
14:O:10:LYS:HZ3	14:O:11:GLN:HB2	1.85	0.42
19:T:15:ASP:O	19:T:16:SER:OG	2.34	0.42
20:U:54:ASN:OD1	20:U:77:GLY:HA2	2.19	0.42
21:V:26:MET:HE2	21:V:26:MET:HB3	1.90	0.42
24:1:38:LYS:HE2	24:1:40:TYR:HE1	1.85	0.42
27:X:478:G:H2'	27:X:479:G:O4'	2.20	0.42
27:X:568:G:H2'	27:X:569:C:O4'	2.20	0.42
27:X:758:G:C2'	27:X:759:C:H5'	2.49	0.42
27:X:1124:U:H2'	27:X:1125:G:H8	1.85	0.42
27:X:1386:A:OP1	27:X:2191:A:N6	2.42	0.42
27:X:1467:U:H3'	27:X:1467:U:C6	2.55	0.42
27:X:1731:C:N3	27:X:1735:G:N1	2.68	0.42
27:X:2526:U:H2'	27:X:2527:G:C8	2.54	0.42
27:X:2794:G:O2'	27:X:2795:A:H5''	2.20	0.42
28:Y:54:U:C4	28:Y:55:C:C4	3.08	0.42
2:B:37:LYS:HD2	2:B:42:ASP:CG	2.45	0.42
2:B:84:PHE:C	2:B:86:PRO:HD3	2.45	0.42
2:B:155:ARG:HH11	2:B:155:ARG:HG3	1.84	0.42
3:C:33:TRP:CE2	3:C:95:LEU:HB2	2.55	0.42
7:H:76:ARG:HB3	7:H:91:PHE:HD1	1.85	0.42
8:I:55:ARG:H	8:I:55:ARG:HG2	1.69	0.42
10:K:63:ARG:HD3	27:X:1469:U:O2	2.20	0.42
13:N:15:LYS:NZ	27:X:1230:C:OP1	2.44	0.42
13:N:61:TRP:O	13:N:65:ILE:HG13	2.19	0.42
17:R:44:GLN:HE21	17:R:78:ALA:HB2	1.84	0.42
24:1:38:LYS:HD2	27:X:2265:A:N6	2.34	0.42
27:X:1073:G:N2	27:X:1087:C:H42	2.12	0.42
27:X:1675:C:H2'	27:X:1676:U:H6	1.84	0.42
27:X:1713:G:C6	27:X:1714:A:C5	3.08	0.42
27:X:1776:A:C8	27:X:1778:U:C5	3.08	0.42
27:X:1935:A:C5	27:X:1936:A:N1	2.88	0.42
27:X:2504:G:C2	27:X:2518:C:C2	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:4:PRO:HD3	7:H:24:VAL:HG23	2.02	0.42
7:H:134:LEU:HA	7:H:134:LEU:HD23	1.72	0.42
8:I:93:LEU:O	8:I:97:ARG:HG3	2.20	0.42
13:N:20:ARG:HH22	14:O:72:ARG:HD3	1.85	0.42
15:P:14:ARG:NE	27:X:514:G:O6	2.51	0.42
15:P:32:ARG:HG3	27:X:1335:A:OP1	2.20	0.42
18:S:73:LYS:O	18:S:74:ARG:HB2	2.20	0.42
22:W:23:LEU:HD23	22:W:23:LEU:HA	1.85	0.42
26:3:13:ARG:HG3	26:3:13:ARG:O	2.20	0.42
26:3:13:ARG:CZ	26:3:25:PHE:HB2	2.50	0.42
26:3:49:VAL:HG13	27:X:2339:A:OP1	2.20	0.42
27:X:304:A:C6	27:X:359:G:C2	3.08	0.42
27:X:314:G:H2'	27:X:315:G:H8	1.84	0.42
27:X:486:U:H4'	27:X:519:C:H2'	2.01	0.42
27:X:513:A:C6	27:X:516:G:C6	3.08	0.42
27:X:537:C:O2'	27:X:538:A:C4	2.62	0.42
27:X:580:A:C8	27:X:2013:A:N6	2.88	0.42
27:X:988:G:N3	27:X:1012:A:H2	2.18	0.42
27:X:1312:G:H5'	27:X:1314:A:O4'	2.20	0.42
27:X:1402:G:H2'	27:X:1403:U:O4'	2.20	0.42
27:X:1539:U:H2'	27:X:1540:C:H6	1.84	0.42
27:X:1625:A:H1'	27:X:1632:A:O4'	2.20	0.42
27:X:2010:G:H1'	27:X:2020:G:N2	2.34	0.42
27:X:2270:U:H2'	27:X:2271:C:C6	2.55	0.42
2:B:168:GLN:O	27:X:2710:C:O2'	2.24	0.41
3:C:23:ASN:O	3:C:27:LEU:HD13	2.20	0.41
6:G:49:VAL:HG12	6:G:50:PRO:O	2.20	0.41
7:H:5:GLN:HG2	27:X:1685:A:H5''	2.01	0.41
10:K:99:ARG:HG2	10:K:99:ARG:HH11	1.84	0.41
14:O:26:GLN:HG2	14:O:27:GLY:N	2.34	0.41
15:P:27:VAL:HG23	15:P:126:HIS:O	2.19	0.41
15:P:90:LEU:HD22	15:P:131:VAL:HG12	2.02	0.41
16:Q:43:GLN:HG2	16:Q:48:VAL:O	2.20	0.41
27:X:456:C:H2'	27:X:457:C:H6	1.84	0.41
27:X:875:G:O2'	28:Y:80:A:N3	2.53	0.41
27:X:1152:C:H4'	27:X:1153:A:OP2	2.20	0.41
27:X:1310:C:C2	27:X:1311:C:C5	3.08	0.41
27:X:1469:U:H5''	27:X:1470:G:C8	2.55	0.41
27:X:1544:A:C4	27:X:1560:A:C6	3.08	0.41
27:X:1852:G:H2'	27:X:1853:C:C6	2.54	0.41
27:X:1948:C:H3'	27:X:1949:A:H8	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2262:C:C2	27:X:2368:G:C2	3.08	0.41
27:X:2387:U:H2'	27:X:2388:G:C8	2.55	0.41
27:X:2533:U:H2'	27:X:2534:U:C6	2.55	0.41
27:X:2871:U:H2'	27:X:2872:U:C6	2.54	0.41
28:Y:46:G:H21	28:Y:50:U:H1'	1.85	0.41
1:A:219:PRO:HG2	27:X:1782:A:OP1	2.19	0.41
1:A:251:GLY:HA3	1:A:255:LYS:CE	2.50	0.41
3:C:84:PHE:CE1	27:X:596:C:H5''	2.54	0.41
4:D:40:LEU:HD23	4:D:41:GLY:N	2.36	0.41
6:G:67:ARG:CD	6:G:70:PHE:HA	2.50	0.41
11:L:31:VAL:HG11	11:L:89:PHE:CZ	2.55	0.41
13:N:46:GLU:HG3	27:X:544:U:H4'	2.02	0.41
13:N:59:ARG:NH1	27:X:1019:U:H1'	2.35	0.41
14:O:5:ILE:N	14:O:10:LYS:HE3	2.36	0.41
14:O:11:GLN:H	14:O:37:ALA:HB3	1.84	0.41
14:O:39:PHE:CE2	14:O:46:VAL:HB	2.55	0.41
15:P:44:VAL:HG11	23:Z:27:ALA:HB2	2.01	0.41
16:Q:4:TYR:CD2	21:V:23:LYS:HB2	2.54	0.41
22:W:3:ILE:HD12	22:W:3:ILE:HA	1.64	0.41
23:Z:36:CYS:SG	23:Z:46:CYS:SG	3.10	0.41
26:3:23:MET:HA	26:3:48:PHE:CD2	2.55	0.41
27:X:36:G:N3	27:X:462:G:O2'	2.52	0.41
27:X:224:G:C2	27:X:229:G:C6	3.08	0.41
27:X:343:A:O2'	27:X:346:C:N4	2.53	0.41
27:X:537:C:O2	27:X:537:C:H2'	2.19	0.41
27:X:670:U:H2'	27:X:671:A:H8	1.84	0.41
27:X:1033:G:O2'	27:X:1035:G:O6	2.29	0.41
27:X:1281:A:H2'	27:X:1282:A:O4'	2.20	0.41
27:X:1481:U:H4'	27:X:1562:G:H21	1.85	0.41
27:X:1824:C:N4	27:X:1825:C:C4	2.88	0.41
27:X:1997:A:H2'	27:X:1998:A:C8	2.55	0.41
27:X:2791:C:O2'	27:X:2792:C:H5'	2.19	0.41
28:Y:48:A:C6	28:Y:49:C:C5	3.07	0.41
1:A:249:PRO:HD3	27:X:2218:G:H5'	2.02	0.41
4:D:77:PHE:O	4:D:79:LEU:HD12	2.20	0.41
8:I:49:PHE:HE2	27:X:229:G:OP1	2.03	0.41
8:I:102:LYS:C	8:I:104:ARG:H	2.28	0.41
9:J:34:GLY:HA2	9:J:106:GLU:HA	2.02	0.41
13:N:13:ARG:O	13:N:16:LYS:HB2	2.20	0.41
13:N:39:LEU:O	14:O:72:ARG:NH2	2.33	0.41
13:N:45:TYR:O	13:N:49:ASP:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:22:LYS:N	27:X:506:G:OP1	2.52	0.41
18:S:22:VAL:O	18:S:83:PHE:HB2	2.19	0.41
19:T:24:LYS:HA	19:T:24:LYS:HD3	1.84	0.41
19:T:60:PHE:CE1	27:X:2344:G:H4'	2.55	0.41
24:1:35:LEU:HB3	24:1:37:LEU:HG	2.02	0.41
27:X:10:A:H2'	27:X:11:G:O4'	2.20	0.41
27:X:836:G:C4	27:X:837:U:C5	3.08	0.41
27:X:1039:A:H61	27:X:1136:G:H2'	1.85	0.41
27:X:1303:U:H2'	27:X:1304:U:H6	1.84	0.41
27:X:1672:A:H3'	27:X:1673:C:H6	1.85	0.41
27:X:1682:A:H2'	27:X:1683:G:O4'	2.21	0.41
27:X:1740:G:H2'	27:X:1741:G:H8	1.84	0.41
1:A:85:ASP:HB2	1:A:92:ILE:HD12	2.01	0.41
3:C:7:ILE:HB	3:C:121:ASP:HB2	2.01	0.41
4:D:16:LEU:HD12	4:D:28:VAL:HG13	2.01	0.41
4:D:83:MET:O	4:D:85:VAL:N	2.53	0.41
13:N:76:TYR:CZ	13:N:80:ILE:HG13	2.56	0.41
15:P:31:VAL:HG21	15:P:127:ILE:HD13	2.02	0.41
17:R:96:LYS:O	17:R:104:VAL:HA	2.19	0.41
21:V:17:GLU:HB3	21:V:53:LEU:HD11	2.02	0.41
27:X:307:C:C2'	27:X:308:C:H5'	2.51	0.41
27:X:825:C:H1'	27:X:1263:G:N2	2.35	0.41
27:X:859:U:O2'	27:X:860:U:O2	2.31	0.41
27:X:1322:G:H21	27:X:1627:C:H5'	1.86	0.41
27:X:1330:G:C4	27:X:1331:G:C8	3.09	0.41
27:X:1925:C:C4	27:X:1926:U:N3	2.88	0.41
27:X:1975:G:O2'	27:X:1976:U:OP2	2.29	0.41
27:X:2660:C:C2	27:X:2704:U:O4	2.74	0.41
28:Y:34:C:H1'	28:Y:54:U:O4	2.20	0.41
2:B:51:TYR:N	2:B:75:THR:OG1	2.53	0.41
2:B:60:ASN:CG	2:B:62:PRO:HD2	2.45	0.41
3:C:189:ASP:HB3	3:C:190:ALA:H	1.63	0.41
4:D:64:LYS:HG2	4:D:65:PRO:O	2.21	0.41
5:E:133:VAL:HG11	5:E:144:VAL:HG11	2.02	0.41
6:G:91:THR:HB	6:G:92:GLY:H	1.76	0.41
6:G:154:GLU:C	6:G:157:PRO:HD2	2.46	0.41
7:H:100:ASN:ND2	7:H:104:GLU:HG3	2.36	0.41
13:N:96:ALA:O	13:N:99:ALA:N	2.53	0.41
14:O:10:LYS:HZ2	14:O:13:ARG:HH12	1.67	0.41
14:O:11:GLN:CD	14:O:38:LEU:HB3	2.45	0.41
15:P:46:ARG:HA	15:P:92:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:89:ARG:HG2	15:P:134:LYS:H	1.85	0.41
22:W:2:LYS:HD3	22:W:33:GLU:OE1	2.20	0.41
27:X:246:C:H1'	27:X:437:G:H22	1.85	0.41
27:X:658:G:H2'	27:X:659:G:C8	2.55	0.41
27:X:1128:G:H2'	27:X:1129:A:H5''	2.03	0.41
27:X:1210:C:C2	27:X:1211:G:C8	3.08	0.41
27:X:1623:C:H5''	27:X:1624:A:H5'	2.02	0.41
27:X:1643:A:N6	27:X:1656:U:H3	2.17	0.41
27:X:1734:C:H5'	27:X:1735:G:OP2	2.20	0.41
27:X:2856:U:H2'	27:X:2857:C:C6	2.55	0.41
1:A:161:THR:HG21	27:X:1811:A:H3'	2.02	0.41
5:E:89:LEU:HD23	5:E:89:LEU:HA	1.89	0.41
5:E:107:ILE:HD11	5:E:151:VAL:HG12	2.02	0.41
6:G:103:TYR:CD2	27:X:1142:G:O4'	2.73	0.41
8:I:71:THR:O	8:I:104:ARG:HB3	2.20	0.41
8:I:129:ALA:O	8:I:133:VAL:HG23	2.21	0.41
11:L:15:ARG:HH21	27:X:2272:A:P	2.43	0.41
11:L:64:LYS:HA	11:L:64:LYS:HD3	1.89	0.41
13:N:90:LEU:HD23	13:N:92:ARG:HG3	2.02	0.41
14:O:62:GLU:HG2	14:O:63:HIS:N	2.36	0.41
18:S:64:ALA:HB2	18:S:85:MET:HG2	2.02	0.41
20:U:25:ARG:HD3	20:U:25:ARG:HA	1.79	0.41
24:1:51:ARG:HH11	24:1:51:ARG:HB2	1.86	0.41
27:X:13:A:H1'	27:X:14:A:N7	2.34	0.41
27:X:648:A:H2	27:X:649:G:H21	1.68	0.41
27:X:717:G:H1'	27:X:739:G:H22	1.83	0.41
27:X:832:A:C5	27:X:833:A:C8	3.09	0.41
27:X:930:A:H4'	28:Y:100:G:N3	2.36	0.41
27:X:1059:A:HO2'	27:X:1060:C:P	2.41	0.41
27:X:1255:A:H2'	27:X:1256:C:C6	2.55	0.41
27:X:1333:G:N2	27:X:1344:C:H41	2.19	0.41
27:X:1958:G:H2'	27:X:1959:U:C6	2.55	0.41
27:X:2062:U:H2'	27:X:2063:A:C8	2.55	0.41
1:A:262:LYS:H	1:A:262:LYS:HE2	1.86	0.41
2:B:105:THR:HG22	2:B:166:THR:OG1	2.21	0.41
4:D:38:GLU:HB3	4:D:87:ILE:HB	2.02	0.41
6:G:75:ILE:HB	6:G:147:ARG:NH1	2.36	0.41
7:H:23:ARG:HE	27:X:2540:A:H2	1.69	0.41
13:N:17:VAL:HG11	13:N:36:PHE:HB2	2.02	0.41
15:P:104:LYS:HZ3	15:P:119:ILE:HG22	1.85	0.41
16:Q:63:LYS:HB2	16:Q:69:ILE:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:94:VAL:HA	27:X:309:G:OP1	2.20	0.41
18:S:38:ALA:HA	18:S:41:ARG:HB3	2.03	0.41
25:2:16:HIS:HB3	25:2:43:THR:OG1	2.21	0.41
27:X:39:C:H2'	27:X:40:U:C6	2.55	0.41
27:X:144:U:H2'	27:X:145:C:H6	1.85	0.41
27:X:321:A:N6	27:X:323:G:N3	2.68	0.41
27:X:587:A:H2'	27:X:588:G:H5''	2.03	0.41
27:X:669:G:H8	27:X:669:G:OP2	2.04	0.41
27:X:825:C:H2'	27:X:826:U:H6	1.86	0.41
27:X:2250:G:H2'	27:X:2251:U:C6	2.56	0.41
1:A:206:LEU:HD23	1:A:206:LEU:HA	1.94	0.41
3:C:39:ARG:HH21	3:C:91:TYR:CB	2.33	0.41
4:D:108:LEU:HA	4:D:111:ILE:HD11	2.03	0.41
7:H:3:MET:HE1	27:X:1683:G:N2	2.28	0.41
7:H:10:VAL:HG23	7:H:17:ARG:O	2.21	0.41
7:H:116:ARG:HD3	12:M:40:ARG:HB2	2.02	0.41
8:I:84:GLU:HB3	8:I:85:ASP:H	1.59	0.41
10:K:36:THR:HG23	10:K:37:THR:O	2.21	0.41
11:L:31:VAL:HG21	11:L:100:VAL:HG23	2.02	0.41
20:U:51:ILE:H	20:U:52:ARG:NH2	2.18	0.41
23:Z:51:TYR:CD2	23:Z:55:ARG:HB2	2.55	0.41
26:3:30:ARG:HH21	26:3:31:HIS:CD2	2.39	0.41
27:X:537:C:H1'	27:X:538:A:C5	2.55	0.41
27:X:545:C:H2'	27:X:546:A:C8	2.55	0.41
27:X:676:G:C6	27:X:677:G:C5	3.09	0.41
27:X:829:C:H2'	27:X:830:C:O4'	2.21	0.41
27:X:1035:G:C6	27:X:1036:G:C6	3.09	0.41
27:X:1287:A:N3	27:X:1310:C:H1'	2.36	0.41
27:X:1578:U:H2'	27:X:1579:G:C8	2.56	0.41
27:X:1640:C:H2'	27:X:1641:C:H6	1.86	0.41
27:X:1655:C:H4'	27:X:2689:C:O2	2.20	0.41
27:X:1693:A:N6	27:X:1694:A:C6	2.88	0.41
27:X:1965:U:H2'	27:X:1966:C:C6	2.54	0.41
27:X:2039:G:H2'	27:X:2039:G:N3	2.36	0.41
2:B:151:TYR:HD1	6:G:106:TYR:CE1	2.38	0.41
3:C:114:GLY:O	3:C:116:LYS:HE3	2.20	0.41
4:D:92:ARG:CZ	28:Y:47:A:H1'	2.51	0.41
4:D:123:ASP:OD2	4:D:127:ASN:HB2	2.20	0.41
8:I:62:LYS:HG3	8:I:62:LYS:HZ2	1.70	0.41
8:I:108:LEU:O	8:I:109:LEU:HD23	2.21	0.41
11:L:96:TYR:HA	11:L:100:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:50:ARG:HA	13:N:53:LYS:HE3	2.03	0.41
15:P:15:LYS:HG3	27:X:514:G:C2	2.55	0.41
18:S:73:LYS:C	18:S:75:LYS:H	2.29	0.41
20:U:41:VAL:HG23	20:U:43:ARG:HD2	2.02	0.41
22:W:1:MET:HE3	22:W:36:ASP:OD2	2.21	0.41
22:W:19:THR:OG1	27:X:863:C:O2'	2.05	0.41
25:2:15:THR:O	25:2:16:HIS:HB2	2.21	0.41
27:X:3:U:O2'	27:X:4:C:P	2.79	0.41
27:X:106:G:C2	27:X:107:G:C5	3.09	0.41
27:X:309:G:N2	27:X:352:G:O6	2.54	0.41
27:X:313:U:C2	27:X:314:G:C8	3.09	0.41
27:X:538:A:N3	27:X:2025:A:C6	2.89	0.41
27:X:753:U:H2'	27:X:754:G:C8	2.56	0.41
27:X:820:U:H1'	27:X:2424:G:OP1	2.20	0.41
27:X:1327:C:H42	27:X:1351:G:H1	1.67	0.41
27:X:1537:U:H2'	27:X:1538:A:O4'	2.21	0.41
27:X:1538:A:H2'	27:X:1539:U:O4'	2.20	0.41
27:X:1763:G:H2'	27:X:1764:A:H4'	2.02	0.41
27:X:1984:A:H2'	27:X:1985:G:O4'	2.21	0.41
27:X:2489:C:C4	27:X:2490:U:C5	3.09	0.41
27:X:2492:G:H2'	27:X:2493:U:H6	1.81	0.41
27:X:2870:C:H2'	27:X:2871:U:C6	2.56	0.41
2:B:147:PRO:HB2	2:B:149:ARG:HG2	2.03	0.41
3:C:102:LEU:HD23	3:C:102:LEU:O	2.21	0.41
4:D:142:THR:HG22	4:D:143:TYR:H	1.85	0.41
6:G:72:PRO:HG2	13:N:60:LEU:HG	2.03	0.41
7:H:27:SER:HB2	7:H:50:ILE:H	1.84	0.41
8:I:16:ARG:HG2	8:I:17:LYS:H	1.85	0.41
9:J:23:LYS:HE2	9:J:23:LYS:HB3	1.95	0.41
12:M:22:ARG:H	12:M:84:ALA:HB2	1.85	0.41
12:M:34:ARG:NH1	12:M:34:ARG:HA	2.36	0.41
14:O:66:GLY:O	14:O:87:ARG:NE	2.48	0.41
25:2:1:MET:HE1	27:X:765:C:OP2	2.21	0.41
27:X:109:A:C6	27:X:110:U:C4	3.09	0.41
27:X:235:C:H2'	27:X:236:C:O4'	2.21	0.41
27:X:389:G:H2'	27:X:390:U:C6	2.56	0.41
27:X:521:U:H5	27:X:522:G:C5	2.38	0.41
27:X:762:A:H4'	27:X:1284:G:N3	2.36	0.41
27:X:933:G:H2'	27:X:934:G:C8	2.56	0.41
27:X:1225:G:H2'	27:X:1249:G:H22	1.85	0.41
27:X:1672:A:H3'	27:X:1673:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1705:U:O4'	27:X:1718:A:N6	2.54	0.41
27:X:1804:U:H2'	27:X:1805:G:H8	1.86	0.41
27:X:2304:G:H8	27:X:2304:G:P	2.44	0.41
27:X:2434:G:H2'	27:X:2435:C:C6	2.56	0.41
27:X:2628:C:H2'	27:X:2629:U:H6	1.86	0.41
27:X:2779:C:O2'	27:X:2780:A:O4'	2.37	0.41
2:B:8:LYS:HE2	2:B:190:GLY:O	2.21	0.40
8:I:57:ILE:HD12	26:3:9:MET:SD	2.61	0.40
11:L:27:LEU:HB2	11:L:87:VAL:HG12	2.04	0.40
12:M:31:ASP:HA	12:M:52:GLY:O	2.22	0.40
15:P:18:VAL:HG12	15:P:20:LEU:H	1.86	0.40
17:R:28:LYS:HG2	17:R:29:HIS:H	1.87	0.40
19:T:26:PHE:CD1	27:X:934:G:H1'	2.56	0.40
19:T:36:ILE:HD11	27:X:2343:C:O2	2.21	0.40
26:3:8:LYS:HE2	26:3:12:ARG:NH2	2.35	0.40
27:X:67:G:N2	27:X:73:A:C4	2.90	0.40
27:X:114:C:OP1	27:X:126:C:N4	2.53	0.40
27:X:492:G:O2'	27:X:493:A:O5'	2.35	0.40
27:X:659:G:H2'	27:X:660:G:O4'	2.21	0.40
27:X:877:G:O2'	27:X:878:C:H5'	2.20	0.40
27:X:1171:A:H2'	27:X:1172:U:C6	2.56	0.40
27:X:1287:A:H2	27:X:1661:C:O2	2.03	0.40
27:X:2821:G:C6	27:X:2846:G:C6	3.09	0.40
28:Y:15:A:O2'	28:Y:16:U:H5''	2.21	0.40
28:Y:75:A:OP1	28:Y:75:A:H4'	2.21	0.40
1:A:168:LYS:HE2	1:A:168:LYS:HB2	1.84	0.40
3:C:17:LEU:HD12	3:C:17:LEU:HA	1.93	0.40
4:D:16:LEU:HD22	4:D:20:PHE:CE1	2.56	0.40
7:H:29:ILE:HA	7:H:34:LEU:HA	2.03	0.40
7:H:104:GLU:HB3	7:H:125:LYS:HD2	2.03	0.40
10:K:100:VAL:HG23	10:K:112:LEU:HG	2.03	0.40
13:N:65:ILE:CD1	13:N:95:LEU:HB3	2.51	0.40
14:O:82:ARG:HD3	14:O:82:ARG:HA	1.67	0.40
26:3:27:SER:OG	27:X:2340:C:OP1	2.27	0.40
27:X:75:C:H2'	27:X:76:C:H6	1.82	0.40
27:X:1030:U:OP1	27:X:1046:U:O2'	2.32	0.40
27:X:1211:G:H2'	27:X:1212:U:C6	2.55	0.40
27:X:1652:G:N2	27:X:1752:U:O2	2.44	0.40
27:X:2329:C:N4	27:X:2330:G:C6	2.89	0.40
27:X:2355:A:H8	27:X:2355:A:OP1	2.04	0.40
27:X:2380:U:H3	27:X:2394:G:H1	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2753:C:O2'	27:X:2754:C:H5'	2.21	0.40
28:Y:17:A:H1'	28:Y:112:A:C8	2.56	0.40
1:A:44:ASN:HA	27:X:1805:G:O2'	2.21	0.40
1:A:100:GLY:HA2	27:X:1517:C:H1'	2.03	0.40
1:A:212:SER:O	1:A:215:LEU:HD12	2.21	0.40
2:B:11:MET:HB3	2:B:11:MET:HE2	1.90	0.40
2:B:58:LYS:HE3	27:X:2805:G:OP1	2.21	0.40
2:B:129:HIS:HE1	27:X:1976:U:O2'	2.04	0.40
6:G:111:LYS:HD2	6:G:111:LYS:O	2.21	0.40
8:I:63:ARG:HD2	26:3:30:ARG:NH1	2.37	0.40
19:T:17:ASN:HA	19:T:18:PRO:HD3	1.79	0.40
25:2:15:THR:OG1	25:2:16:HIS:N	2.53	0.40
27:X:81:C:H5''	27:X:307:C:H5'	2.03	0.40
27:X:536:A:N6	27:X:2605:C:H4'	2.36	0.40
27:X:565:A:O5'	27:X:565:A:H8	2.04	0.40
27:X:644:A:N3	27:X:2382:C:H4'	2.36	0.40
27:X:759:C:O2'	27:X:2591:C:H5'	2.22	0.40
27:X:822:G:H2'	27:X:823:U:H6	1.86	0.40
27:X:1011:A:C8	27:X:1165:G:N2	2.90	0.40
27:X:1164:C:H2'	27:X:1165:G:O4'	2.22	0.40
27:X:1224:A:H4'	27:X:1225:G:OP2	2.21	0.40
27:X:1325:U:H4'	27:X:1326:U:O5'	2.22	0.40
27:X:2652:G:H2'	27:X:2653:A:H8	1.86	0.40
1:A:208:LYS:HB3	27:X:742:G:O6	2.22	0.40
2:B:93:VAL:C	2:B:95:ILE:H	2.29	0.40
2:B:119:ARG:HG2	2:B:120:TRP:NE1	2.36	0.40
6:G:94:LYS:HB3	6:G:94:LYS:HE3	1.54	0.40
8:I:62:LYS:HB2	26:3:13:ARG:H	1.86	0.40
8:I:76:LYS:HB2	8:I:79:GLN:HG2	2.03	0.40
11:L:26:ARG:NH1	27:X:2357:A:H4'	2.37	0.40
12:M:34:ARG:HH12	12:M:91:VAL:HA	1.86	0.40
16:Q:5:ASP:C	16:Q:7:LEU:H	2.30	0.40
19:T:45:PHE:CE2	19:T:69:PHE:HE2	2.39	0.40
23:Z:25:LEU:HD12	23:Z:25:LEU:HA	1.86	0.40
23:Z:42:SER:O	23:Z:44:HIS:HD2	2.03	0.40
24:1:17:GLY:O	24:1:19:GLY:N	2.52	0.40
27:X:193:A:C2	27:X:194:G:H1'	2.57	0.40
27:X:836:G:N2	27:X:847:C:O2	2.54	0.40
27:X:1226:A:N1	27:X:1250:A:H1'	2.35	0.40
27:X:1885:C:N3	27:X:1886:G:H1'	2.36	0.40
27:X:2013:A:H4'	27:X:2014:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2189:A:H8	27:X:2189:A:O5'	2.03	0.40
27:X:2299:A:N6	27:X:2312:A:O2'	2.55	0.40
1:A:15:GLN:O	1:A:24:LEU:HA	2.21	0.40
1:A:151:LYS:HD2	1:A:151:LYS:HA	1.92	0.40
2:B:172:VAL:HG22	2:B:182:ILE:HD11	2.02	0.40
10:K:98:LEU:O	10:K:111:ALA:HB1	2.22	0.40
13:N:52:ASN:HA	13:N:55:ARG:HG3	2.03	0.40
13:N:74:MET:SD	13:N:79:PHE:HD1	2.45	0.40
16:Q:4:TYR:CE2	21:V:23:LYS:HB2	2.57	0.40
19:T:53:MET:HA	19:T:58:THR:O	2.21	0.40
23:Z:51:TYR:CE1	23:Z:55:ARG:HG3	2.57	0.40
26:3:62:LEU:HD12	26:3:62:LEU:HA	1.90	0.40
27:X:165:G:N2	27:X:185:C:N3	2.54	0.40
27:X:200:A:O2'	27:X:421:G:N2	2.55	0.40
27:X:428:A:H2'	27:X:429:C:C6	2.56	0.40
27:X:540:G:N2	27:X:2004:U:H1'	2.37	0.40
27:X:773:G:C2'	27:X:774:A:H5'	2.52	0.40
27:X:1173:G:H2'	27:X:1174:G:H8	1.86	0.40
27:X:1671:A:C1'	27:X:2798:A:H5'	2.51	0.40
27:X:1698:C:O2	27:X:1753:A:H2'	2.21	0.40
27:X:1712:G:N2	27:X:1713:G:C8	2.89	0.40
27:X:1967:U:H2'	27:X:1968:G:H8	1.87	0.40
27:X:2186:G:H2'	27:X:2187:A:C8	2.56	0.40
27:X:2560:G:H4'	27:X:2561:G:C8	2.57	0.40
27:X:2794:G:C2	27:X:2803:C:N3	2.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	258/275 (94%)	223 (86%)	34 (13%)	1 (0%)	30	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	203/211 (96%)	182 (90%)	20 (10%)	1 (0%)	24	55
3	C	192/205 (94%)	165 (86%)	25 (13%)	2 (1%)	12	41
4	D	175/180 (97%)	153 (87%)	21 (12%)	1 (1%)	21	51
5	E	169/185 (91%)	155 (92%)	13 (8%)	1 (1%)	21	51
6	G	140/174 (80%)	126 (90%)	14 (10%)	0	100	100
7	H	132/134 (98%)	123 (93%)	8 (6%)	1 (1%)	16	45
8	I	132/156 (85%)	101 (76%)	28 (21%)	3 (2%)	5	26
9	J	134/141 (95%)	115 (86%)	19 (14%)	0	100	100
10	K	111/116 (96%)	102 (92%)	9 (8%)	0	100	100
11	L	102/114 (90%)	86 (84%)	16 (16%)	0	100	100
12	M	106/166 (64%)	101 (95%)	5 (5%)	0	100	100
13	N	115/118 (98%)	103 (90%)	10 (9%)	2 (2%)	7	31
14	O	92/100 (92%)	81 (88%)	11 (12%)	0	100	100
15	P	128/137 (93%)	109 (85%)	17 (13%)	2 (2%)	7	32
16	Q	91/95 (96%)	78 (86%)	11 (12%)	2 (2%)	5	27
17	R	108/114 (95%)	86 (80%)	22 (20%)	0	100	100
18	S	173/237 (73%)	152 (88%)	21 (12%)	0	100	100
19	T	72/91 (79%)	61 (85%)	9 (12%)	2 (3%)	4	23
20	U	70/81 (86%)	52 (74%)	14 (20%)	4 (6%)	1	12
21	V	63/67 (94%)	59 (94%)	4 (6%)	0	100	100
22	W	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
23	Z	54/60 (90%)	48 (89%)	6 (11%)	0	100	100
24	1	51/55 (93%)	37 (72%)	11 (22%)	3 (6%)	1	12
25	2	44/47 (94%)	40 (91%)	4 (9%)	0	100	100
26	3	57/66 (86%)	46 (81%)	11 (19%)	0	100	100
All	All	3025/3380 (90%)	2633 (87%)	367 (12%)	25 (1%)	16	45

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	Q	6	ILE
13	N	94	VAL
15	P	127	ILE

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Mol	Chain	Res	Type
24	1	9	ILE
24	1	10	VAL
16	Q	69	ILE
19	T	19	LYS
20	U	60	VAL
2	B	121	ASN
4	D	146	VAL
5	E	165	VAL
8	I	53	ARG
20	U	15	VAL
20	U	39	LYS
1	A	219	PRO
7	H	42	LYS
24	1	18	THR
15	P	129	ILE
3	C	15	ILE
13	N	8	ILE
20	U	30	VAL
19	T	75	GLY
3	C	22	VAL
8	I	19	VAL
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%)	157 (78%)	45 (22%)	1	6
2	B	155/157 (99%)	130 (84%)	25 (16%)	2	13
3	C	154/163 (94%)	121 (79%)	33 (21%)	1	7
4	D	153/156 (98%)	140 (92%)	13 (8%)	10	32
5	E	136/144 (94%)	120 (88%)	16 (12%)	5	22
6	G	118/146 (81%)	95 (80%)	23 (20%)	1	8
7	H	103/103 (100%)	84 (82%)	19 (18%)	1	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	101/121 (84%)	79 (78%)	22 (22%)	1	6
9	J	110/115 (96%)	87 (79%)	23 (21%)	1	7
10	K	90/93 (97%)	74 (82%)	16 (18%)	2	11
11	L	74/82 (90%)	54 (73%)	20 (27%)	0	3
12	M	94/134 (70%)	66 (70%)	28 (30%)	0	2
13	N	96/97 (99%)	79 (82%)	17 (18%)	2	11
14	O	75/79 (95%)	65 (87%)	10 (13%)	4	19
15	P	112/118 (95%)	87 (78%)	25 (22%)	1	6
16	Q	75/76 (99%)	55 (73%)	20 (27%)	0	3
17	R	91/95 (96%)	80 (88%)	11 (12%)	5	21
18	S	149/192 (78%)	125 (84%)	24 (16%)	2	13
19	T	55/67 (82%)	48 (87%)	7 (13%)	4	20
20	U	57/66 (86%)	41 (72%)	16 (28%)	0	2
21	V	53/55 (96%)	49 (92%)	4 (8%)	12	37
22	W	48/48 (100%)	45 (94%)	3 (6%)	16	41
23	Z	50/53 (94%)	43 (86%)	7 (14%)	3	17
24	1	46/48 (96%)	31 (67%)	15 (33%)	0	1
25	2	39/40 (98%)	30 (77%)	9 (23%)	1	5
26	3	46/52 (88%)	39 (85%)	7 (15%)	3	15
All	All	2482/2716 (91%)	2024 (82%)	458 (18%)	1	10

All (458) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	21	PHE
1	A	22	SER
1	A	27	LYS
1	A	33	LEU
1	A	34	THR
1	A	40	THR
1	A	43	ARG
1	A	48	ARG
1	A	64	ILE
1	A	68	LYS

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Mol	Chain	Res	Type
1	A	84	TYR
1	A	88	ARG
1	A	96	HIS
1	A	104	TYR
1	A	111	LEU
1	A	116	THR
1	A	118	ASN
1	A	129	ASN
1	A	131	LEU
1	A	134	ARG
1	A	138	VAL
1	A	151	LYS
1	A	154	GLN
1	A	157	ARG
1	A	161	THR
1	A	164	GLN
1	A	171	ASP
1	A	183	ARG
1	A	198	ASN
1	A	203	ASN
1	A	206	LEU
1	A	214	TRP
1	A	215	LEU
1	A	218	LYS
1	A	240	THR
1	A	244	ARG
1	A	245	VAL
1	A	247	VAL
1	A	248	THR
1	A	250	TRP
1	A	252	LYS
1	A	259	THR
1	A	261	ARG
1	A	262	LYS
2	B	14	ILE
2	B	24	THR
2	B	25	VAL
2	B	26	VAL
2	B	35	GLN
2	B	47	VAL
2	B	60	ASN
2	B	69	LYS

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Mol	Chain	Res	Type
2	B	72	VAL
2	B	77	ILE
2	B	79	ARG
2	B	84	PHE
2	B	87	ASP
2	B	113	THR
2	B	118	LYS
2	B	119	ARG
2	B	132	LYS
2	B	141	ILE
2	B	143	GLN
2	B	150	VAL
2	B	165	VAL
2	B	198	LEU
2	B	199	ARG
2	B	200	SER
2	B	203	LYS
3	C	3	GLN
3	C	5	ASN
3	C	14	THR
3	C	17	LEU
3	C	31	VAL
3	C	45	THR
3	C	48	ARG
3	C	51	VAL
3	C	53	LYS
3	C	56	ARG
3	C	57	LYS
3	C	62	LYS
3	C	64	THR
3	C	74	VAL
3	C	82	VAL
3	C	99	VAL
3	C	108	ILE
3	C	116	LYS
3	C	118	VAL
3	C	120	VAL
3	C	124	ASP
3	C	143	ASP
3	C	152	THR
3	C	157	THR
3	C	164	VAL

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Mol	Chain	Res	Type
3	C	165	SER
3	C	172	VAL
3	C	176	ASN
3	C	180	ILE
3	C	182	ARG
3	C	188	ILE
3	C	189	ASP
3	C	193	LEU
4	D	9	ASN
4	D	46	ASP
4	D	50	ILE
4	D	62	LEU
4	D	80	ARG
4	D	89	VAL
4	D	90	THR
4	D	112	ARG
4	D	130	LEU
4	D	137	ILE
4	D	144	ASP
4	D	146	VAL
4	D	157	VAL
5	E	6	LYS
5	E	16	THR
5	E	35	VAL
5	E	43	VAL
5	E	50	LEU
5	E	85	ILE
5	E	86	ASN
5	E	89	LEU
5	E	113	VAL
5	E	116	GLU
5	E	127	GLU
5	E	136	ILE
5	E	158	HIS
5	E	164	PHE
5	E	165	VAL
5	E	175	LYS
6	G	30	LYS
6	G	39	GLN
6	G	40	ASN
6	G	42	VAL
6	G	43	VAL

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Mol	Chain	Res	Type
6	G	47	SER
6	G	53	ARG
6	G	63	ARG
6	G	71	THR
6	G	75	ILE
6	G	82	VAL
6	G	94	LYS
6	G	99	VAL
6	G	101	THR
6	G	102	ARG
6	G	111	LYS
6	G	116	ARG
6	G	119	LEU
6	G	126	VAL
6	G	132	PHE
6	G	145	HIS
6	G	156	HIS
6	G	158	HIS
7	H	8	LEU
7	H	20	MET
7	H	46	HIS
7	H	51	ILE
7	H	54	SER
7	H	69	VAL
7	H	81	ILE
7	H	87	SER
7	H	89	ILE
7	H	98	ILE
7	H	104	GLU
7	H	108	THR
7	H	109	ARG
7	H	110	VAL
7	H	118	LEU
7	H	119	ARG
7	H	120	ASP
7	H	126	ILE
7	H	127	VAL
8	I	19	VAL
8	I	26	THR
8	I	32	ARG
8	I	39	SER
8	I	49	PHE

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Mol	Chain	Res	Type
8	I	50	GLU
8	I	54	SER
8	I	55	ARG
8	I	56	LEU
8	I	60	LEU
8	I	62	LYS
8	I	77	LEU
8	I	80	LEU
8	I	94	GLU
8	I	96	TYR
8	I	98	LEU
8	I	99	VAL
8	I	109	LEU
8	I	114	ILE
8	I	120	VAL
8	I	141	VAL
8	I	142	LEU
9	J	8	THR
9	J	9	LYS
9	J	10	PHE
9	J	11	ARG
9	J	15	ARG
9	J	27	TYR
9	J	28	VAL
9	J	38	MET
9	J	44	LYS
9	J	45	SER
9	J	54	VAL
9	J	77	LYS
9	J	84	MET
9	J	88	LYS
9	J	93	TYR
9	J	103	VAL
9	J	110	VAL
9	J	111	THR
9	J	113	GLU
9	J	128	ILE
9	J	133	VAL
9	J	135	ARG
9	J	140	GLU
10	K	5	LYS
10	K	8	ARG

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Mol	Chain	Res	Type
10	K	9	LYS
10	K	12	ARG
10	K	17	ARG
10	K	20	LEU
10	K	37	THR
10	K	45	ARG
10	K	53	THR
10	K	59	ASP
10	K	73	LYS
10	K	75	VAL
10	K	95	THR
10	K	98	LEU
10	K	109	THR
10	K	115	LEU
11	L	8	ARG
11	L	11	LEU
11	L	12	ARG
11	L	13	THR
11	L	15	ARG
11	L	17	VAL
11	L	18	ARG
11	L	31	VAL
11	L	37	HIS
11	L	38	ILE
11	L	43	ILE
11	L	45	ASP
11	L	50	THR
11	L	60	LYS
11	L	65	THR
11	L	67	THR
11	L	87	VAL
11	L	90	ASP
11	L	91	ARG
11	L	93	SER
12	M	2	GLN
12	M	3	THR
12	M	6	LYS
12	M	13	LEU
12	M	16	ILE
12	M	19	ASP
12	M	20	HIS
12	M	25	PRO

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Mol	Chain	Res	Type
12	M	28	ARG
12	M	33	VAL
12	M	34	ARG
12	M	37	THR
12	M	38	LYS
12	M	39	VAL
12	M	45	THR
12	M	46	ARG
12	M	57	ILE
12	M	60	SER
12	M	71	ILE
12	M	83	PHE
12	M	87	LEU
12	M	90	GLN
12	M	92	THR
12	M	93	ILE
12	M	96	ARG
12	M	98	LYS
12	M	101	ARG
12	M	103	LYS
13	N	3	ARG
13	N	11	ARG
13	N	13	ARG
13	N	18	LEU
13	N	22	LYS
13	N	30	LYS
13	N	40	LEU
13	N	55	ARG
13	N	60	LEU
13	N	70	ARG
13	N	75	ASN
13	N	83	LEU
13	N	90	LEU
13	N	92	ARG
13	N	93	LYS
13	N	97	ASP
13	N	102	GLU
14	O	11	GLN
14	O	20	ILE
14	O	21	ARG
14	O	22	VAL
14	O	28	GLU

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Mol	Chain	Res	Type
14	O	56	VAL
14	O	69	ILE
14	O	88	GLN
14	O	91	THR
14	O	96	LEU
15	P	9	ARG
15	P	16	GLN
15	P	27	VAL
15	P	31	VAL
15	P	36	ARG
15	P	39	ARG
15	P	40	LEU
15	P	42	VAL
15	P	45	ILE
15	P	60	ILE
15	P	86	LEU
15	P	91	PHE
15	P	97	VAL
15	P	102	THR
15	P	104	LYS
15	P	106	LEU
15	P	107	ILE
15	P	110	VAL
15	P	119	ILE
15	P	121	LYS
15	P	122	LYS
15	P	123	ARG
15	P	124	THR
15	P	129	ILE
15	P	130	ILE
16	Q	5	ASP
16	Q	6	ILE
16	Q	7	LEU
16	Q	12	ILE
16	Q	15	LYS
16	Q	26	SER
16	Q	27	PHE
16	Q	30	SER
16	Q	38	ILE
16	Q	44	GLN
16	Q	51	ILE
16	Q	58	VAL

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Mol	Chain	Res	Type
16	Q	62	ARG
16	Q	64	ARG
16	Q	67	ARG
16	Q	69	ILE
16	Q	73	ASN
16	Q	75	ARG
16	Q	82	LEU
16	Q	84	GLU
17	R	38	LEU
17	R	48	VAL
17	R	55	THR
17	R	56	LYS
17	R	71	GLN
17	R	81	VAL
17	R	85	ASP
17	R	88	THR
17	R	92	THR
17	R	105	ARG
17	R	106	VAL
18	S	6	LYS
18	S	13	LYS
18	S	15	ASP
18	S	22	VAL
18	S	25	ASN
18	S	28	ASN
18	S	48	THR
18	S	53	ASP
18	S	56	VAL
18	S	70	GLN
18	S	71	MET
18	S	79	ILE
18	S	94	VAL
18	S	100	THR
18	S	109	GLN
18	S	114	ASP
18	S	120	LEU
18	S	122	ILE
18	S	130	ILE
18	S	151	ASP
18	S	158	CYS
18	S	160	LEU
18	S	163	ASP

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Mol	Chain	Res	Type
18	S	169	VAL
19	T	14	ARG
19	T	19	LYS
19	T	40	GLN
19	T	41	ARG
19	T	62	LEU
19	T	64	ASP
19	T	79	ILE
20	U	8	THR
20	U	10	LYS
20	U	17	SER
20	U	18	VAL
20	U	19	ILE
20	U	21	ARG
20	U	27	ASP
20	U	32	ARG
20	U	35	THR
20	U	43	ARG
20	U	47	HIS
20	U	48	LYS
20	U	49	LYS
20	U	53	GLU
20	U	63	SER
20	U	67	LEU
21	V	12	THR
21	V	29	ARG
21	V	46	LEU
21	V	53	LEU
22	W	3	ILE
22	W	6	VAL
22	W	37	THR
23	Z	6	VAL
23	Z	21	SER
23	Z	25	LEU
23	Z	40	LYS
23	Z	53	ASP
23	Z	56	GLN
23	Z	57	VAL
24	1	7	ARG
24	1	8	ILE
24	1	12	MET
24	1	20	PHE

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Mol	Chain	Res	Type
24	1	21	TYR
24	1	25	THR
24	1	28	ARG
24	1	30	ASN
24	1	32	GLN
24	1	36	GLU
24	1	41	ASP
24	1	43	VAL
24	1	50	PHE
24	1	51	ARG
24	1	54	LYS
25	2	1	MET
25	2	10	ARG
25	2	12	ARG
25	2	15	THR
25	2	28	ARG
25	2	31	LEU
25	2	41	GLN
25	2	43	THR
25	2	46	ASP
26	3	7	HIS
26	3	9	MET
26	3	11	LYS
26	3	19	THR
26	3	34	THR
26	3	55	TRP
26	3	62	LEU

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

Mol	Chain	Res	Type
1	A	15	GLN
1	A	129	ASN
1	A	164	GLN
1	A	166	GLN
1	A	186	HIS
1	A	227	ASN
2	B	13	GLN
2	B	35	GLN
2	B	66	HIS
2	B	129	HIS
3	C	10	ASN

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Mol	Chain	Res	Type
3	C	34	GLN
3	C	132	ASN
3	C	156	ASN
3	C	163	ASN
3	C	176	ASN
4	D	37	ASN
5	E	74	ASN
5	E	139	GLN
6	G	39	GLN
6	G	40	ASN
6	G	66	HIS
6	G	107	GLN
6	G	129	HIS
6	G	140	GLN
8	I	103	ASN
9	J	58	HIS
9	J	124	HIS
10	K	3	HIS
10	K	24	GLN
12	M	23	GLN
13	N	34	ASN
13	N	37	GLN
13	N	41	ASN
13	N	63	GLN
13	N	66	ASN
13	N	81	ASN
14	O	63	HIS
14	O	88	GLN
15	P	16	GLN
15	P	73	ASN
15	P	78	ASN
15	P	81	HIS
15	P	126	HIS
16	Q	43	GLN
16	Q	57	ASN
16	Q	73	ASN
17	R	15	HIS
17	R	29	HIS
17	R	44	GLN
17	R	71	GLN
18	S	46	GLN
18	S	70	GLN

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Mol	Chain	Res	Type
18	S	109	GLN
18	S	118	HIS
18	S	121	GLN
20	U	16	ASN
21	V	54	ASN
22	W	15	ASN
23	Z	35	GLN
23	Z	44	HIS
25	2	6	GLN
25	2	8	ASN
25	2	29	ASN
26	3	7	HIS
26	3	31	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	X	2657/2880 (92%)	612 (23%)	39 (1%)
28	Y	121/123 (98%)	31 (25%)	2 (1%)
All	All	2778/3003 (92%)	643 (23%)	41 (1%)

All (643) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
27	X	4	C
27	X	13	A
27	X	14	A
27	X	15	G
27	X	17	G
27	X	34	U
27	X	37	C
27	X	39	C
27	X	45	C
27	X	48	A
27	X	49	U
27	X	50	G
27	X	51	A
27	X	59	G
27	X	63	A
27	X	68	C
27	X	69	G

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Mol	Chain	Res	Type
27	X	73	A
27	X	74	G
27	X	75	C
27	X	83	A
27	X	88	G
27	X	89	A
27	X	90	G
27	X	91	A
27	X	95	G
27	X	100	G
27	X	101	A
27	X	108	G
27	X	110	U
27	X	116	A
27	X	118	U
27	X	123	A
27	X	124	A
27	X	129	A
27	X	134	G
27	X	136	A
27	X	137	A
27	X	143	A
27	X	147	G
27	X	173	A
27	X	176	A
27	X	178	C
27	X	181	A
27	X	182	G
27	X	192	G
27	X	193	A
27	X	198	A
27	X	199	A
27	X	206	U
27	X	207	U
27	X	209	G
27	X	210	A
27	X	219	G
27	X	220	U
27	X	222	G
27	X	225	G
27	X	229	G
27	X	241	C

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Mol	Chain	Res	Type
27	X	242	A
27	X	243	G
27	X	304	A
27	X	306	G
27	X	310	A
27	X	312	G
27	X	319	G
27	X	321	A
27	X	323	G
27	X	333	A
27	X	334	G
27	X	335	A
27	X	337	G
27	X	340	G
27	X	342	G
27	X	343	A
27	X	344	G
27	X	360	A
27	X	388	G
27	X	397	U
27	X	398	C
27	X	399	G
27	X	400	U
27	X	408	U
27	X	409	G
27	X	413	G
27	X	414	A
27	X	418	C
27	X	419	G
27	X	421	G
27	X	424	G
27	X	425	A
27	X	435	A
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	483	A
27	X	484	G

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Mol	Chain	Res	Type
27	X	492	G
27	X	493	A
27	X	500	G
27	X	504	G
27	X	514	G
27	X	515	A
27	X	518	A
27	X	519	C
27	X	520	C
27	X	521	U
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	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	597	U
27	X	611	C
27	X	613	A
27	X	614	G
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	636	G

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Mol	Chain	Res	Type
27	X	638	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
27	X	664	C
27	X	665	A
27	X	666	U
27	X	667	U
27	X	668	A
27	X	669	G
27	X	682	G
27	X	689	A
27	X	690	A
27	X	695	G
27	X	699	G
27	X	712	A
27	X	736	G
27	X	739	G
27	X	743	A
27	X	747	A
27	X	752	G
27	X	753	U
27	X	759	C
27	X	760	U
27	X	766	A
27	X	774	A
27	X	788	G
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	805	G
27	X	806	A

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Mol	Chain	Res	Type
27	X	814	G
27	X	818	G
27	X	824	U
27	X	825	C
27	X	832	A
27	X	840	U
27	X	841	G
27	X	845	U
27	X	846	A
27	X	856	A
27	X	859	U
27	X	872	G
27	X	879	A
27	X	891	A
27	X	922	A
27	X	931	G
27	X	938	G
27	X	939	C
27	X	940	G
27	X	944	A
27	X	952	A
27	X	956	A
27	X	957	G
27	X	964	A
27	X	966	A
27	X	967	G
27	X	972	C
27	X	973	U
27	X	976	C
27	X	979	A
27	X	985	G
27	X	994	A
27	X	996	C
27	X	1006	C
27	X	1007	A
27	X	1014	G
27	X	1016	C
27	X	1019	U
27	X	1021	A
27	X	1023	U
27	X	1028	G
27	X	1032	A

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Mol	Chain	Res	Type
27	X	1033	G
27	X	1034	U
27	X	1037	U
27	X	1044	U
27	X	1051	U
27	X	1054	C
27	X	1056	U
27	X	1057	A
27	X	1058	G
27	X	1060	C
27	X	1066	G
27	X	1068	A
27	X	1077	U
27	X	1079	G
27	X	1082	G
27	X	1083	C
27	X	1086	C
27	X	1087	C
27	X	1090	C
27	X	1097	A
27	X	1099	A
27	X	1108	U
27	X	1109	A
27	X	1123	G
27	X	1129	A
27	X	1130	U
27	X	1133	G
27	X	1139	A
27	X	1142	G
27	X	1143	A
27	X	1144	U
27	X	1145	C
27	X	1146	G
27	X	1152	C
27	X	1153	A
27	X	1166	A
27	X	1183	C
27	X	1185	C
27	X	1192	A
27	X	1208	A
27	X	1209	G
27	X	1226	A

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Mol	Chain	Res	Type
27	X	1247	U
27	X	1249	G
27	X	1250	A
27	X	1256	C
27	X	1266	G
27	X	1268	U
27	X	1269	G
27	X	1278	A
27	X	1284	G
27	X	1285	A
27	X	1288	A
27	X	1289	A
27	X	1301	U
27	X	1313	U
27	X	1314	A
27	X	1322	G
27	X	1325	U
27	X	1334	A
27	X	1336	G
27	X	1342	U
27	X	1354	A
27	X	1372	A
27	X	1378	A
27	X	1381	G
27	X	1391	A
27	X	1392	U
27	X	1397	A
27	X	1398	G
27	X	1399	C
27	X	1404	C
27	X	1409	U
27	X	1413	U
27	X	1425	G
27	X	1428	G
27	X	1429	A
27	X	1430	G
27	X	1433	A
27	X	1434	U
27	X	1435	G
27	X	1442	C
27	X	1443	G
27	X	1459	U

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Mol	Chain	Res	Type
27	X	1460	G
27	X	1465	G
27	X	1466	C
27	X	1468	A
27	X	1469	U
27	X	1470	G
27	X	1471	G
27	X	1475	U
27	X	1482	U
27	X	1490	U
27	X	1497	C
27	X	1498	G
27	X	1522	C
27	X	1523	A
27	X	1524	C
27	X	1525	A
27	X	1528	C
27	X	1531	C
27	X	1545	G
27	X	1551	U
27	X	1552	C
27	X	1553	G
27	X	1554	G
27	X	1562	G
27	X	1564	U
27	X	1570	C
27	X	1571	G
27	X	1574	A
27	X	1575	C
27	X	1582	A
27	X	1585	A
27	X	1594	U
27	X	1601	U
27	X	1602	G
27	X	1603	A
27	X	1608	U
27	X	1624	A
27	X	1626	A
27	X	1629	G
27	X	1632	A
27	X	1634	A
27	X	1648	C

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Mol	Chain	Res	Type
27	X	1651	U
27	X	1656	U
27	X	1657	A
27	X	1661	C
27	X	1665	C
27	X	1674	C
27	X	1680	U
27	X	1682	A
27	X	1686	A
27	X	1688	U
27	X	1691	G
27	X	1710	U
27	X	1713	G
27	X	1717	A
27	X	1718	A
27	X	1735	G
27	X	1747	G
27	X	1749	G
27	X	1755	G
27	X	1760	G
27	X	1764	A
27	X	1767	G
27	X	1770	U
27	X	1775	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	1802	A
27	X	1807	A
27	X	1808	C
27	X	1812	U
27	X	1813	A
27	X	1819	U
27	X	1821	A
27	X	1825	C
27	X	1831	G
27	X	1846	A
27	X	1861	G

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Mol	Chain	Res	Type
27	X	1867	A
27	X	1868	A
27	X	1874	G
27	X	1882	G
27	X	1886	G
27	X	1887	G
27	X	1888	C
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	1938	U
27	X	1943	A
27	X	1944	C
27	X	1945	C
27	X	1946	U
27	X	1948	C
27	X	1949	A
27	X	1950	C
27	X	1953	A
27	X	1954	A
27	X	1955	G
27	X	1965	U
27	X	1970	G
27	X	1974	U
27	X	1976	U
27	X	1980	A
27	X	1999	U
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	2026	C
27	X	2032	G

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Mol	Chain	Res	Type
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	2075	U
27	X	2076	G
27	X	2083	G
27	X	2089	C
27	X	2171	U
27	X	2181	A
27	X	2189	A
27	X	2190	A
27	X	2191	A
27	X	2192	U
27	X	2195	C
27	X	2196	U
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	2222	U
27	X	2225	G
27	X	2247	A
27	X	2262	C
27	X	2265	A
27	X	2266	A
27	X	2268	G
27	X	2284	U
27	X	2285	U
27	X	2286	G
27	X	2287	G
27	X	2290	A
27	X	2294	U
27	X	2298	U
27	X	2300	G
27	X	2301	A

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Mol	Chain	Res	Type
27	X	2305	C
27	X	2306	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	2329	C
27	X	2330	G
27	X	2333	A
27	X	2351	G
27	X	2358	C
27	X	2361	G
27	X	2362	G
27	X	2364	C
27	X	2369	U
27	X	2371	A
27	X	2375	G
27	X	2381	A
27	X	2386	G
27	X	2387	U
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	2408	G
27	X	2410	U
27	X	2413	A
27	X	2420	C
27	X	2424	G
27	X	2427	A
27	X	2429	A
27	X	2449	G
27	X	2452	U
27	X	2453	C
27	X	2455	A
27	X	2457	A
27	X	2458	U
27	X	2463	G

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Mol	Chain	Res	Type
27	X	2471	U
27	X	2477	C
27	X	2479	U
27	X	2480	C
27	X	2481	G
27	X	2482	A
27	X	2483	U
27	X	2484	G
27	X	2497	A
27	X	2498	U
27	X	2504	G
27	X	2508	G
27	X	2522	G
27	X	2532	G
27	X	2542	U
27	X	2545	A
27	X	2546	G
27	X	2551	A
27	X	2552	C
27	X	2553	G
27	X	2556	A
27	X	2557	G
27	X	2561	G
27	X	2564	U
27	X	2565	C
27	X	2578	G
27	X	2581	A
27	X	2582	G
27	X	2583	U
27	X	2588	U
27	X	2591	C
27	X	2593	A
27	X	2594	U
27	X	2600	A
27	X	2608	A
27	X	2611	A
27	X	2624	G
27	X	2633	A
27	X	2634	G
27	X	2642	G
27	X	2650	G
27	X	2664	G

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Mol	Chain	Res	Type
27	X	2668	U
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	2713	A
27	X	2728	A
27	X	2731	G
27	X	2732	C
27	X	2738	A
27	X	2744	A
27	X	2745	A
27	X	2756	A
27	X	2757	G
27	X	2758	A
27	X	2759	U
27	X	2760	G
27	X	2769	C
27	X	2770	A
27	X	2771	C
27	X	2780	A
27	X	2781	G
27	X	2782	G
27	X	2783	U
27	X	2787	A
27	X	2795	A
27	X	2796	A
27	X	2798	A
27	X	2807	U
27	X	2809	A
27	X	2811	G
27	X	2814	G
27	X	2824	C
27	X	2825	A
27	X	2832	G
27	X	2842	C
27	X	2847	G
27	X	2849	C
27	X	2851	G
27	X	2852	G

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Mol	Chain	Res	Type
27	X	2854	G
27	X	2858	A
27	X	2860	C
27	X	2861	A
27	X	2866	A
27	X	2868	G
27	X	2869	U
28	Y	14	C
28	Y	15	A
28	Y	17	A
28	Y	18	G
28	Y	26	G
28	Y	28	A
28	Y	29	C
28	Y	37	C
28	Y	42	U
28	Y	43	G
28	Y	45	C
28	Y	46	G
28	Y	47	A
28	Y	49	C
28	Y	51	G
28	Y	54	U
28	Y	59	A
28	Y	68	A
28	Y	69	G
28	Y	72	C
28	Y	75	A
28	Y	86	A
28	Y	97	C
28	Y	102	A
28	Y	108	G
28	Y	110	U
28	Y	111	C
28	Y	112	A
28	Y	113	G
28	Y	115	G
28	Y	123	U

All (41) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
27	X	38	G
27	X	48	A
27	X	50	G
27	X	123	A
27	X	218	A
27	X	219	G
27	X	334	G
27	X	434	C
27	X	458	G
27	X	492	G
27	X	499	G
27	X	537	C
27	X	553	C
27	X	788	G
27	X	789	G
27	X	1031	C
27	X	1053	G
27	X	1059	A
27	X	1141	U
27	X	1182	U
27	X	1225	G
27	X	1313	U
27	X	1391	A
27	X	1398	G
27	X	1441	A
27	X	1496	G
27	X	1607	A
27	X	1811	A
27	X	1923	U
27	X	1975	G
27	X	2190	A
27	X	2228	U
27	X	2299	A
27	X	2312	A
27	X	2404	A
27	X	2409	A
27	X	2705	A
27	X	2756	A
27	X	2824	C
28	Y	27	A
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 51 ligands modelled in this entry, 51 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	260/275 (94%)	0.57	30 (11%) 9 9	45, 101, 165, 255	0
2	B	205/211 (97%)	0.05	7 (3%) 48 29	26, 43, 97, 208	0
3	C	194/205 (94%)	0.26	11 (5%) 29 19	38, 101, 172, 256	0
4	D	177/180 (98%)	0.47	13 (7%) 21 15	108, 173, 225, 261	0
5	E	171/185 (92%)	0.07	9 (5%) 32 20	51, 120, 177, 236	0
6	G	142/174 (81%)	0.41	13 (9%) 14 11	35, 72, 151, 204	0
7	H	134/134 (100%)	-0.07	3 (2%) 62 37	31, 42, 85, 136	0
8	I	134/156 (85%)	0.84	22 (16%) 4 5	53, 125, 199, 245	0
9	J	136/141 (96%)	0.46	15 (11%) 10 10	56, 88, 168, 221	0
10	K	113/116 (97%)	-0.03	3 (2%) 56 33	25, 30, 61, 99	0
11	L	104/114 (91%)	0.81	12 (11%) 9 9	128, 160, 197, 232	0
12	M	108/166 (65%)	-0.05	2 (1%) 66 40	29, 37, 93, 143	0
13	N	117/118 (99%)	0.27	9 (7%) 19 13	40, 78, 123, 213	0
14	O	94/100 (94%)	0.43	8 (8%) 16 12	51, 96, 164, 191	0
15	P	130/137 (94%)	0.03	3 (2%) 61 36	31, 51, 149, 168	0
16	Q	93/95 (97%)	-0.05	2 (2%) 62 37	45, 83, 145, 192	0
17	R	110/114 (96%)	0.51	9 (8%) 17 13	66, 97, 187, 238	0
18	S	175/237 (73%)	0.28	9 (5%) 33 21	89, 141, 204, 258	0
19	T	74/91 (81%)	0.56	6 (8%) 18 13	70, 110, 148, 231	0
20	U	72/81 (88%)	0.78	9 (12%) 8 8	73, 123, 178, 252	0
21	V	65/67 (97%)	-0.09	0 100 100	67, 111, 168, 222	0
22	W	55/55 (100%)	-0.16	1 (1%) 67 41	72, 94, 147, 177	0
23	Z	56/60 (93%)	0.00	1 (1%) 67 41	30, 36, 87, 100	0
24	1	53/55 (96%)	1.09	12 (22%) 2 3	98, 127, 189, 275	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	2	46/47 (97%)	0.50	4 (8%) 16 12	39, 69, 102, 127	0
26	3	59/66 (89%)	1.19	14 (23%) 2 2	79, 99, 176, 252	0
27	X	2667/2880 (92%)	0.09	71 (2%) 56 33	25, 73, 176, 304	0
28	Y	122/123 (99%)	0.56	8 (6%) 24 16	74, 150, 189, 279	0
All	All	5866/6383 (91%)	0.23	306 (5%) 33 21	25, 87, 182, 304	0

All (306) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	T	15	ASP	9.6
9	J	84	MET	9.5
1	A	220	HIS	8.6
9	J	21	ASP	7.9
6	G	129	HIS	7.9
14	O	23	GLU	7.4
4	D	39	GLY	7.3
1	A	85	ASP	6.6
25	2	40	HIS	6.6
2	B	135	HIS	6.6
4	D	43	SER	6.5
17	R	93	ARG	6.5
4	D	42	SER	6.4
1	A	84	TYR	6.2
5	E	37	TYR	6.1
8	I	31	GLY	6.1
8	I	53	ARG	6.0
6	G	110	LEU	6.0
1	A	237	GLU	5.8
8	I	63	ARG	5.5
27	X	1073	G	5.4
1	A	18	THR	5.3
28	Y	2	C	5.3
24	1	14	SER	5.3
18	S	92	VAL	5.2
26	3	14	ILE	5.2
1	A	22	SER	5.1
8	I	100	ARG	5.1
27	X	1082	G	5.1
26	3	54	GLU	5.0
3	C	66	ASN	4.9
2	B	142	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
20	U	16	ASN	4.8
20	U	46	LEU	4.8
26	3	55	TRP	4.8
1	A	236	GLY	4.8
25	2	1	MET	4.7
2	B	136	ARG	4.7
27	X	1574	A	4.7
27	X	1087	C	4.7
11	L	12	ARG	4.6
6	G	107	GLN	4.6
28	Y	111	C	4.5
27	X	2290	A	4.5
27	X	940	G	4.4
1	A	91	ARG	4.3
28	Y	58	G	4.3
27	X	304	A	4.2
9	J	27	TYR	4.2
8	I	11	GLY	4.1
1	A	250	TRP	4.1
8	I	45	LYS	4.1
10	K	3	HIS	4.0
6	G	162	LYS	4.0
1	A	44	ASN	4.0
17	R	83	LEU	3.9
18	S	116	VAL	3.9
3	C	48	ARG	3.8
27	X	871	U	3.8
8	I	36	GLY	3.7
8	I	27	ASP	3.7
8	I	56	LEU	3.7
3	C	189	ASP	3.7
8	I	21	ARG	3.7
11	L	97	HIS	3.7
1	A	249	PRO	3.6
17	R	78	ALA	3.6
8	I	39	SER	3.6
11	L	34	SER	3.6
27	X	225	G	3.6
27	X	1099	A	3.5
22	W	7	ARG	3.5
27	X	1086	C	3.5
23	Z	4	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
3	C	19	LEU	3.5
24	1	27	ASN	3.5
27	X	774	A	3.5
27	X	1067	G	3.5
13	N	88	ILE	3.5
1	A	20	ASP	3.4
27	X	1068	A	3.4
28	Y	68	A	3.4
3	C	172	VAL	3.4
13	N	23	GLY	3.4
13	N	12	ARG	3.4
26	3	52	LYS	3.4
1	A	238	GLY	3.4
27	X	305	A	3.4
13	N	48	ARG	3.4
3	C	193	LEU	3.3
19	T	19	LYS	3.3
15	P	123	ARG	3.3
27	X	1089	C	3.3
11	L	33	ARG	3.3
2	B	205	SER	3.2
27	X	1429	A	3.2
27	X	2189	A	3.2
8	I	97	ARG	3.2
18	S	32	PHE	3.2
3	C	43	ALA	3.2
19	T	61	ALA	3.2
26	3	63	PRO	3.2
27	X	1074	G	3.2
4	D	86	GLY	3.2
3	C	44	SER	3.2
26	3	32	GLN	3.1
27	X	1104	G	3.1
20	U	8	THR	3.1
1	A	28	ARG	3.1
28	Y	29	C	3.1
3	C	49	ALA	3.1
9	J	12	LYS	3.1
26	3	11	LYS	3.0
1	A	217	ARG	3.0
9	J	16	GLY	3.0
27	X	1080	A	3.0

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Mol	Chain	Res	Type	RSRZ
6	G	68	PRO	3.0
27	X	1085	G	3.0
1	A	241	GLY	3.0
14	O	98	ILE	3.0
27	X	1912	G	3.0
19	T	59	LEU	3.0
27	X	1058	G	2.9
27	X	248	A	2.9
27	X	2287	G	2.9
27	X	2731	G	2.9
9	J	32	ASP	2.9
9	J	106	GLU	2.9
24	1	19	GLY	2.9
26	3	33	ASN	2.9
8	I	52	GLY	2.9
24	1	3	LYS	2.9
18	S	29	ASN	2.8
18	S	114	ASP	2.8
16	Q	56	MET	2.8
4	D	94	GLU	2.8
27	X	38	G	2.8
24	1	22	TYR	2.8
5	E	68	THR	2.8
27	X	665	A	2.8
15	P	37	LYS	2.8
2	B	137	ARG	2.8
14	O	39	PHE	2.8
26	3	31	HIS	2.8
1	A	54	ILE	2.8
27	X	542	A	2.8
7	H	11	ALA	2.8
9	J	15	ARG	2.7
20	U	28	GLY	2.7
11	L	104	ALA	2.7
8	I	17	LYS	2.7
8	I	88	PHE	2.7
6	G	105	GLY	2.7
13	N	110	VAL	2.7
5	E	5	GLY	2.7
27	X	1603	A	2.7
17	R	66	GLN	2.7
1	A	47	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
7	H	40	GLY	2.7
24	1	2	ALA	2.7
26	3	9	MET	2.6
13	N	58	ARG	2.6
17	R	77	HIS	2.6
9	J	78	LYS	2.6
5	E	64	LEU	2.6
6	G	72	PRO	2.6
27	X	416	U	2.6
27	X	147	G	2.6
27	X	2477	C	2.6
6	G	161	GLN	2.6
13	N	91	ASN	2.6
11	L	111	GLY	2.6
27	X	1477	C	2.6
27	X	2199	C	2.6
4	D	40	LEU	2.6
25	2	42	LEU	2.6
27	X	560	G	2.5
4	D	121	ALA	2.5
19	T	14	ARG	2.5
4	D	85	VAL	2.5
6	G	165	VAL	2.5
27	X	432	C	2.5
6	G	109	GLY	2.5
27	X	1225	G	2.5
4	D	103	LEU	2.5
20	U	52	ARG	2.5
20	U	34	THR	2.5
5	E	136	ILE	2.4
1	A	219	PRO	2.4
11	L	18	ARG	2.4
27	X	417	C	2.4
27	X	1469	U	2.4
27	X	2088	U	2.4
4	D	125	ARG	2.4
13	N	76	TYR	2.4
27	X	661	C	2.4
6	G	163	PRO	2.4
1	A	23	GLY	2.4
27	X	2582	G	2.4
24	1	40	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
17	R	102	LYS	2.4
27	X	2444	C	2.4
5	E	111	HIS	2.4
27	X	1102	G	2.4
3	C	41	GLY	2.4
8	I	48	PHE	2.4
8	I	15	ASP	2.4
11	L	40	ALA	2.4
18	S	165	GLU	2.4
4	D	75	SER	2.3
27	X	303	C	2.3
27	X	434	C	2.3
9	J	82	THR	2.3
8	I	40	ARG	2.3
16	Q	62	ARG	2.3
15	P	19	LYS	2.3
19	T	69	PHE	2.3
4	D	84	PRO	2.3
17	R	67	GLY	2.3
18	S	86	VAL	2.3
9	J	7	ARG	2.3
27	X	1365	U	2.3
27	X	1467	U	2.3
26	3	44	LYS	2.3
27	X	984	A	2.3
18	S	167	THR	2.3
27	X	1266	G	2.3
1	A	24	LEU	2.3
14	O	11	GLN	2.3
9	J	72	ASP	2.3
12	M	40	ARG	2.3
27	X	48	A	2.3
27	X	71	A	2.3
8	I	81	GLN	2.3
9	J	91	VAL	2.3
24	1	35	LEU	2.3
27	X	1083	C	2.3
11	L	89	PHE	2.2
10	K	94	TYR	2.2
1	A	252	LYS	2.2
25	2	3	ARG	2.2
26	3	30	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
6	G	97	ASP	2.2
27	X	2289	A	2.2
5	E	139	GLN	2.2
27	X	537	C	2.2
20	U	79	GLU	2.2
20	U	62	LEU	2.2
20	U	47	HIS	2.2
28	Y	46	G	2.2
11	L	51	LEU	2.2
27	X	1663	C	2.2
28	Y	14	C	2.2
2	B	61	LYS	2.2
11	L	85	LYS	2.2
13	N	49	ASP	2.2
26	3	62	LEU	2.2
4	D	119	PRO	2.2
14	O	9	GLY	2.2
27	X	656	U	2.2
9	J	134	LYS	2.2
27	X	955	G	2.2
27	X	2330	G	2.2
1	A	239	ARG	2.2
17	R	74	LEU	2.2
24	1	47	HIS	2.1
1	A	21	PHE	2.1
6	G	137	LYS	2.1
8	I	64	GLY	2.1
7	H	117	GLU	2.1
27	X	1070	G	2.1
27	X	2018	G	2.1
26	3	10	ALA	2.1
14	O	21	ARG	2.1
24	1	11	LYS	2.1
24	1	46	LYS	2.1
28	Y	123	U	2.1
1	A	244	ARG	2.1
5	E	10	ALA	2.1
11	L	31	VAL	2.1
27	X	436	A	2.1
27	X	2268	G	2.1
27	X	246	C	2.1
27	X	332	C	2.1

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Mol	Chain	Res	Type	RSRZ
27	X	346	C	2.1
1	A	33	LEU	2.1
5	E	71	LEU	2.1
10	K	31	GLU	2.1
9	J	11	ARG	2.1
8	I	41	SER	2.1
14	O	80	TYR	2.1
27	X	1185	C	2.1
27	X	413	G	2.1
3	C	47	THR	2.1
14	O	46	VAL	2.1
1	A	52	ARG	2.0
1	A	263	ARG	2.0
12	M	38	LYS	2.0
18	S	22	VAL	2.0
27	X	1069	G	2.0
1	A	46	ARG	2.0
2	B	159	HIS	2.0
17	R	60	PRO	2.0
8	I	54	SER	2.0
1	A	102	LYS	2.0
24	1	23	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
29	MG	X	2944	1/1	0.65	0.71	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MG	X	2926	1/1	0.66	0.76	32,32,32,32	0
29	MG	X	2908	1/1	0.68	0.56	31,31,31,31	0
29	MG	X	2948	1/1	0.71	0.40	48,48,48,48	0
29	MG	X	2924	1/1	0.72	0.42	77,77,77,77	0
29	MG	X	2922	1/1	0.73	0.35	30,30,30,30	0
29	MG	X	2950	1/1	0.74	0.31	37,37,37,37	0
29	MG	X	2910	1/1	0.75	0.60	39,39,39,39	0
29	MG	X	2904	1/1	0.76	0.29	29,29,29,29	0
29	MG	X	2919	1/1	0.76	0.37	59,59,59,59	0
29	MG	X	2947	1/1	0.77	0.36	49,49,49,49	0
29	MG	X	2912	1/1	0.78	0.39	27,27,27,27	0
29	MG	X	2914	1/1	0.78	0.35	26,26,26,26	0
29	MG	K	201	1/1	0.80	0.27	25,25,25,25	0
29	MG	X	2930	1/1	0.82	0.39	30,30,30,30	0
29	MG	X	2934	1/1	0.83	0.38	42,42,42,42	0
29	MG	X	2941	1/1	0.83	0.46	115,115,115,115	0
29	MG	X	2925	1/1	0.83	0.38	32,32,32,32	0
29	MG	X	2917	1/1	0.84	1.26	55,55,55,55	0
29	MG	X	2931	1/1	0.84	0.26	25,25,25,25	0
29	MG	X	2909	1/1	0.85	0.29	51,51,51,51	0
29	MG	X	2903	1/1	0.85	0.39	30,30,30,30	0
29	MG	X	2937	1/1	0.86	0.20	36,36,36,36	0
29	MG	X	2915	1/1	0.86	0.30	28,28,28,28	0
29	MG	X	2911	1/1	0.86	0.70	40,40,40,40	0
29	MG	X	2933	1/1	0.87	0.28	55,55,55,55	0
29	MG	X	2905	1/1	0.87	0.28	27,27,27,27	0
29	MG	X	2902	1/1	0.87	0.37	33,33,33,33	0
29	MG	X	2932	1/1	0.87	0.37	39,39,39,39	0
29	MG	X	2906	1/1	0.88	0.61	27,27,27,27	0
29	MG	X	2901	1/1	0.88	0.26	37,37,37,37	0
29	MG	X	2945	1/1	0.88	0.56	61,61,61,61	0
29	MG	X	2935	1/1	0.89	0.40	74,74,74,74	0
29	MG	X	2929	1/1	0.89	0.45	37,37,37,37	0
29	MG	X	2938	1/1	0.89	0.52	27,27,27,27	0
29	MG	X	2940	1/1	0.89	0.49	54,54,54,54	0
29	MG	X	2949	1/1	0.89	0.24	32,32,32,32	0
29	MG	X	2928	1/1	0.89	0.21	36,36,36,36	0
29	MG	X	2927	1/1	0.90	0.12	69,69,69,69	0
29	MG	X	2921	1/1	0.91	0.51	51,51,51,51	0
29	MG	X	2907	1/1	0.91	0.91	42,42,42,42	0
29	MG	X	2913	1/1	0.91	0.31	27,27,27,27	0
29	MG	X	2918	1/1	0.92	0.41	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MG	X	2936	1/1	0.93	0.24	33,33,33,33	0
29	MG	X	2939	1/1	0.93	0.21	32,32,32,32	0
29	MG	X	2923	1/1	0.95	0.21	33,33,33,33	0
29	MG	X	2916	1/1	0.95	0.29	26,26,26,26	0
29	MG	X	2920	1/1	0.95	0.30	41,41,41,41	0
29	MG	X	2946	1/1	0.95	0.96	27,27,27,27	0
29	MG	X	2943	1/1	0.97	0.20	31,31,31,31	0
29	MG	X	2942	1/1	0.97	0.17	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.