



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:03 AM UTC

PDB ID : 4IOC / pdb_00004ioc
Title : Crystal structure of compound 4f bound to large ribosomal subunit (50S) from *Deinococcus radiodurans*
Authors : Han, S.; Marr, E.S.
Deposited on : 2013-01-07
Resolution : 3.60 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

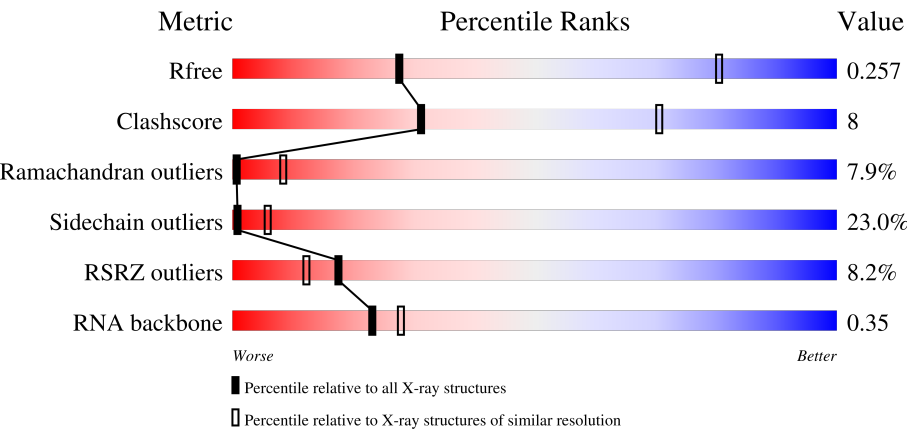
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)
RNA backbone	3983	1014 (4.14-3.06)

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	X	2880	4% 43%34%14%•7%
2	Y	123	4% 48%29%18%••
3	A	274	9% 45%29%11%•12%
4	B	211	% 59%26%9%••

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	141	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	
29	3	66	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	4	37	62% 68% 30%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	M	201	-	-	-	X
31	MG	X	2903	-	-	-	X
31	MG	X	2905	-	-	-	X
31	MG	X	2906	-	-	-	X
31	MG	X	2907	-	-	-	X
31	MG	X	2909	-	-	-	X
31	MG	X	2910	-	-	-	X
31	MG	X	2913	-	-	-	X
31	MG	X	2917	-	-	-	X
31	MG	X	2920	-	-	-	X
31	MG	X	2924	-	-	-	X
31	MG	X	2928	-	-	-	X
31	MG	Y	202	-	-	-	X
31	MG	Y	204	-	-	-	X

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 83877 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2686	Total	C	N	O	P	0	0	0
			57651	25718	10642	18606	2685			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	122	Total	C	N	O	P	0	0	0
			2598	1161	476	840	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	240	Total	C	N	O	S	0	0	0
			1826	1137	366	321	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	197	Total	C	N	O	S	0	0	0
			1506	935	287	282	2			

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

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

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

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

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	71	Total	C	N	O	S	0	0	0
			503	310	91	99	3			

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	141	Total	C	N	O	S	0	0	0
			1067	655	216	196				

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

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

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	127	Total	C	N	O	S	0	0	0
			1014	639	199	174	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

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

- Molecule 20 is a protein called 50S ribosomal protein L24.

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

- Molecule 21 is a protein called 50S ribosomal protein L25.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	84	Total	C	N	O	S	0	0	0
			625	393	122	109	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	66	Total	C	N	O	S	0	0	0
			533	327	107	96	3			

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	1	53	Total C	0	0	53
			53 53			

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	2	46	Total C 46 46	0	0	46

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	3	63	Total C 63 63	0	0	63

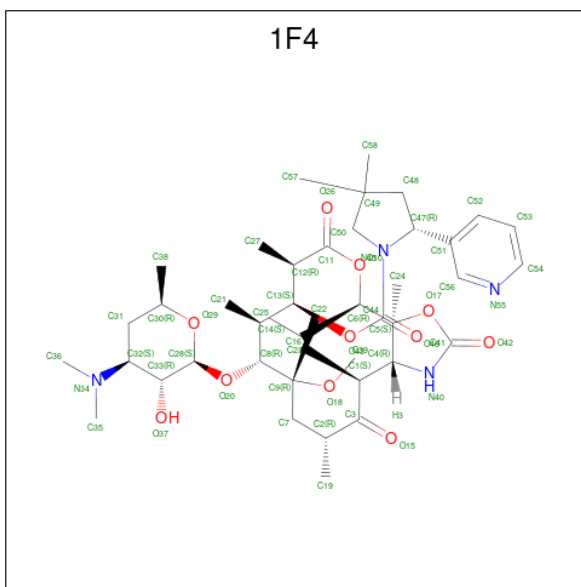
- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	4	37	Total C N O S 297 179 66 47 5	0	0	0

- Molecule 31 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	28	Total Mg 28 28	0	0
31	Y	6	Total Mg 6 6	0	0
31	M	1	Total Mg 1 1	0	0

- Molecule 32 is (3aS,4R,7R,8S,9S,10R,11R,13R,15S,15aR)-4-ethyl-11-methoxy-3a,7,9,11,13,15-hexamethyl-2,6,14-trioxo-10-[[3,4,6-trideoxy-3-(dimethylamino)-beta-D-xylo-hexopyranosyl]oxy]tetradecahydro-2H-oxacyclotetradecino[4,3-d][1,3]oxazol-8-yl (2R)-4,4-dimethyl-2-(pyridin-3-yl)pyrrolidine-1-carboxylate (CCD ID: 1F4) (formula: C₄₃H₆₈N₄O₁₁).

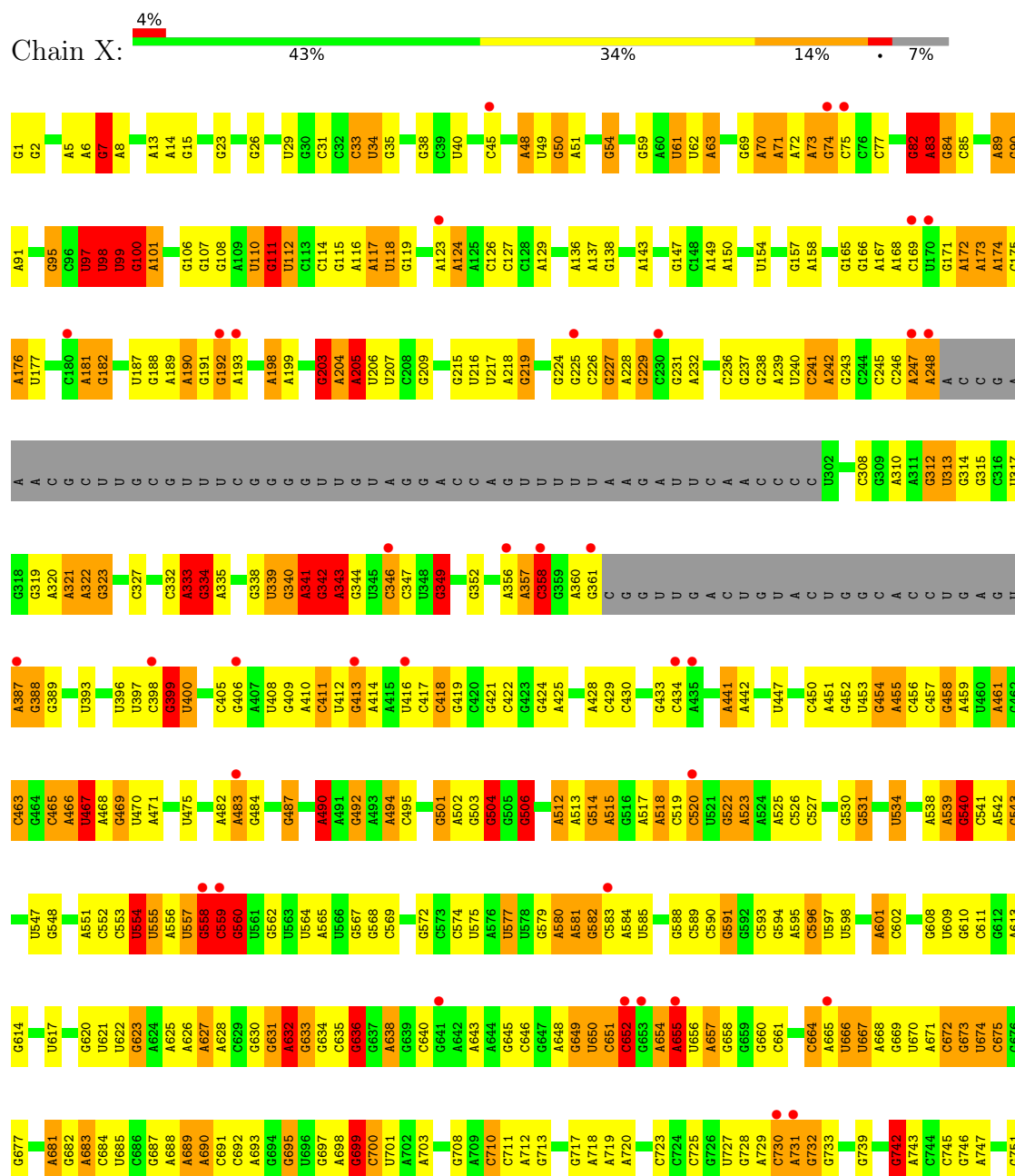


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	X	1	Total	C	N	O	0	0
			58	43	4	11		

3 Residue-property plots

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

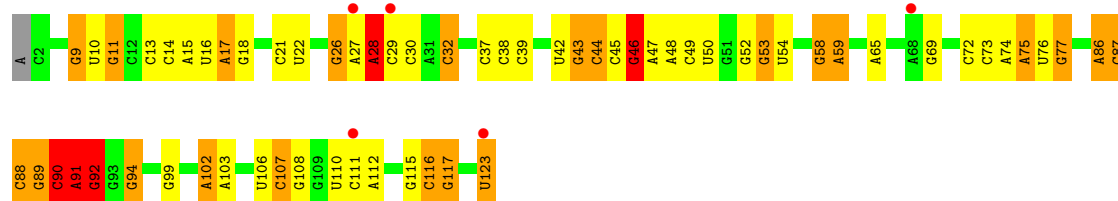
- Molecule 1: 23S ribosomal RNA



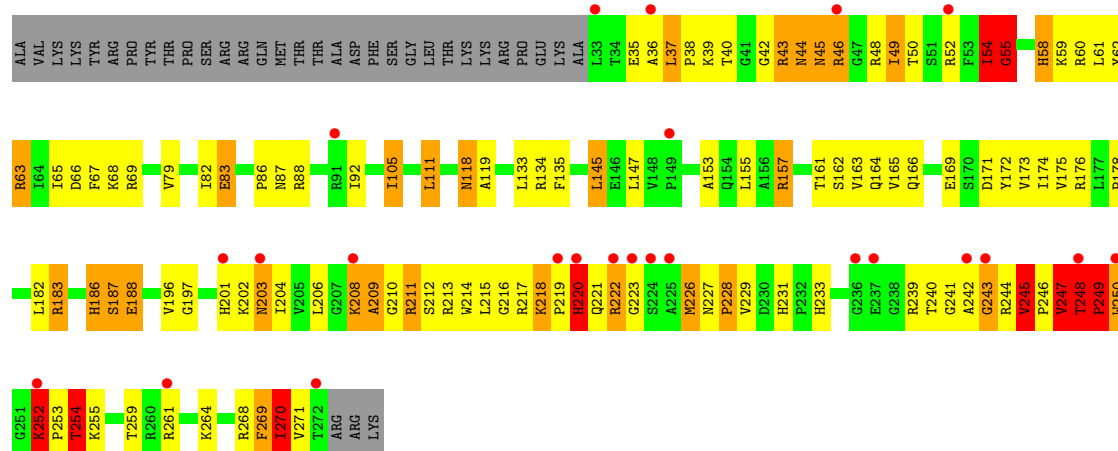
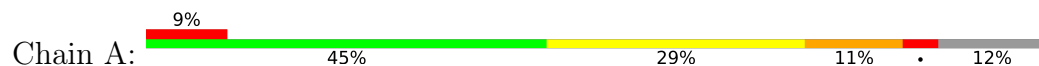


A1800	C1801	U1804	G1805	G1806	A1807	C1808	U1809	U1810	A1811	U1812	A1813	U1817	U1818	U1819	G1820	A1821	C1825	C1830	G1832	G1831	U1833	C1835	C1836	G1839	A1840	A1845	A1846	G1847	G1850	A1851	G1852	U1856	A1859	A1860	G1861	A1867	G1874	U1881	G1882	A1883	A1884	G1885	G1886	G1887	G1888	G										
G	C	C	C	G	U	A	U	A	U	A	A	C	G	G	U	C	U1909	G1903	G1911	G1912	G1913	G1918	A1919	U1920	A1921	U1922	U1923	C1924	C1925	U1926	U1927	U1928	U1929	C1930	A1935	A1936	G1937	U1938	U1939	C1940	A1943	U1946	G1947	C1948	A1949	C1950	G1951	A1952	A1953	A1954	G1955	G1958				
U1959	A1960	G1963	U1964	A1965	C1966	C1971	G1972	C1973	U1974	G1975	U1976	C1977	U1978	U1979	A1980	A1981	C1982	G1983	A1984	G1985	G1986	G1987	A1988	C1989	U1990	C1991	G1992	U1993	U1994	G1995	A1996	A1997	A1998	U1999	A2002	A2003	U2004	U2005	G2006	G2007	U2007	C2008	U2009	G2010	U2011	A2012	A2013	G2014	A2015	A2016	U2017	G2018	C2019	U2024	A2025	C2026
C2027	C2028	G2029	U2030	A2031	C2032	C2033	A2034	C2035	C2038	G2039	A2040	A2041	A2042	G2043	G2044	A2045	C2046	C2047	C2048	U2051	G2052	G2053	A2054	C2055	C2056	U2062	A2063	U2064	A2065	G2066	G2070	G2071	C2072	U2075	G2076	G2077	G2078	A2079	U2080	C2081	C2082	G2083	U2088	C2089	C	U	A	G	C	U	G	G				
G	A	U	A	G	U	U	G	G	A	C	C	C	U	U	G	G	A	A	C	C	C	G	C	U	U	U	U	U	G	G	G	C	U	U	G	U	U	C	C	G	G	U	C	C	C	C	C	C	C	C	C					
A	C	C	C	U	G	A2165	G2166	C2170	U2171	U2172	G2173	G2174	A2181	U2185	A2189	A2190	A2191	U2192	C2193	A2194	C2195	U2196	U2197	U2198	C2199	G2200	G2201	A2204	C2205	U2208	G2209	C2210	U2211	U2212	G2213	G2214	C2215	G2216	G2217	U2218	U2219	A2220	G2221	U2222	U2223	U2224	G2225	A2226	C2227	U2228	G2229	G2230	U2322			
G2235	U2236	C2237	U2241	A2245	A2246	A2247	A2252	A2253	C2254	G2255	G2256	A2257	G2258	G2261	C2262	A2265	A2266	A2267	G2268	U2269	U2270	C2271	A2277	A2278	G2283	U2284	U2285	G2286	G2287	A2288	A2289	A2290	U2291	C2295	U2298	A2299	G2300	A2301	C2305	A2306	A2312	G2313	G2314	A2315	G2320	C2321	U2322									
U2323	G2324	A2325	U2326	U2327	C2328	C2329	G2330	A2333	C2338	A2339	C2340	C2343	G2344	G2351	A2352	G2353	A2357	C2358	G2362	G2363	C2364	A2367	C2368	U2369	G2370	A2371	C2372	G2373	C2374	G2375	G2376	A2381	C2382	G2383	C2384	U2386	G2386	U2387	G2388	G2389	G2392	G2393	G2394	C2395	C2396	A2397	U2398	G2399	G2400	A2401						
U2402	C2403	A2404	A2405	C2406	G2407	A2408	A2409	U2410	A2413	A2414	G2415	A2418	C2420	C2421	G2422	G2423	G2426	A2427	U2428	A2438	U2439	C2446	A2448	U2452	C2453	C2454	A2455	U2456	A2457	U2458	C2459	G2460	G2461	C2462	G2463	G2466	U2470	U2471	U2472	C2477	C2480	G2481	A2482	U2483	G2484	U2485	C2486									
G2487	G2488	C2489	U2490	C2491	G2492	U2493	C2494	G2495	A2496	C2497	U2498	C2499	G2504	C2505	C2506	U2507	G2508	A2509	A2510	G2511	A2512	G2513	G2514	G2515	U2516	C2517	G2518	C2519	G2522	G2523	U2526	G2527	G2528	G2529	C2530	A2543	A2544	A2545	G2546	C2547	G2548	A2551	C2552	G2553	A2556	G2557	C2558	U2559	G2560	G2561	U2562	U2564				
C2565	A2566	C2567	A2568	U2572	C2573	G2574	A2577	C2578	U2579	A2580	A2581	G2582	C2585	C2586	U2587	U2588	C2589	U2590	C2591	U2592	A2593	U2594	C2595	C2596	C2597	C2598	U2599	G2604	C2605	U2608	G2609	G2610	A2611	G2612	A2613	U2614	U2615	U2616	G2617	A2618	U2619	G2620	C2621	G2627	C2628	A2633	G2634	G2640	U2641	U2642	U2643	G2643				
A2644	A2649	C2650	A2653	A2654	C2655	G2656	G2657	A2658	C2659	C2660	G2661	U2662	U2663	C2667	U2668	C2669	C2670	C2671	C2678	C2683	A2684	C2687	U2688	C2689	A2690	C2691	U2692	U2693	C2694	C2695	A2696	G2697	G2698	C2699	U2700	C2703	U2704	A2705	U2706	G2707	U2708	A2713	U2714	C2715	U2718	U2719	U2720	A2721	G2724							
U2728	A2729	U2730	G2731	C2732	C2735	U2736	A2737	U2745	C2748	U2758	U2759	G2760	C2767	C2768	C2769	A2770	C2771	U2774	U2775	U2776	A2777	U2778	C2779	A2780	C2781	U2782	U2783	A2784	A2785	C2788	C2791	U2792	G2793	U2794	A2795	U2796	U2797	A2798	C2799	C2800	C2803	U2804	G2805	U2807	U2808	A2809	U2810	G2811								
G2813	G2821	U2822	G2823	C2824	A2825	G2832	G2837	U2841	C2842	A2843	G2846	U2847	C2848	U2849	G2854	C2855	U2856	C2857	A2858	U2859	C2860	A2861	C2864	C2865	A2866	C2867	G2868	A2877	C	U	C																									

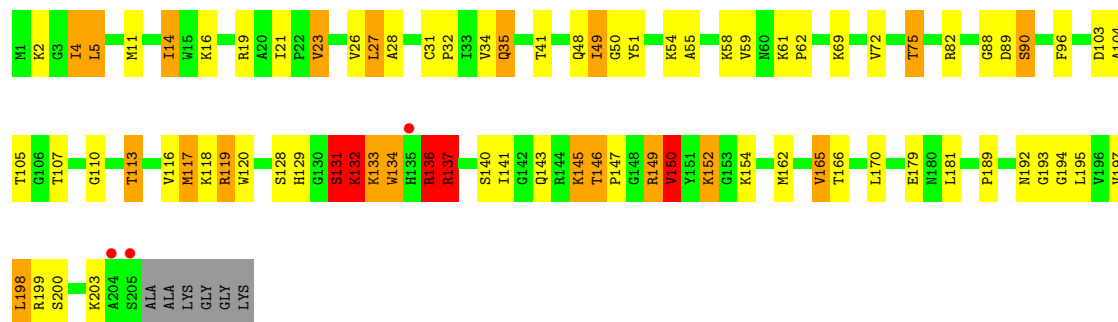
• Molecule 2: 5S ribosomal RNA



• Molecule 3: 50S ribosomal protein L2

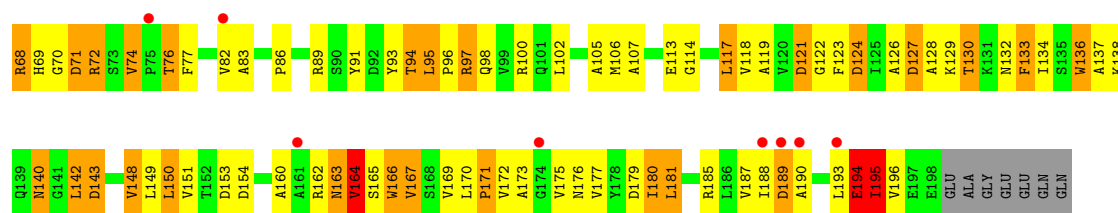


• Molecule 4: 50S ribosomal protein L3

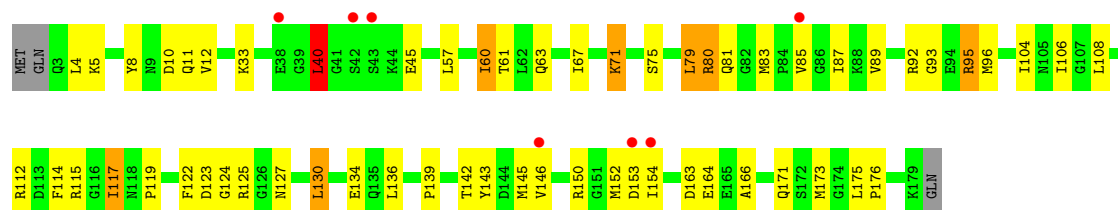


• Molecule 5: 50S ribosomal protein L4

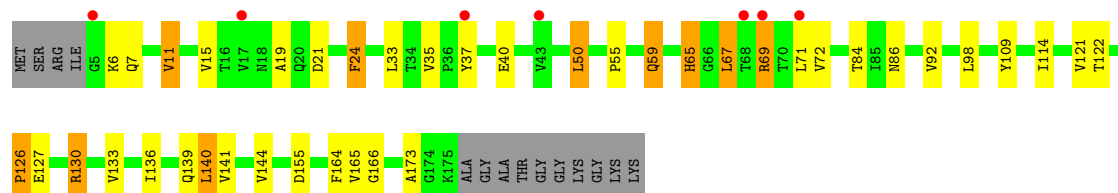




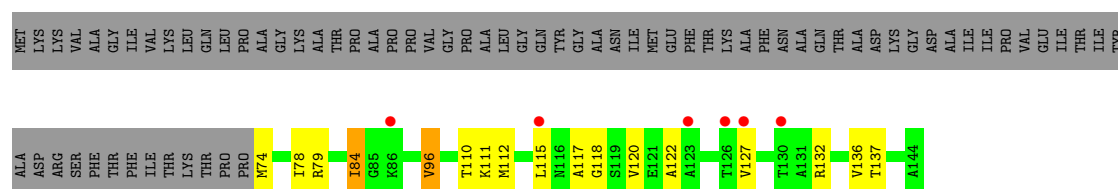
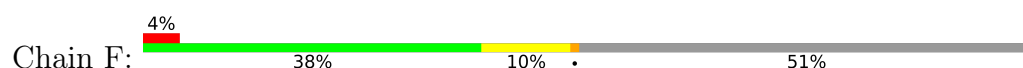
• Molecule 6: 50S ribosomal protein L5



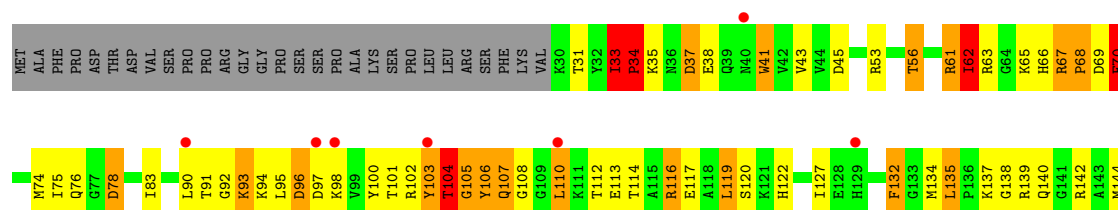
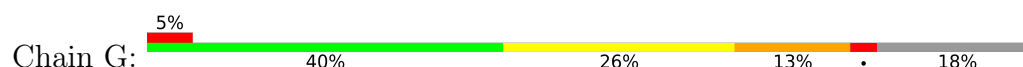
• Molecule 7: 50S ribosomal protein L6

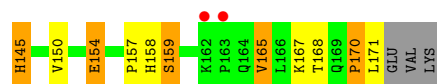


• Molecule 8: 50S ribosomal protein L11



• Molecule 9: 50S ribosomal protein L13

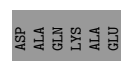
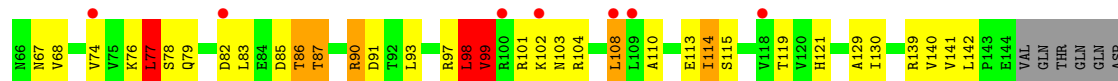
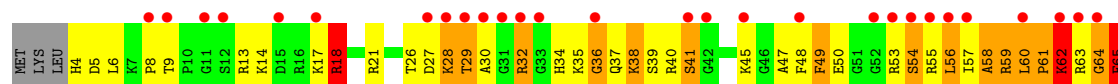




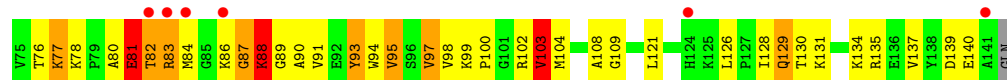
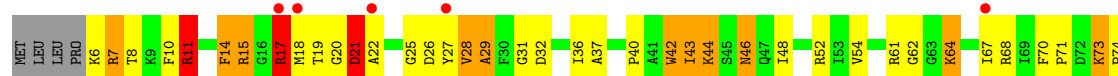
- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L16



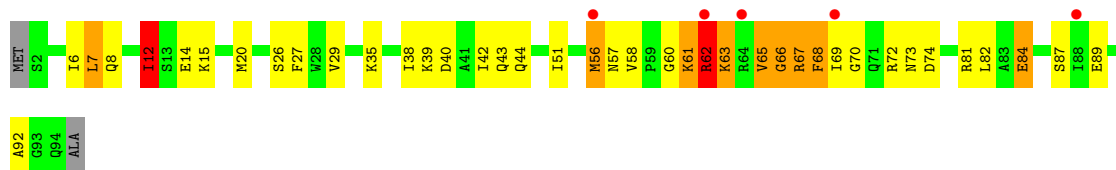
- Molecule 13: 50S ribosomal protein L17



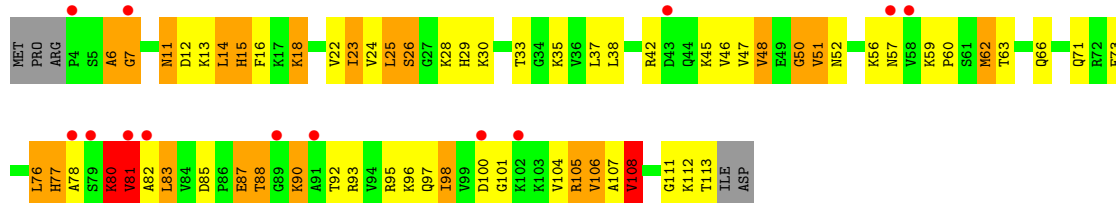
- Molecule 14: 50S ribosomal protein L18



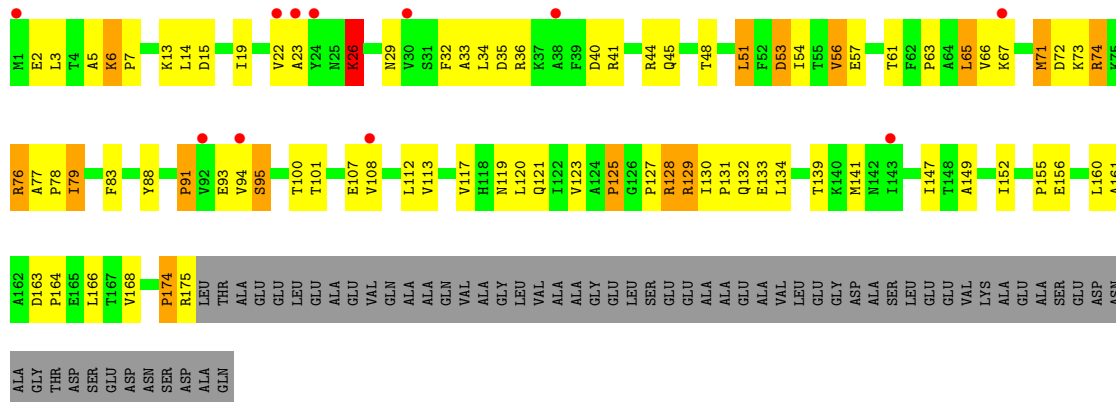
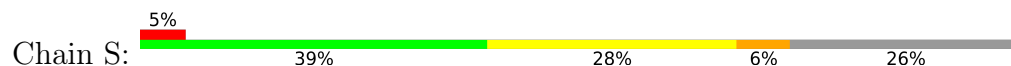
- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24



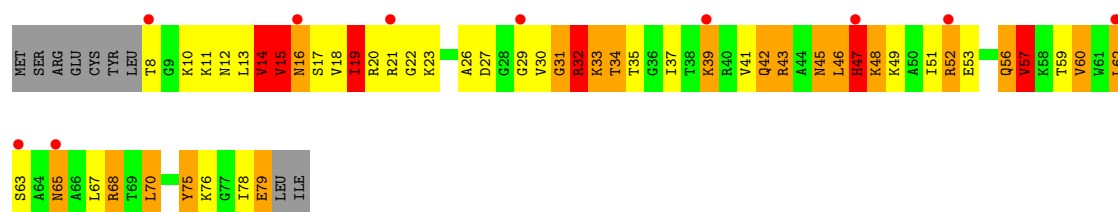
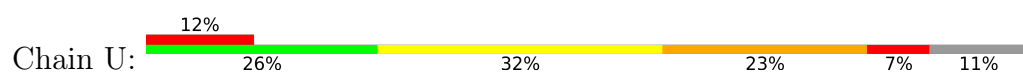
- Molecule 21: 50S ribosomal protein L25



- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



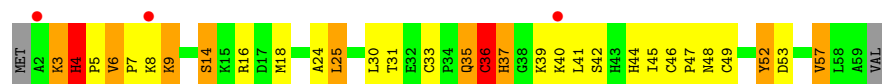
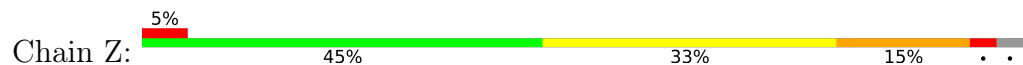
- Molecule 24: 50S ribosomal protein L29



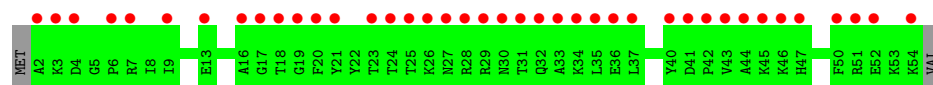
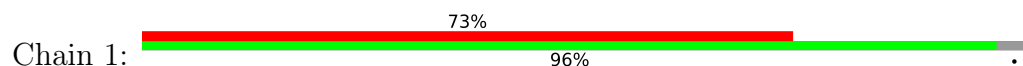
- Molecule 25: 50S ribosomal protein L30



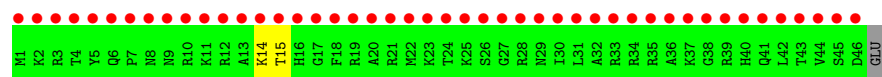
- Molecule 26: 50S ribosomal protein L32



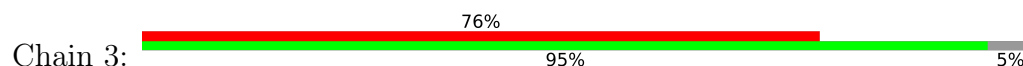
- Molecule 27: 50S ribosomal protein L33

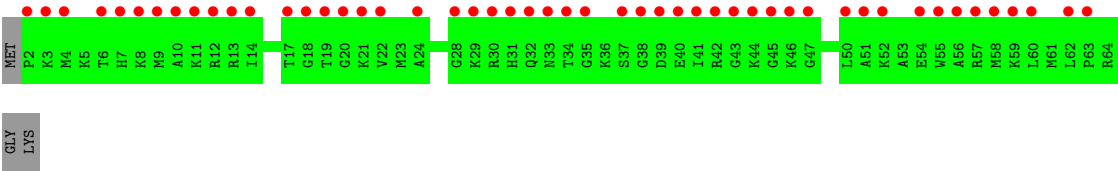


- Molecule 28: 50S ribosomal protein L34

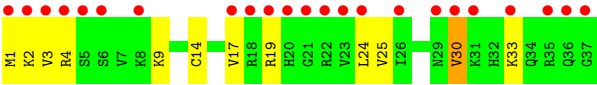


- Molecule 29: 50S ribosomal protein L35





● Molecule 30: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.64Å 408.49Å 692.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.60 30.00 – 3.61	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.60) 88.3 (30.00-3.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 3.65Å)	Xtriage
Refinement program	autoBUSTER	Depositor
R, R_{free}	0.198 , 0.239 0.215 , 0.257	Depositor DCC
R_{free} test set	12232 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å ²)	129.2	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 91.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	83877	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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: 1F4, 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	X	0.71	27/64561 (0.0%)	1.39	857/100708 (0.9%)
2	Y	0.82	2/2904 (0.1%)	1.35	31/4525 (0.7%)
3	A	0.97	6/1862 (0.3%)	1.58	38/2510 (1.5%)
4	B	0.94	1/1567 (0.1%)	1.51	16/2105 (0.8%)
5	C	1.03	3/1529 (0.2%)	1.70	28/2070 (1.4%)
6	D	0.87	0/1419	1.35	5/1903 (0.3%)
7	E	0.86	0/1308	1.39	5/1771 (0.3%)
8	F	0.93	0/508	1.36	1/683 (0.1%)
9	G	0.94	1/1138 (0.1%)	1.62	18/1539 (1.2%)
10	H	0.90	2/1007 (0.2%)	1.44	11/1352 (0.8%)
11	I	1.14	4/1081 (0.4%)	1.80	32/1448 (2.2%)
12	J	1.46	7/1113 (0.6%)	1.75	36/1486 (2.4%)
13	K	1.08	5/886 (0.6%)	1.64	20/1188 (1.7%)
14	L	0.90	0/785	1.71	17/1048 (1.6%)
15	M	0.97	1/884 (0.1%)	1.66	18/1186 (1.5%)
16	N	0.87	0/994	1.57	14/1323 (1.1%)
17	O	0.89	0/750	1.62	14/1000 (1.4%)
18	P	0.95	1/1027 (0.1%)	1.57	11/1373 (0.8%)
19	Q	0.93	0/737	1.67	14/988 (1.4%)
20	R	1.09	1/835 (0.1%)	1.78	25/1121 (2.2%)
21	S	1.11	0/1370	1.50	12/1862 (0.6%)
22	T	0.93	0/633	1.54	11/838 (1.3%)
23	U	1.28	4/556 (0.7%)	1.94	27/741 (3.6%)
24	V	0.91	0/537	1.62	6/714 (0.8%)
25	W	0.88	0/426	1.53	3/568 (0.5%)
26	Z	1.02	0/469	1.68	8/629 (1.3%)
30	4	0.98	0/298	1.33	0/390
All	All	0.80	65/91184 (0.1%)	1.44	1278/137069 (0.9%)

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	X	0	3

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	R	77	HIS	CA-C	9.55	1.56	1.52
4	B	117	MET	SD-CE	9.25	2.02	1.79
11	I	29	THR	CA-C	7.92	1.63	1.52
1	X	559	C	C3'-O3'	7.65	1.53	1.42
1	X	655	A	C3'-O3'	7.32	1.53	1.42
11	I	28	LYS	CA-C	7.00	1.61	1.53
15	M	29	PRO	CA-C	6.92	1.62	1.52
3	A	242	ALA	CA-C	6.85	1.61	1.52
13	K	12	ARG	CA-C	6.79	1.61	1.52
1	X	393	U	C1'-N1	6.63	1.58	1.48
23	U	46	LEU	CA-C	6.56	1.61	1.52
12	J	19	THR	CA-C	6.52	1.60	1.52
13	K	8	ARG	C-N	6.30	1.42	1.33
1	X	236	C	C1'-N1	6.30	1.57	1.48
1	X	434	C	C1'-N1	6.22	1.56	1.47
1	X	346	C	C1'-N1	6.17	1.57	1.48
1	X	1674	C	C3'-O3'	-6.03	1.33	1.42
23	U	47	HIS	C-N	6.02	1.41	1.33
1	X	646	C	C1'-N1	5.99	1.57	1.48
1	X	927	C	C1'-N1	5.92	1.57	1.48
11	I	63	ARG	CA-C	5.88	1.59	1.52
1	X	868	U	C1'-N1	5.85	1.57	1.48
1	X	2189	A	C3'-O3'	5.81	1.50	1.42
1	X	917	U	C1'-N1	5.80	1.57	1.48
1	X	1522	C	C1'-N1	5.72	1.57	1.48
5	C	66	ASN	C-N	5.70	1.41	1.33
10	H	1	MET	SD-CE	-5.70	1.65	1.79
3	A	203	ASN	CA-CB	5.68	1.63	1.53
1	X	1946	U	C1'-N1	5.65	1.56	1.48
1	X	1909	U	C1'-N1	5.59	1.55	1.47
10	H	124	MET	SD-CE	5.51	1.93	1.79
23	U	18	VAL	CA-C	5.50	1.57	1.52
1	X	31	C	C1'-N1	5.50	1.56	1.48
12	J	83	ARG	C-N	5.50	1.41	1.33
12	J	11	ARG	CA-C	5.50	1.60	1.52
12	J	86	LYS	CA-C	5.49	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	241	GLY	C-N	5.49	1.41	1.33
2	Y	32	C	C1'-N1	5.47	1.56	1.48
9	G	110	LEU	CA-CB	5.47	1.59	1.52
11	I	29	THR	C-N	5.46	1.40	1.33
1	X	422	C	C1'-N1	5.38	1.56	1.48
23	U	46	LEU	C-N	5.37	1.41	1.33
12	J	17	ARG	CA-C	5.35	1.59	1.52
18	P	60	ILE	C-N	5.35	1.37	1.33
1	X	327	C	C1'-N1	5.35	1.56	1.48
1	X	2072	C	C1'-N1	5.34	1.56	1.48
1	X	1182	U	C1'-N1	5.34	1.56	1.48
1	X	2321	C	C1'-N1	5.34	1.56	1.48
1	X	1825	C	C1'-N1	5.31	1.56	1.48
1	X	358	C	C1'-N1	5.28	1.56	1.48
3	A	54	ILE	CA-CB	5.26	1.61	1.54
1	X	430	C	C1'-N1	5.26	1.56	1.48
5	C	66	ASN	CA-CB	5.24	1.62	1.53
3	A	239	ARG	CA-C	5.18	1.59	1.52
1	X	1467	U	C1'-N1	5.17	1.56	1.48
13	K	3	HIS	CA-C	5.11	1.63	1.52
1	X	916	U	C1'-N1	5.10	1.56	1.48
5	C	66	ASN	CA-C	5.08	1.59	1.52
2	Y	87	C	C3'-O3'	5.08	1.49	1.42
12	J	18	MET	CA-C	5.07	1.59	1.52
3	A	54	ILE	CA-C	5.05	1.59	1.52
13	K	8	ARG	CA-C	5.04	1.59	1.52
13	K	52	ILE	CG1-CD1	5.04	1.71	1.51
12	J	15	ARG	CA-C	5.03	1.59	1.52
1	X	2208	U	C1'-N1	5.01	1.55	1.48

All (1278) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1288	A	C1'-O4'-C4'	-24.41	85.29	109.70
1	X	1288	A	C5'-C4'-O4'	15.03	131.64	109.10
1	X	1019	U	P-O3'-C3'	14.88	142.51	120.20
1	X	559	C	C4'-C3'-C2'	-14.06	88.54	102.60
3	A	203	ASN	CA-CB-CG	12.60	125.20	112.60
1	X	1468	A	O4'-C1'-C2'	-12.60	95.00	107.60
1	X	2564	U	P-O3'-C3'	12.50	138.95	120.20
1	X	176	A	P-O3'-C3'	12.44	138.86	120.20
1	X	655	A	P-O3'-C3'	12.29	138.64	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1975	G	C2'-C3'-O3'	12.00	127.50	109.50
1	X	558	G	P-O3'-C3'	11.99	138.18	120.20
1	X	1775	A	P-O3'-C3'	11.78	137.87	120.20
1	X	1473	U	P-O3'-C3'	11.29	137.13	120.20
1	X	204	A	P-O3'-C3'	11.23	137.05	120.20
1	X	33	C	P-O3'-C3'	11.12	136.88	120.20
1	X	1288	A	C4'-C3'-C2'	-11.03	91.57	102.60
1	X	841	G	O4'-C4'-C3'	-11.00	93.00	104.00
1	X	1634	A	P-O3'-C3'	10.99	136.69	120.20
1	X	100	G	P-O3'-C3'	10.98	136.66	120.20
1	X	2497	A	P-O3'-C3'	10.79	136.38	120.20
1	X	2736	U	P-O3'-C3'	10.66	136.19	120.20
1	X	2018	G	P-O3'-C3'	10.64	136.16	120.20
1	X	814	G	P-O3'-C3'	10.61	136.11	120.20
1	X	1790	G	P-O3'-C3'	10.61	136.11	120.20
1	X	342	G	P-O3'-C3'	10.48	135.92	120.20
1	X	2312	A	P-O3'-C3'	10.32	135.68	120.20
1	X	994	A	P-O3'-C3'	10.31	135.66	120.20
1	X	334	G	P-O3'-C3'	10.19	135.48	120.20
1	X	788	G	P-O3'-C3'	10.12	135.38	120.20
1	X	1475	U	P-O3'-C3'	10.05	135.28	120.20
1	X	1288	A	O4'-C4'-C3'	-10.05	96.05	106.10
1	X	2854	G	N9-C1'-C2'	10.03	129.04	114.00
1	X	181	A	P-O3'-C3'	9.99	135.19	120.20
1	X	664	C	P-O3'-C3'	9.92	135.08	120.20
1	X	48	A	P-O3'-C3'	9.80	134.89	120.20
1	X	683	A	P-O3'-C3'	9.75	134.82	120.20
1	X	1036	G	P-O3'-C3'	9.73	134.79	120.20
1	X	1938	U	P-O3'-C3'	9.68	134.71	120.20
1	X	469	G	P-O3'-C3'	9.67	134.71	120.20
1	X	2323	U	P-O3'-C3'	9.65	134.68	120.20
1	X	2854	G	C1'-O4'-C4'	-9.65	100.05	109.70
1	X	2330	G	N9-C1'-C2'	9.59	126.38	112.00
1	X	559	C	P-O3'-C3'	9.56	134.54	120.20
9	G	70	PHE	CA-CB-CG	9.49	123.29	113.80
1	X	2691	C	P-O3'-C3'	9.48	134.42	120.20
1	X	399	G	P-O3'-C3'	9.46	134.40	120.20
1	X	1249	G	P-O3'-C3'	9.43	134.34	120.20
1	X	822	G	P-O3'-C3'	9.42	134.34	120.20
1	X	2261	G	P-O3'-C3'	9.31	134.17	120.20
5	C	66	ASN	CA-CB-CG	9.30	121.90	112.60
1	X	1249	G	C2'-C3'-O3'	9.16	123.23	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	218	A	P-O3'-C3'	9.14	133.91	120.20
1	X	73	A	P-O3'-C3'	9.13	133.90	120.20
1	X	1442	C	P-O3'-C3'	9.12	133.88	120.20
1	X	454	G	P-O3'-C3'	9.12	133.87	120.20
1	X	841	G	N9-C1'-C2'	9.11	125.66	112.00
1	X	559	C	O4'-C1'-N1	9.09	122.14	108.50
1	X	514	G	P-O3'-C3'	9.03	133.74	120.20
1	X	1441	A	P-O3'-C3'	9.02	133.72	120.20
2	Y	58	G	P-O3'-C3'	9.02	133.72	120.20
1	X	1811	A	C2'-C3'-O3'	8.95	122.92	109.50
1	X	2593	A	O3'-P-O5'	-8.87	90.69	104.00
1	X	940	G	P-O5'-C5'	8.85	134.17	120.90
11	I	48	PHE	CA-CB-CG	8.82	122.62	113.80
1	X	2298	U	P-O3'-C3'	8.81	133.41	120.20
1	X	2808	U	O4'-C1'-N1	8.80	121.41	108.20
1	X	1288	A	O4'-C1'-N9	8.78	121.37	108.20
1	X	204	A	C2'-C3'-O3'	8.75	122.63	109.50
1	X	2189	A	P-O3'-C3'	8.74	133.30	120.20
1	X	98	U	P-O3'-C3'	8.71	133.26	120.20
1	X	1096	A	P-O3'-C3'	8.71	133.26	120.20
1	X	490	A	P-O3'-C3'	8.71	133.26	120.20
23	U	18	VAL	CA-C-N	8.70	137.63	121.97
23	U	18	VAL	C-N-CA	8.70	137.63	121.97
1	X	1391	A	P-O3'-C3'	8.69	133.24	120.20
1	X	2426	G	P-O3'-C3'	8.68	133.21	120.20
1	X	1574	A	C4'-C3'-C2'	-8.67	93.93	102.60
11	I	28	LYS	N-CA-C	8.66	122.60	109.62
1	X	1122	A	P-O3'-C3'	8.64	133.16	120.20
1	X	346	C	N1-C1'-C2'	8.64	124.96	112.00
1	X	817	A	O4'-C4'-C3'	-8.57	95.43	104.00
1	X	683	A	C2'-C3'-O3'	8.54	122.31	109.50
1	X	242	A	C1'-O4'-C4'	-8.50	101.40	109.90
3	A	211	ARG	N-CA-C	-8.48	101.62	111.03
2	Y	16	U	P-O3'-C3'	8.47	132.91	120.20
11	I	63	ARG	N-CA-C	-8.45	102.91	113.55
4	B	150	VAL	N-CA-CB	8.44	121.12	110.99
1	X	343	A	O4'-C1'-C2'	-8.43	99.17	107.60
1	X	1716	G	O3'-P-O5'	-8.41	91.38	104.00
1	X	577	U	C4'-C3'-C2'	-8.39	94.21	102.60
1	X	1467	U	N1-C1'-C2'	8.37	124.56	112.00
1	X	1923	U	P-O3'-C3'	8.37	132.76	120.20
1	X	554	U	P-O3'-C3'	8.36	132.74	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Q	62	ARG	CA-C-N	8.29	137.38	121.54
19	Q	62	ARG	C-N-CA	8.29	137.38	121.54
1	X	1261	G	P-O3'-C3'	8.29	132.64	120.20
1	X	2824	C	C2'-C3'-O3'	8.28	121.92	109.50
22	T	44	LYS	N-CA-C	-8.28	102.22	111.07
1	X	71	A	P-O3'-C3'	8.25	132.57	120.20
15	M	28	ARG	N-CA-C	-8.25	95.69	108.55
1	X	2770	A	P-O3'-C3'	8.23	132.55	120.20
9	G	120	SER	N-CA-C	-8.20	102.17	112.90
1	X	1186	G	P-O3'-C3'	8.18	132.47	120.20
1	X	2559	U	C4'-C3'-O3'	-8.13	100.80	113.00
1	X	2560	G	C2'-C3'-O3'	8.13	121.70	109.50
1	X	2748	C	C3'-C2'-O2'	8.10	122.85	110.70
15	M	103	LYS	N-CA-C	8.09	123.45	113.50
1	X	774	A	P-O5'-C5'	8.07	133.00	120.90
1	X	333	A	P-O3'-C3'	8.05	132.27	120.20
1	X	2460	G	P-O5'-C5'	8.04	132.97	120.90
1	X	1820	G	P-O3'-C3'	8.02	132.22	120.20
1	X	1923	U	C2'-C3'-O3'	8.01	121.52	109.50
3	A	248	THR	CB-CA-C	8.01	125.95	110.17
1	X	1732	U	P-O3'-C3'	8.01	132.21	120.20
1	X	2544	A	O3'-P-O5'	-8.00	92.00	104.00
1	X	815	A	C4'-C3'-O3'	-7.99	101.02	113.00
1	X	2258	G	C4'-C3'-C2'	-7.98	94.62	102.60
1	X	1053	G	P-O3'-C3'	7.97	132.16	120.20
1	X	2477	C	P-O5'-C5'	7.96	132.84	120.90
1	X	242	A	C4'-C3'-C2'	-7.96	94.64	102.60
1	X	788	G	C2'-C3'-O3'	7.95	121.42	109.50
1	X	483	A	P-O3'-C3'	-7.93	108.30	120.20
1	X	1935	A	N9-C1'-C2'	7.92	123.87	112.00
25	W	48	LYS	CA-C-N	7.90	131.91	120.38
25	W	48	LYS	C-N-CA	7.90	131.91	120.38
1	X	1280	U	P-O3'-C3'	7.89	132.04	120.20
1	X	1055	A	P-O3'-C3'	7.88	132.01	120.20
12	J	93	TYR	N-CA-C	7.87	120.10	108.14
1	X	1469	U	P-O5'-C5'	7.87	132.70	120.90
1	X	1993	G	C1'-C2'-O2'	7.83	120.15	108.40
1	X	33	C	C4'-C3'-O3'	7.83	121.14	109.40
1	X	558	G	C2'-C3'-O3'	7.82	121.23	109.50
1	X	1278	A	O4'-C1'-N9	7.81	119.92	108.20
1	X	2018	G	C1'-O4'-C4'	-7.81	101.89	109.70
5	C	167	VAL	N-CA-C	7.80	120.72	108.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1684	G	P-O3'-C3'	7.80	131.90	120.20
1	X	2731	G	P-O3'-C3'	7.79	131.89	120.20
1	X	1403	U	P-O3'-C3'	7.79	131.88	120.20
1	X	334	G	C2'-C3'-O3'	7.78	121.17	109.50
1	X	1409	U	P-O3'-C3'	7.78	131.87	120.20
1	X	341	A	P-O3'-C3'	7.78	131.87	120.20
2	Y	90	C	P-O3'-C3'	-7.78	108.53	120.20
1	X	504	G	C3'-C2'-O2'	7.77	122.36	110.70
1	X	2593	A	P-O3'-C3'	7.75	131.83	120.20
1	X	321	A	P-O3'-C3'	7.75	131.83	120.20
1	X	1474	A	P-O3'-C3'	7.75	131.82	120.20
1	X	1770	U	C1'-O4'-C4'	-7.74	102.16	109.90
1	X	1775	A	C2'-C3'-O3'	7.67	121.01	109.50
1	X	465	C	P-O5'-C5'	-7.67	109.40	120.90
1	X	1278	A	C1'-O4'-C4'	-7.67	102.03	109.70
1	X	466	A	C2'-C3'-O3'	7.66	121.00	109.50
1	X	610	G	O3'-P-O5'	-7.66	92.51	104.00
22	T	15	ASP	CA-CB-CG	7.65	120.25	112.60
7	E	24	PHE	CA-C-N	7.64	131.56	120.71
7	E	24	PHE	C-N-CA	7.64	131.56	120.71
1	X	690	A	C4'-C3'-C2'	-7.63	94.97	102.60
1	X	1799	A	C1'-O4'-C4'	-7.61	102.09	109.70
1	X	399	G	C2'-C3'-O3'	7.61	120.91	109.50
1	X	2472	U	P-O3'-C3'	-7.60	108.79	120.20
1	X	434	C	P-O3'-C3'	7.60	131.60	120.20
1	X	1278	A	C3'-C2'-C1'	-7.60	93.90	101.50
1	X	1019	U	C4'-C3'-O3'	7.60	120.80	109.40
1	X	89	A	P-O3'-C3'	7.59	131.59	120.20
1	X	813	A	P-O3'-C3'	7.58	131.57	120.20
18	P	115	ASN	CA-CB-CG	7.55	120.15	112.60
1	X	651	C	P-O3'-C3'	7.53	131.50	120.20
1	X	2228	U	P-O3'-C3'	7.53	131.50	120.20
12	J	22	ALA	N-CA-C	7.50	120.85	110.35
1	X	1470	G	P-O5'-C5'	-7.49	109.66	120.90
1	X	2229	G	P-O3'-C3'	7.48	131.42	120.20
1	X	540	G	P-O3'-C3'	7.47	131.41	120.20
1	X	1574	A	C1'-O4'-C4'	-7.46	102.44	109.90
1	X	467	U	P-O3'-C3'	7.45	131.38	120.20
1	X	2730	A	P-O3'-C3'	7.45	131.37	120.20
1	X	2724	G	O5'-C5'-C4'	-7.43	100.36	111.50
5	C	142	LEU	CA-C-N	7.42	130.09	120.44
5	C	142	LEU	C-N-CA	7.42	130.09	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1601	U	P-O3'-C3'	7.41	131.32	120.20
1	X	2493	U	C3'-C2'-O2'	7.40	121.80	110.70
12	J	87	GLY	CA-C-N	7.40	135.67	121.54
12	J	87	GLY	C-N-CA	7.40	135.67	121.54
1	X	1086	C	P-O3'-C3'	7.39	131.29	120.20
1	X	755	C	P-O3'-C3'	-7.39	109.11	120.20
1	X	1353	A	P-O3'-C3'	7.39	131.28	120.20
20	R	81	VAL	N-CA-C	7.38	118.45	108.11
4	B	132	LYS	CA-C-N	7.37	135.23	122.56
4	B	132	LYS	C-N-CA	7.37	135.23	122.56
1	X	557	U	C1'-O4'-C4'	-7.36	102.34	109.70
1	X	2662	C	C4'-C3'-C2'	-7.36	95.24	102.60
1	X	796	A	C4'-C3'-C2'	-7.33	95.27	102.60
7	E	11	VAL	N-CA-C	7.33	114.23	107.56
12	J	19	THR	N-CA-C	7.33	121.09	109.50
1	X	2689	C	P-O3'-C3'	7.33	131.20	120.20
1	X	638	A	P-O3'-C3'	7.33	131.19	120.20
1	X	825	C	P-O3'-C3'	-7.32	109.22	120.20
1	X	1975	G	P-O3'-C3'	7.31	131.17	120.20
1	X	2018	G	N9-C1'-C2'	7.31	124.96	114.00
23	U	48	LYS	N-CA-C	7.31	118.18	107.88
1	X	483	A	N9-C1'-C2'	7.29	122.94	112.00
1	X	2634	G	C3'-C2'-C1'	-7.29	94.21	101.50
1	X	1036	G	C2'-C3'-O3'	7.29	120.43	109.50
17	O	50	ASP	N-CA-C	-7.28	103.66	112.54
1	X	731	A	P-O3'-C3'	7.28	131.12	120.20
1	X	1811	A	P-O3'-C3'	7.26	131.09	120.20
23	U	33	LYS	CA-C-N	7.26	135.40	121.54
23	U	33	LYS	C-N-CA	7.26	135.40	121.54
1	X	172	A	P-O3'-C3'	7.25	131.08	120.20
3	A	220	HIS	CA-CB-CG	7.25	121.05	113.80
15	M	29	PRO	N-CA-C	7.25	127.41	112.47
1	X	803	C	P-O3'-C3'	7.23	131.04	120.20
13	K	83	VAL	N-CA-C	7.23	117.21	110.42
1	X	2039	G	O4'-C1'-C2'	-7.22	100.38	107.60
3	A	171	ASP	N-CA-C	-7.21	103.64	113.30
12	J	89	GLY	CA-C-N	7.21	130.91	120.38
12	J	89	GLY	C-N-CA	7.21	130.91	120.38
1	X	939	C	P-O3'-C3'	7.21	131.01	120.20
1	X	1575	C	P-O3'-C3'	7.21	131.01	120.20
1	X	2552	C	O3'-P-O5'	-7.21	93.19	104.00
1	X	454	G	C2'-C3'-O3'	7.19	120.29	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1288	A	C5'-C4'-C3'	7.19	125.99	115.20
1	X	2590	U	P-O5'-C5'	7.18	131.67	120.90
19	Q	60	GLY	CA-C-N	7.17	135.24	121.54
19	Q	60	GLY	C-N-CA	7.17	135.24	121.54
1	X	1308	C	P-O5'-C5'	-7.14	110.19	120.90
1	X	1468	A	N9-C1'-C2'	7.13	122.70	112.00
1	X	817	A	C1'-O4'-C4'	-7.13	102.77	109.90
11	I	58	ALA	N-CA-C	-7.12	99.94	110.48
21	S	129	ARG	CA-C-N	7.11	127.71	122.59
21	S	129	ARG	C-N-CA	7.11	127.71	122.59
1	X	99	U	C2'-C3'-O3'	7.11	120.16	109.50
1	X	1459	U	P-O3'-C3'	7.10	130.85	120.20
20	R	28	LYS	N-CA-C	-7.10	101.16	110.53
1	X	247	A	C1'-O4'-C4'	-7.09	102.61	109.70
1	X	1338	G	P-O3'-C3'	7.09	130.84	120.20
1	X	2620	G	C4'-C3'-C2'	-7.09	95.51	102.60
23	U	53	GLU	N-CA-C	7.09	121.24	108.48
4	B	23	VAL	N-CA-C	7.08	118.09	108.17
18	P	86	LEU	CA-C-N	7.07	131.43	120.82
18	P	86	LEU	C-N-CA	7.07	131.43	120.82
1	X	1439	G	P-O3'-C3'	7.05	130.78	120.20
1	X	822	G	C4'-C3'-C2'	-7.04	95.56	102.60
1	X	2199	C	P-O5'-C5'	7.04	131.45	120.90
1	X	2255	G	C3'-C2'-O2'	7.03	121.25	110.70
1	X	1685	A	C4'-C3'-O3'	7.03	119.94	109.40
2	Y	75	A	P-O5'-C5'	7.01	131.42	120.90
3	A	245	VAL	N-CA-CB	-7.00	105.72	111.67
1	X	2324	G	P-O3'-C3'	7.00	130.71	120.20
2	Y	123	U	N1-C1'-C2'	7.00	122.50	112.00
1	X	312	G	C1'-O4'-C4'	-6.99	102.71	109.70
11	I	38	LYS	CA-C-N	6.99	134.66	121.87
11	I	38	LYS	C-N-CA	6.99	134.66	121.87
1	X	788	G	O4'-C4'-C3'	-6.99	99.11	106.10
1	X	2566	A	P-O3'-C3'	6.97	130.65	120.20
1	X	666	U	C1'-O4'-C4'	-6.96	102.94	109.90
1	X	399	G	C4'-C3'-C2'	6.96	109.56	102.60
1	X	1468	A	P-O5'-C5'	6.96	131.34	120.90
3	A	214	TRP	CB-CA-C	6.96	119.85	111.22
1	X	1984	A	C3'-C2'-C1'	-6.96	94.34	101.30
1	X	2040	A	C3'-C2'-O2'	6.96	121.13	110.70
1	X	1985	G	C3'-C2'-O2'	6.95	121.12	110.70
1	X	1774	A	C4'-C3'-O3'	-6.95	102.58	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2496	C	O3'-P-O5'	-6.95	93.58	104.00
1	X	1706	A	P-O5'-C5'	-6.94	110.48	120.90
3	A	245	VAL	N-CA-C	6.94	116.78	108.45
9	G	103	TYR	CA-C-N	6.94	134.80	121.54
9	G	103	TYR	C-N-CA	6.94	134.80	121.54
1	X	973	U	O3'-P-O5'	-6.94	93.59	104.00
1	X	74	G	O4'-C4'-C3'	-6.93	97.07	104.00
1	X	494	A	P-O3'-C3'	6.93	130.60	120.20
17	O	6	GLN	CA-C-N	6.90	134.72	121.54
17	O	6	GLN	C-N-CA	6.90	134.72	121.54
3	A	243	GLY	CA-C-N	6.88	134.68	121.54
3	A	243	GLY	C-N-CA	6.88	134.68	121.54
1	X	1288	A	C3'-C2'-C1'	-6.88	94.62	101.50
1	X	1496	G	C2'-C3'-O3'	6.85	123.98	113.70
1	X	2018	G	O4'-C1'-C2'	-6.85	98.95	105.80
20	R	57	ASN	N-CA-C	6.85	119.57	108.34
1	X	1991	C	P-O3'-C3'	-6.84	109.94	120.20
1	X	559	C	C5'-C4'-C3'	6.83	126.25	116.00
1	X	656	U	P-O3'-C3'	6.83	130.44	120.20
11	I	28	LYS	CA-C-N	6.83	134.57	121.54
11	I	28	LYS	C-N-CA	6.83	134.57	121.54
3	A	49	ILE	N-CA-CB	6.82	118.76	111.46
18	P	19	LYS	N-CA-C	6.82	121.68	112.88
1	X	956	A	P-O5'-C5'	6.82	131.13	120.90
2	Y	90	C	C4'-C3'-O3'	6.82	123.23	113.00
1	X	82	G	O3'-P-O5'	-6.80	93.80	104.00
1	X	2582	G	P-O5'-C5'	6.80	131.09	120.90
15	M	28	ARG	CA-C-O	-6.79	114.25	120.50
23	U	16	ASN	N-CA-C	6.79	119.33	110.43
1	X	883	A	C5'-C4'-O4'	6.79	119.99	109.80
1	X	98	U	C2'-C3'-O3'	6.79	119.68	109.50
1	X	1407	G	N9-C1'-C2'	6.78	122.17	112.00
1	X	2578	G	P-O5'-C5'	6.78	131.07	120.90
1	X	343	A	N9-C1'-C2'	6.78	122.16	112.00
1	X	1637	U	O3'-P-O5'	-6.77	93.84	104.00
1	X	761	G	C1'-O4'-C4'	-6.76	103.14	109.90
1	X	650	U	P-O5'-C5'	6.75	131.02	120.90
1	X	173	A	C1'-O4'-C4'	-6.74	102.97	109.70
1	X	1473	U	O4'-C1'-C2'	6.72	112.52	105.80
1	X	1496	G	C4'-C3'-O3'	6.72	123.08	113.00
1	X	2261	G	C2'-C3'-O3'	6.72	119.58	109.50
1	X	1958	G	O4'-C4'-C3'	-6.71	97.29	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1790	G	C1'-O4'-C4'	-6.71	102.99	109.70
1	X	2808	U	P-O5'-C5'	6.70	130.95	120.90
1	X	1268	U	P-O3'-C3'	6.68	130.22	120.20
1	X	1744	G	C4'-C3'-C2'	-6.68	95.92	102.60
1	X	1359	G	C5'-C4'-C3'	-6.68	105.98	116.00
1	X	2004	U	O3'-P-O5'	-6.68	93.99	104.00
2	Y	86	A	C3'-C2'-O2'	6.67	120.71	110.70
1	X	582	G	O3'-P-O5'	-6.67	94.00	104.00
1	X	1574	A	O4'-C1'-N9	6.66	118.49	108.50
1	X	938	G	P-O3'-C3'	6.65	130.18	120.20
1	X	1820	G	C4'-C3'-O3'	6.64	119.37	109.40
1	X	343	A	O4'-C1'-N9	6.64	118.46	108.50
1	X	1307	U	C3'-C2'-O2'	6.62	120.63	110.70
1	X	1469	U	N1-C1'-C2'	6.62	121.93	112.00
1	X	2034	A	P-O3'-C3'	6.61	130.12	120.20
1	X	1496	G	P-O3'-C3'	6.60	130.11	120.20
1	X	1663	C	O3'-P-O5'	-6.60	94.09	104.00
1	X	1467	U	P-O3'-C3'	-6.60	110.30	120.20
20	R	90	LYS	N-CA-C	6.60	116.98	108.34
1	X	1412	C	C2'-C3'-O3'	6.59	123.59	113.70
21	S	72	ASP	CA-CB-CG	6.59	119.19	112.60
1	X	1336	G	C3'-C2'-O2'	6.58	120.57	110.70
1	X	794	A	N9-C1'-C2'	6.57	121.86	112.00
12	J	82	THR	CA-C-N	6.57	134.09	121.54
12	J	82	THR	C-N-CA	6.57	134.09	121.54
13	K	93	GLY	CA-C-N	-6.56	112.21	121.99
13	K	93	GLY	C-N-CA	-6.56	112.21	121.99
1	X	1223	G	C3'-C2'-C1'	6.55	108.05	101.50
9	G	120	SER	CA-C-N	6.55	129.38	120.54
9	G	120	SER	C-N-CA	6.55	129.38	120.54
1	X	2204	A	P-O3'-C3'	6.55	130.02	120.20
1	X	2497	A	C1'-O4'-C4'	-6.55	103.15	109.70
1	X	956	A	O3'-P-O5'	-6.54	94.19	104.00
1	X	99	U	P-O3'-C3'	6.53	130.00	120.20
1	X	1288	A	C2'-C3'-O3'	6.53	119.30	109.50
3	A	249	PRO	CA-C-N	6.53	134.01	121.54
3	A	249	PRO	C-N-CA	6.53	134.01	121.54
11	I	99	VAL	N-CA-CB	6.53	122.00	111.23
16	N	87	ASN	CA-C-N	6.53	129.40	120.46
16	N	87	ASN	C-N-CA	6.53	129.40	120.46
1	X	2824	C	P-O3'-C3'	6.52	129.98	120.20
1	X	1710	U	P-O3'-C3'	6.51	129.97	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1185	C	P-O5'-C5'	6.51	130.66	120.90
1	X	2459	C	C1'-C2'-O2'	6.51	118.17	108.40
1	X	1473	U	C2'-C3'-O3'	6.50	119.25	109.50
1	X	560	G	N9-C1'-C2'	6.49	121.74	112.00
1	X	1953	A	P-O5'-C5'	-6.49	111.17	120.90
5	C	163	ASN	CA-C-N	6.49	133.65	121.97
5	C	163	ASN	C-N-CA	6.49	133.65	121.97
23	U	67	LEU	N-CA-C	-6.49	104.84	112.89
4	B	136	ARG	N-CA-C	6.47	120.22	110.64
1	X	2414	A	P-O3'-C3'	6.46	129.89	120.20
20	R	7	GLY	CA-C-N	6.45	129.45	120.29
20	R	7	GLY	C-N-CA	6.45	129.45	120.29
14	L	90	ASP	CA-CB-CG	6.45	119.05	112.60
1	X	2825	A	C4'-C3'-O3'	-6.44	103.33	113.00
1	X	1783	G	C1'-C2'-O2'	6.44	118.06	108.40
1	X	2559	U	C2'-C3'-O3'	-6.44	104.04	113.70
11	I	27	ASP	CA-CB-CG	6.44	119.04	112.60
1	X	1072	U	P-O3'-C3'	6.43	129.85	120.20
1	X	525	A	C1'-C2'-O2'	6.42	118.03	108.40
1	X	841	G	C1'-O4'-C4'	-6.42	103.48	109.90
1	X	2452	U	P-O3'-C3'	6.42	129.83	120.20
1	X	2481	G	P-O3'-C3'	6.42	129.82	120.20
12	J	97	VAL	N-CA-C	6.42	113.08	106.21
1	X	1468	A	P-O3'-C3'	6.41	129.82	120.20
1	X	1019	U	C2'-C3'-O3'	6.41	119.11	109.50
1	X	343	A	P-O5'-C5'	6.41	130.51	120.90
1	X	747	A	C3'-C2'-O2'	6.40	120.31	110.70
1	X	1960	A	C3'-C2'-O2'	6.39	120.29	110.70
1	X	515	A	P-O3'-C3'	6.39	129.79	120.20
1	X	248	A	P-O5'-C5'	6.39	130.49	120.90
1	X	117	A	P-O3'-C3'	6.39	129.78	120.20
1	X	926	C	C1'-C2'-O2'	6.39	117.98	108.40
1	X	2229	G	P-O5'-C5'	-6.38	111.33	120.90
1	X	1345	G	C5'-C4'-O4'	6.38	118.66	109.10
1	X	111	G	P-O5'-C5'	6.37	130.45	120.90
1	X	1291	G	O4'-C4'-C3'	-6.37	97.63	104.00
1	X	2032	G	O4'-C4'-C3'	-6.36	97.64	104.00
1	X	1526	U	P-O5'-C5'	6.36	130.44	120.90
1	X	788	G	N9-C1'-C2'	6.36	123.54	114.00
23	U	18	VAL	N-CA-C	6.36	116.29	108.53
6	D	163	ASP	CA-C-N	6.35	128.70	120.44
6	D	163	ASP	C-N-CA	6.35	128.70	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	S	76	ARG	N-CA-C	6.35	119.88	111.75
1	X	673	G	C3'-C2'-O2'	6.35	120.22	110.70
1	X	1211	G	P-O3'-C3'	-6.35	110.68	120.20
1	X	1036	G	C4'-C3'-C2'	6.35	108.95	102.60
1	X	581	A	O3'-P-O5'	-6.34	94.49	104.00
1	X	2649	A	C5'-C4'-C3'	-6.34	106.49	116.00
2	Y	13	C	C3'-C2'-O2'	6.34	120.21	110.70
1	X	1122	A	N9-C1'-C2'	6.34	121.51	112.00
1	X	520	C	C4'-C3'-C2'	-6.34	96.26	102.60
1	X	518	A	P-O3'-C3'	6.33	129.70	120.20
1	X	852	U	P-O5'-C5'	-6.33	111.41	120.90
1	X	1439	G	C2'-C3'-O3'	6.33	123.19	113.70
1	X	2409	A	C1'-O4'-C4'	-6.33	103.38	109.70
1	X	2813	G	C3'-C2'-O2'	6.32	120.17	110.70
3	A	242	ALA	N-CA-C	6.31	124.25	110.80
12	J	88	LYS	N-CA-C	6.31	124.24	110.80
1	X	1468	A	C3'-C2'-C1'	-6.31	94.99	101.30
1	X	1749	G	O4'-C1'-C2'	-6.30	99.50	105.80
1	X	33	C	O4'-C1'-N1	6.30	117.65	108.20
1	X	1524	C	P-O3'-C3'	6.30	129.65	120.20
5	C	143	ASP	CA-CB-CG	6.30	118.90	112.60
1	X	2196	U	P-O3'-C3'	6.29	129.64	120.20
1	X	2599	U	P-O5'-C5'	-6.29	111.47	120.90
9	G	106	TYR	N-CA-CB	6.28	121.11	110.49
23	U	14	VAL	CA-C-N	6.28	133.28	121.97
23	U	14	VAL	C-N-CA	6.28	133.28	121.97
1	X	2375	G	O4'-C4'-C3'	-6.28	97.72	104.00
1	X	1982	C	O4'-C4'-C3'	-6.28	97.72	104.00
1	X	2778	U	P-O3'-C3'	6.27	129.61	120.20
1	X	1669	A	O4'-C4'-C3'	-6.27	97.73	104.00
1	X	2758	A	C1'-O4'-C4'	-6.27	103.43	109.70
1	X	1749	G	C1'-O4'-C4'	-6.27	103.43	109.70
18	P	87	GLU	N-CA-C	6.26	121.70	111.37
1	X	2237	C	P-O3'-C3'	6.26	129.59	120.20
1	X	2693	U	O3'-P-O5'	-6.26	94.61	104.00
1	X	672	C	O4'-C4'-C3'	-6.25	97.75	104.00
1	X	2198	U	P-O3'-C3'	6.25	129.58	120.20
1	X	1662	G	O3'-P-O5'	-6.25	94.62	104.00
1	X	1938	U	C4'-C3'-C2'	6.25	108.85	102.60
13	K	11	ASN	CA-C-N	6.25	133.48	121.54
13	K	11	ASN	C-N-CA	6.25	133.48	121.54
1	X	582	G	P-O3'-C3'	6.25	129.57	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	P	91	PHE	CA-CB-CG	6.24	120.04	113.80
1	X	2258	G	O4'-C4'-C3'	-6.24	97.76	104.00
1	X	1313	U	C1'-O4'-C4'	-6.24	103.46	109.70
1	X	2376	G	P-O5'-C5'	6.23	130.24	120.90
5	C	193	LEU	N-CA-C	-6.23	104.40	112.68
1	X	192	G	P-O3'-C3'	6.22	129.53	120.20
1	X	1473	U	C4'-C3'-C2'	6.22	108.82	102.60
1	X	2667	C	C4'-C3'-C2'	-6.22	96.38	102.60
2	Y	90	C	C4'-C3'-C2'	6.22	108.82	102.60
1	X	173	A	O5'-C5'-C4'	-6.22	102.38	111.70
1	X	969	U	C2'-C3'-O3'	6.21	118.82	109.50
20	R	14	LEU	CA-C-N	6.21	133.40	121.54
20	R	14	LEU	C-N-CA	6.21	133.40	121.54
4	B	113	THR	CB-CA-C	6.20	121.72	111.31
1	X	518	A	N9-C1'-C2'	6.20	123.29	114.00
5	C	171	PRO	CA-C-N	6.20	133.12	121.97
5	C	171	PRO	C-N-CA	6.20	133.12	121.97
1	X	2693	U	C1'-O4'-C4'	-6.19	103.51	109.70
1	X	2861	A	O4'-C1'-C2'	-6.19	101.41	107.60
23	U	33	LYS	N-CA-C	-6.19	106.95	114.75
1	X	2477	C	O5'-C5'-C4'	-6.18	102.23	111.50
1	X	2261	G	C4'-C3'-O3'	6.18	118.67	109.40
1	X	110	U	O3'-P-O5'	-6.18	94.73	104.00
1	X	1339	U	C3'-C2'-O2'	6.17	119.96	110.70
1	X	514	G	N9-C1'-C2'	6.17	123.25	114.00
1	X	969	U	P-O3'-C3'	6.17	129.45	120.20
1	X	1938	U	N1-C1'-C2'	6.16	123.24	114.00
1	X	1753	A	P-O5'-C5'	6.15	130.13	120.90
1	X	387	A	C5'-C4'-O4'	6.15	119.03	109.80
1	X	1285	A	P-O3'-C3'	6.15	129.43	120.20
1	X	673	G	C2'-C3'-O3'	6.15	122.92	113.70
1	X	1315	A	P-O3'-C3'	6.15	129.42	120.20
1	X	2795	A	P-O3'-C3'	6.15	129.42	120.20
18	P	34	SER	N-CA-C	6.14	117.39	109.65
9	G	96	ASP	CA-CB-CG	6.14	118.74	112.60
1	X	1288	A	O5'-C5'-C4'	-6.14	102.50	111.70
1	X	2426	G	O3'-P-O5'	-6.14	94.80	104.00
1	X	2018	G	C3'-C2'-C1'	-6.13	95.37	101.50
1	X	575	U	O3'-P-O5'	-6.13	94.81	104.00
1	X	1682	A	C1'-C2'-O2'	6.12	117.59	108.40
1	X	352	G	P-O5'-C5'	6.12	130.09	120.90
10	H	26	ASN	CA-C-N	6.12	133.24	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	H	26	ASN	C-N-CA	6.12	133.24	121.54
15	M	3	THR	CA-C-N	-6.12	112.80	122.95
15	M	3	THR	C-N-CA	-6.12	112.80	122.95
1	X	558	G	N9-C1'-C2'	6.11	123.17	114.00
1	X	1661	C	O5'-C5'-C4'	-6.11	102.33	111.50
1	X	591	G	C3'-C2'-O2'	6.11	119.87	110.70
14	L	51	LEU	N-CA-C	6.11	120.44	112.92
20	R	78	ALA	N-CA-C	-6.11	104.24	113.89
1	X	799	C	P-O5'-C5'	-6.11	111.74	120.90
3	A	228	PRO	CA-C-N	6.11	129.09	120.42
3	A	228	PRO	C-N-CA	6.11	129.09	120.42
1	X	1475	U	C2'-C3'-O3'	6.10	118.66	109.50
1	X	794	A	C4'-C3'-O3'	-6.10	103.85	113.00
1	X	1473	U	C4'-C3'-O3'	6.10	118.56	109.40
1	X	1820	G	C2'-C3'-O3'	6.10	118.65	109.50
1	X	2048	C	P-O5'-C5'	-6.10	111.75	120.90
1	X	2724	G	P-O5'-C5'	6.09	130.04	120.90
1	X	421	G	P-O5'-C5'	6.09	130.03	120.90
1	X	810	U	P-O3'-C3'	-6.08	111.08	120.20
1	X	1147	G	C3'-C2'-O2'	6.08	119.82	110.70
1	X	1412	C	P-O3'-C3'	6.08	129.32	120.20
1	X	843	G	P-O3'-C3'	6.08	129.32	120.20
1	X	2028	C	C1'-C2'-O2'	6.08	117.51	108.40
1	X	656	U	P-O5'-C5'	6.07	130.00	120.90
1	X	1668	G	P-O5'-C5'	6.06	129.99	120.90
1	X	531	G	C3'-C2'-O2'	6.06	119.79	110.70
1	X	1474	A	O3'-P-O5'	-6.06	94.91	104.00
5	C	117	LEU	N-CA-C	6.06	117.35	107.23
1	X	531	G	P-O3'-C3'	-6.06	111.11	120.20
1	X	413	G	C4'-C3'-O3'	6.05	122.08	113.00
1	X	483	A	C4'-C3'-C2'	6.05	108.65	102.60
12	J	43	ILE	N-CA-C	6.05	116.52	107.51
1	X	983	G	C4'-C3'-O3'	-6.04	103.93	113.00
3	A	216	GLY	CA-C-N	6.04	133.07	121.54
3	A	216	GLY	C-N-CA	6.04	133.07	121.54
1	X	1989	C	O4'-C4'-C3'	-6.03	97.97	104.00
1	X	2008	C	O3'-P-O5'	-6.03	94.95	104.00
1	X	1656	U	P-O3'-C3'	6.03	129.24	120.20
1	X	2190	A	C1'-O4'-C4'	-6.02	103.88	109.90
1	X	543	G	O5'-C5'-C4'	-6.02	102.47	111.50
1	X	1523	A	P-O3'-C3'	6.01	129.22	120.20
1	X	1575	C	C2'-C3'-O3'	6.01	118.52	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	92	G	P-O3'-C3'	-6.01	111.19	120.20
1	X	814	G	N9-C1'-C2'	6.00	123.01	114.00
14	L	67	THR	CA-C-N	6.00	133.01	121.54
14	L	67	THR	C-N-CA	6.00	133.01	121.54
1	X	1139	A	N9-C1'-C2'	6.00	122.99	114.00
16	N	25	TRP	N-CA-C	5.99	118.39	109.59
1	X	1850	G	P-O3'-C3'	5.99	129.18	120.20
1	X	2018	G	C4'-C3'-O3'	5.98	118.37	109.40
1	X	2586	G	C4'-C3'-C2'	-5.98	96.62	102.60
1	X	1469	U	O3'-P-O5'	5.98	112.96	104.00
20	R	106	VAL	CA-C-N	5.97	132.95	121.54
20	R	106	VAL	C-N-CA	5.97	132.95	121.54
1	X	1664	G	C2'-C3'-O3'	5.97	118.46	109.50
1	X	1496	G	C3'-C2'-C1'	-5.97	95.33	101.30
1	X	1966	C	P-O3'-C3'	-5.97	111.25	120.20
1	X	1607	A	C2'-C3'-O3'	5.97	122.65	113.70
1	X	994	A	C4'-C3'-O3'	-5.96	104.05	113.00
1	X	1777	A	C1'-O4'-C4'	-5.96	103.73	109.70
1	X	458	G	P-O3'-C3'	5.96	129.14	120.20
1	X	471	A	C3'-C2'-O2'	5.96	119.64	110.70
1	X	1392	U	N1-C1'-C2'	5.96	120.93	112.00
1	X	2856	U	C1'-C2'-O2'	5.95	117.33	108.40
1	X	1188	A	P-O3'-C3'	5.95	129.12	120.20
1	X	1142	G	O4'-C1'-C2'	-5.94	99.86	105.80
1	X	1339	U	P-O3'-C3'	5.94	129.11	120.20
1	X	2507	U	P-O3'-C3'	5.94	129.11	120.20
1	X	1830	C	P-O3'-C3'	5.94	129.10	120.20
1	X	1790	G	C4'-C3'-O3'	5.93	118.30	109.40
15	M	33	VAL	N-CA-CB	5.93	118.93	111.46
23	U	35	THR	CB-CA-C	5.93	120.00	111.82
15	M	30	GLY	CA-C-N	5.92	132.85	121.54
15	M	30	GLY	C-N-CA	5.92	132.85	121.54
1	X	1152	C	P-O3'-C3'	5.92	129.08	120.20
1	X	2564	U	C1'-O4'-C4'	-5.92	103.98	109.90
14	L	20	THR	CA-C-N	5.92	132.84	121.54
14	L	20	THR	C-N-CA	5.92	132.84	121.54
1	X	398	C	P-O5'-C5'	5.91	129.76	120.90
1	X	1275	A	P-O5'-C5'	5.91	129.76	120.90
4	B	88	GLY	N-CA-C	5.90	117.09	111.67
1	X	580	A	N9-C1'-C2'	5.89	122.83	114.00
1	X	788	G	C1'-O4'-C4'	-5.89	103.81	109.70
1	X	2018	G	C1'-C2'-O2'	5.89	120.63	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L	13	THR	CA-C-N	5.89	128.65	120.29
14	L	13	THR	C-N-CA	5.89	128.65	120.29
1	X	321	A	C4'-C3'-O3'	-5.88	100.57	109.40
1	X	2662	C	C4'-C3'-O3'	-5.88	104.17	113.00
1	X	2222	U	P-O5'-C5'	5.88	129.72	120.90
5	C	194	GLU	CA-C-N	5.88	132.56	121.97
5	C	194	GLU	C-N-CA	5.88	132.56	121.97
1	X	2204	A	C2'-C3'-O3'	5.88	118.32	109.50
12	J	10	PHE	CA-CB-CG	5.88	119.68	113.80
9	G	93	LYS	N-CA-C	5.87	117.97	108.41
1	X	227	G	N9-C1'-C2'	5.86	120.80	112.00
1	X	1678	G	O4'-C4'-C3'	-5.86	98.14	104.00
1	X	2566	A	C3'-C2'-O2'	5.86	119.49	110.70
1	X	1654	A	C3'-C2'-C1'	-5.86	95.44	101.30
16	N	84	LYS	N-CA-C	-5.86	105.80	113.12
1	X	2488	G	P-O3'-C3'	-5.86	111.42	120.20
21	S	35	ASP	CA-CB-CG	5.86	118.46	112.60
1	X	771	C	C4'-C3'-C2'	-5.85	96.75	102.60
1	X	2579	A	C3'-C2'-O2'	5.85	119.48	110.70
1	X	1782	A	P-O5'-C5'	5.85	129.68	120.90
20	R	108	VAL	CA-C-N	5.85	128.71	120.28
20	R	108	VAL	C-N-CA	5.85	128.71	120.28
1	X	2030	U	P-O3'-C3'	-5.85	111.43	120.20
1	X	2697	G	C3'-C2'-O2'	5.85	119.47	110.70
1	X	560	G	P-O3'-C3'	-5.84	111.44	120.20
13	K	94	TYR	N-CA-C	5.84	117.72	108.67
23	U	75	TYR	CA-C-N	5.84	132.69	121.54
23	U	75	TYR	C-N-CA	5.84	132.69	121.54
5	C	71	ASP	CA-CB-CG	5.84	118.44	112.60
5	C	169	VAL	N-CA-C	5.83	116.50	107.99
1	X	1664	G	P-O5'-C5'	5.83	129.64	120.90
1	X	742	G	C1'-O4'-C4'	-5.82	104.08	109.90
1	X	357	A	P-O3'-C3'	5.82	128.93	120.20
11	I	32	ARG	N-CA-C	-5.82	99.03	108.52
1	X	1882	G	P-O5'-C5'	5.81	129.62	120.90
1	X	2795	A	C3'-C2'-C1'	5.81	107.11	101.30
4	B	136	ARG	N-CA-CB	5.81	118.14	109.19
23	U	62	LEU	N-CA-C	5.81	117.87	108.34
1	X	2288	A	P-O3'-C3'	5.81	128.91	120.20
2	Y	30	C	P-O5'-C5'	5.81	129.62	120.90
1	X	1766	U	P-O5'-C5'	-5.80	112.19	120.90
1	X	1465	G	P-O3'-C3'	-5.80	111.50	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2530	C	P-O3'-C3'	5.80	128.90	120.20
1	X	198	A	P-O3'-C3'	5.79	128.89	120.20
1	X	742	G	P-O3'-C3'	5.79	128.89	120.20
11	I	56	LEU	CA-C-N	5.79	127.86	120.56
11	I	56	LEU	C-N-CA	5.79	127.86	120.56
1	X	1071	U	P-O3'-C3'	5.79	128.89	120.20
12	J	14	PHE	N-CA-C	5.79	119.00	109.85
1	X	1618	U	P-O3'-C3'	5.79	128.88	120.20
12	J	77	LYS	CA-C-N	5.79	131.37	121.35
12	J	77	LYS	C-N-CA	5.79	131.37	121.35
15	M	31	ASP	CA-CB-CG	5.79	118.39	112.60
1	X	1456	C	C3'-C2'-O2'	5.79	119.38	110.70
1	X	1466	C	C4'-C3'-C2'	-5.79	96.81	102.60
1	X	1281	A	O3'-P-O5'	-5.78	95.33	104.00
1	X	567	G	P-O3'-C3'	-5.78	111.53	120.20
2	Y	88	C	P-O5'-C5'	5.77	129.56	120.90
1	X	61	U	C1'-O4'-C4'	-5.77	104.13	109.90
12	J	76	THR	N-CA-C	5.76	119.35	110.42
1	X	2056	C	O3'-P-O5'	-5.76	95.36	104.00
1	X	1466	C	O4'-C1'-C2'	-5.76	101.84	107.60
1	X	2656	G	P-O5'-C5'	-5.76	112.26	120.90
1	X	522	G	O4'-C1'-N9	5.76	116.84	108.20
2	Y	90	C	P-O5'-C5'	5.76	129.54	120.90
13	K	40	LYS	CA-C-N	5.76	130.32	120.71
13	K	40	LYS	C-N-CA	5.76	130.32	120.71
1	X	1253	C	C1'-C2'-O2'	5.75	117.03	108.40
12	J	103	VAL	N-CA-CB	5.75	118.11	111.90
1	X	2560	G	C3'-C2'-O2'	5.75	123.22	114.60
22	T	18	PRO	N-CA-C	5.74	124.30	112.47
16	N	60	LEU	CA-C-N	5.74	127.90	120.44
16	N	60	LEU	C-N-CA	5.74	127.90	120.44
1	X	1243	G	C1'-C2'-O2'	5.74	117.00	108.40
14	L	88	VAL	CA-C-N	5.73	130.90	121.39
14	L	88	VAL	C-N-CA	5.73	130.90	121.39
1	X	506	G	C3'-C2'-O2'	5.73	119.29	110.70
1	X	2367	A	C5'-C4'-C3'	-5.72	107.41	116.00
21	S	45	GLN	CA-C-N	5.72	127.88	120.44
21	S	45	GLN	C-N-CA	5.72	127.88	120.44
1	X	2004	U	P-O5'-C5'	-5.72	112.32	120.90
23	U	45	ASN	CA-CB-CG	5.72	118.32	112.60
6	D	85	VAL	N-CA-C	5.71	116.92	112.12
1	X	2855	C	P-O3'-C3'	-5.71	111.64	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	601	A	P-O5'-C5'	5.71	129.46	120.90
3	A	261	ARG	N-CA-C	5.71	118.91	110.46
1	X	205	A	C4'-C3'-O3'	5.71	121.56	113.00
4	B	179	GLU	N-CA-C	-5.70	105.98	113.17
1	X	1001	A	P-O3'-C3'	5.70	128.75	120.20
1	X	540	G	C2'-C3'-O3'	5.70	118.05	109.50
1	X	2785	A	C3'-C2'-O2'	5.70	119.25	110.70
2	Y	9	G	O5'-C5'-C4'	5.70	120.05	111.50
1	X	2489	C	P-O5'-C5'	-5.70	112.36	120.90
1	X	968	C	C2'-C3'-O3'	5.69	118.04	109.50
1	X	70	A	C2'-C3'-O3'	5.69	118.04	109.50
1	X	1368	G	C3'-C2'-O2'	5.69	119.24	110.70
1	X	1412	C	C3'-C2'-C1'	-5.69	95.61	101.30
11	I	55	ARG	CA-C-N	5.69	132.40	121.54
11	I	55	ARG	C-N-CA	5.69	132.40	121.54
1	X	1743	C	P-O3'-C3'	-5.68	111.67	120.20
1	X	242	A	P-O3'-C3'	5.68	128.71	120.20
1	X	1357	U	P-O3'-C3'	5.67	128.71	120.20
3	A	133	LEU	N-CA-C	5.67	119.72	112.34
15	M	54	VAL	N-CA-CB	5.67	117.12	110.82
1	X	2621	G	C5'-C4'-C3'	5.67	124.51	116.00
1	X	1341	G	C4'-C3'-C2'	5.67	108.27	102.60
13	K	105	GLY	N-CA-C	5.67	120.67	113.24
1	X	1467	U	O4'-C1'-C2'	-5.67	101.93	107.60
1	X	1790	G	O4'-C4'-C3'	-5.67	100.43	106.10
1	X	2015	G	P-O3'-C3'	5.66	128.69	120.20
1	X	925	U	P-O3'-C3'	5.66	128.69	120.20
1	X	1324	G	O4'-C1'-C2'	-5.66	100.14	105.80
1	X	2671	C	C4'-C3'-C2'	-5.66	96.94	102.60
1	X	63	A	C5'-C4'-C3'	-5.66	107.52	116.00
1	X	454	G	C4'-C3'-C2'	5.66	108.26	102.60
11	I	87	THR	CA-C-N	5.66	132.34	121.54
11	I	87	THR	C-N-CA	5.66	132.34	121.54
13	K	38	LEU	CA-C-N	5.66	128.12	120.65
13	K	38	LEU	C-N-CA	5.66	128.12	120.65
1	X	1412	C	C4'-C3'-O3'	5.65	121.48	113.00
26	Z	52	TYR	CA-C-N	5.65	132.34	121.54
26	Z	52	TYR	C-N-CA	5.65	132.34	121.54
1	X	626	A	P-O3'-C3'	5.65	128.68	120.20
1	X	1217	U	C3'-C2'-O2'	5.65	119.18	110.70
10	H	4	PRO	CA-C-N	5.65	132.34	121.54
10	H	4	PRO	C-N-CA	5.65	132.34	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2694	G	P-O3'-C3'	5.65	128.68	120.20
1	X	2704	U	C4'-C3'-O3'	-5.65	104.53	113.00
3	A	44	ASN	CA-CB-CG	5.65	118.25	112.60
17	O	6	GLN	N-CA-C	-5.65	104.26	113.19
1	X	1283	C	P-O3'-C3'	5.65	128.67	120.20
1	X	2017	U	N1-C1'-C2'	5.64	120.47	112.00
1	X	675	C	C3'-C2'-O2'	5.64	119.16	110.70
1	X	1409	U	C5'-C4'-C3'	5.64	123.66	115.20
1	X	2528	G	O4'-C1'-C2'	-5.64	101.96	107.60
11	I	98	LEU	CA-C-N	5.64	132.12	121.97
11	I	98	LEU	C-N-CA	5.64	132.12	121.97
1	X	1223	G	P-O3'-C3'	5.64	128.66	120.20
1	X	1680	U	C3'-C2'-O2'	5.64	119.16	110.70
1	X	2056	C	P-O3'-C3'	5.64	128.66	120.20
1	X	2692	A	C1'-C2'-O2'	5.64	116.86	108.40
1	X	2384	G	P-O3'-C3'	5.63	128.65	120.20
1	X	2426	G	P-O5'-C5'	5.63	129.34	120.90
16	N	8	ILE	N-CA-CB	5.63	120.52	111.23
2	Y	26	G	P-O3'-C3'	5.63	128.64	120.20
26	Z	47	PRO	CA-C-N	5.63	127.75	120.44
26	Z	47	PRO	C-N-CA	5.63	127.75	120.44
1	X	176	A	C4'-C3'-O3'	5.62	117.84	109.40
1	X	1168	G	P-O5'-C5'	5.62	129.33	120.90
1	X	1238	A	P-O5'-C5'	5.62	129.33	120.90
1	X	2088	U	P-O3'-C3'	5.62	128.63	120.20
20	R	100	ASP	CA-CB-CG	5.62	118.22	112.60
1	X	190	A	C1'-O4'-C4'	-5.62	104.28	109.90
1	X	1817	U	O5'-C5'-C4'	-5.62	103.08	111.50
1	X	190	A	O4'-C4'-C3'	-5.61	98.39	104.00
1	X	539	A	C1'-O4'-C4'	-5.61	104.09	109.70
1	X	1439	G	C3'-C2'-C1'	-5.61	95.69	101.30
1	X	1632	A	O4'-C1'-N9	-5.61	99.78	108.20
1	X	1746	A	O4'-C1'-N9	5.61	116.91	108.50
1	X	2580	C	P-O3'-C3'	5.61	128.61	120.20
1	X	2811	G	C3'-C2'-O2'	5.61	119.11	110.70
14	L	36	LYS	N-CA-C	-5.61	104.62	112.25
1	X	1314	A	O4'-C1'-C2'	-5.60	100.20	105.80
1	X	1439	G	C4'-C3'-O3'	5.60	121.40	113.00
1	X	1607	A	P-O3'-C3'	5.59	128.59	120.20
1	X	681	A	C1'-C2'-O2'	5.59	116.79	108.40
1	X	972	C	C1'-O4'-C4'	-5.59	104.11	109.70
1	X	2033	C	P-O3'-C3'	5.59	128.58	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	H	52	VAL	N-CA-C	-5.59	100.42	108.53
1	X	2633	A	P-O3'-C3'	5.59	128.58	120.20
1	X	1681	A	P-O3'-C3'	5.59	128.58	120.20
11	I	48	PHE	CA-C-N	5.58	132.20	121.54
11	I	48	PHE	C-N-CA	5.58	132.20	121.54
1	X	2634	G	C1'-O4'-C4'	-5.58	104.12	109.70
1	X	2579	A	C3'-C2'-C1'	5.58	106.88	101.30
1	X	1080	A	C1'-O4'-C4'	-5.58	104.12	109.70
1	X	1799	A	O4'-C4'-C3'	-5.58	100.52	106.10
1	X	1142	G	P-O3'-C3'	5.58	128.57	120.20
1	X	1442	C	C4'-C3'-O3'	5.57	117.76	109.40
1	X	761	G	N9-C1'-C2'	5.57	120.35	112.00
1	X	48	A	C2'-C3'-O3'	5.57	117.85	109.50
1	X	2498	U	O3'-P-O5'	-5.57	95.65	104.00
1	X	2608	A	C1'-O4'-C4'	-5.57	104.13	109.70
1	X	2634	G	O4'-C1'-N9	5.57	116.55	108.20
12	J	11	ARG	N-CA-C	5.57	122.66	110.80
15	M	58	ASN	CA-CB-CG	5.57	118.17	112.60
1	X	71	A	C2'-C3'-O3'	5.56	117.85	109.50
19	Q	27	PHE	CA-CB-CG	5.56	119.36	113.80
2	Y	28	A	N9-C1'-C2'	5.56	120.34	112.00
11	I	61	PRO	CA-C-N	5.56	132.16	121.54
11	I	61	PRO	C-N-CA	5.56	132.16	121.54
1	X	349	G	P-O5'-C5'	5.56	129.24	120.90
1	X	1278	A	O3'-P-O5'	-5.56	95.66	104.00
1	X	2018	G	C5'-C4'-C3'	-5.56	106.86	115.20
1	X	691	C	O4'-C1'-N1	5.56	116.84	108.50
1	X	2715	C	P-O5'-C5'	5.56	129.24	120.90
1	X	1467	U	C4'-C3'-O3'	5.55	121.33	113.00
1	X	2843	A	C5'-C4'-C3'	-5.55	107.67	116.00
25	W	41	ARG	N-CA-C	-5.55	105.62	112.90
1	X	1761	G	C3'-C2'-O2'	5.55	119.03	110.70
1	X	2511	G	P-O5'-C5'	5.55	129.23	120.90
19	Q	65	VAL	N-CA-CB	5.55	120.29	112.52
1	X	2671	C	P-O5'-C5'	-5.55	112.58	120.90
3	A	87	ASN	CA-CB-CG	5.55	118.15	112.60
1	X	7	G	C3'-C2'-O2'	5.55	119.02	110.70
1	X	2526	U	C1'-C2'-O2'	5.55	116.72	108.40
1	X	1764	A	C2'-C3'-O3'	5.55	122.02	113.70
1	X	1559	G	P-O3'-C3'	5.54	128.52	120.20
1	X	1988	A	C2'-C3'-O3'	-5.54	105.38	113.70
1	X	1745	C	P-O3'-C3'	-5.54	111.89	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2690	A	C4'-C3'-O3'	-5.54	104.69	113.00
11	I	62	LYS	CA-C-N	5.54	132.66	122.79
11	I	62	LYS	C-N-CA	5.54	132.66	122.79
23	U	60	VAL	N-CA-C	5.54	120.87	109.34
17	O	11	GLN	N-CA-C	5.54	122.60	110.80
1	X	2397	A	C3'-C2'-O2'	5.54	119.01	110.70
1	X	2782	G	C1'-O4'-C4'	-5.54	104.36	109.90
4	B	131	SER	N-CA-C	5.54	115.60	108.34
1	X	562	G	O4'-C4'-C3'	-5.54	98.46	104.00
1	X	2470	U	N1-C1'-C2'	5.54	120.31	112.00
1	X	2491	C	O4'-C1'-N1	5.54	116.80	108.50
1	X	1016	C	N1-C1'-C2'	5.53	120.30	112.00
1	X	815	A	P-O3'-C3'	5.53	128.49	120.20
1	X	34	U	P-O5'-C5'	5.53	129.19	120.90
23	U	39	LYS	N-CA-C	5.52	117.59	108.48
1	X	632	A	C4'-C3'-C2'	-5.52	97.08	102.60
9	G	41	TRP	CA-C-N	5.52	128.81	120.75
9	G	41	TRP	C-N-CA	5.52	128.81	120.75
20	R	12	ASP	N-CA-C	-5.52	104.61	111.90
1	X	1217	U	C4'-C3'-O3'	5.52	121.28	113.00
1	X	2700	U	P-O3'-C3'	-5.52	111.92	120.20
1	X	174	A	P-O5'-C5'	5.52	129.17	120.90
1	X	2867	G	C1'-C2'-O2'	5.52	116.67	108.40
1	X	652	C	C5'-C4'-C3'	-5.51	107.73	116.00
1	X	2420	C	P-O5'-C5'	5.51	129.17	120.90
1	X	2800	C	C1'-C2'-O2'	5.51	116.67	108.40
1	X	7	G	C5'-C4'-C3'	-5.51	107.73	116.00
1	X	559	C	C3'-C2'-C1'	5.51	106.81	101.30
1	X	2613	A	C3'-C2'-O2'	5.51	118.96	110.70
1	X	2663	U	P-O3'-C3'	-5.51	111.94	120.20
1	X	1313	U	C3'-C2'-C1'	-5.50	96.00	101.50
1	X	2782	G	O4'-C4'-C3'	-5.50	98.50	104.00
1	X	117	A	C1'-O4'-C4'	-5.50	104.20	109.70
1	X	1289	A	O4'-C4'-C3'	-5.50	98.50	104.00
1	X	2439	U	C3'-C2'-O2'	5.50	118.94	110.70
1	X	539	A	C2'-C3'-O3'	5.49	117.74	109.50
1	X	1294	G	C4'-C3'-C2'	-5.49	97.11	102.60
18	P	71	VAL	N-CA-CB	5.49	117.60	110.57
23	U	31	GLY	CA-C-N	5.49	132.03	121.54
23	U	31	GLY	C-N-CA	5.49	132.03	121.54
1	X	1676	U	C1'-C2'-O2'	5.49	116.64	108.40
1	X	2290	A	P-O3'-C3'	5.49	128.44	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2691	C	C1'-O4'-C4'	-5.49	104.41	109.90
1	X	526	C	C3'-C2'-C1'	-5.49	95.81	101.30
1	X	998	C	C5'-C4'-C3'	5.49	124.23	116.00
1	X	1138	A	P-O5'-C5'	5.49	129.13	120.90
1	X	853	C	C3'-C2'-O2'	5.48	118.92	110.70
4	B	131	SER	CA-C-N	5.48	132.01	121.54
4	B	131	SER	C-N-CA	5.48	132.01	121.54
1	X	940	G	C4'-C3'-C2'	-5.48	97.12	102.60
1	X	1268	U	P-O5'-C5'	5.47	129.11	120.90
1	X	1308	C	C4'-C3'-C2'	-5.47	97.13	102.60
1	X	2371	A	O4'-C1'-N9	5.47	116.71	108.50
1	X	1940	C	P-O3'-C3'	-5.47	111.99	120.20
1	X	2409	A	N9-C1'-C2'	5.47	122.20	114.00
1	X	2805	G	C1'-C2'-O2'	5.46	116.59	108.40
6	D	166	ALA	CA-C-N	5.46	127.92	120.54
6	D	166	ALA	C-N-CA	5.46	127.92	120.54
1	X	1725	C	P-O5'-C5'	-5.46	112.71	120.90
1	X	2660	C	P-O5'-C5'	5.46	129.08	120.90
1	X	182	G	O5'-C5'-C4'	-5.45	103.52	111.70
1	X	596	C	P-O5'-C5'	-5.45	112.72	120.90
1	X	2267	A	P-O3'-C3'	5.45	128.38	120.20
1	X	805	G	O4'-C1'-N9	-5.45	100.02	108.20
1	X	1999	U	P-O3'-C3'	-5.45	112.03	120.20
1	X	1776	A	P-O3'-C3'	5.45	128.37	120.20
1	X	1241	G	P-O3'-C3'	-5.45	112.03	120.20
1	X	1337	G	P-O5'-C5'	5.45	129.07	120.90
3	A	83	GLU	N-CA-C	5.45	117.25	109.14
1	X	1920	A	P-O3'-C3'	5.44	128.37	120.20
1	X	1010	U	P-O5'-C5'	5.44	129.06	120.90
1	X	1946	U	O4'-C1'-C2'	-5.44	102.16	107.60
16	N	7	GLY	CA-C-N	5.44	131.77	121.97
16	N	7	GLY	C-N-CA	5.44	131.77	121.97
1	X	520	C	P-O3'-C3'	5.44	128.36	120.20
1	X	805	G	N9-C1'-C2'	5.44	122.16	114.00
1	X	1792	C	N1-C1'-C2'	5.44	122.16	114.00
23	U	15	VAL	N-CA-CB	5.44	120.21	111.23
12	J	139	ASP	N-CA-C	-5.44	106.32	113.12
1	X	1344	C	C4'-C3'-O3'	-5.44	104.84	113.00
1	X	1686	A	C1'-O4'-C4'	-5.44	104.46	109.90
1	X	2572	U	N1-C1'-C2'	5.44	120.15	112.00
1	X	2854	G	O4'-C1'-C2'	-5.43	100.36	105.80
4	B	128	SER	N-CA-C	5.43	122.37	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	174	A	P-O3'-C3'	5.43	128.34	120.20
1	X	799	C	O3'-P-O5'	-5.43	95.86	104.00
1	X	85	C	C3'-C2'-O2'	5.43	118.84	110.70
1	X	1036	G	C4'-C3'-O3'	5.42	117.54	109.40
1	X	1269	G	O4'-C1'-C2'	-5.42	102.18	107.60
1	X	1314	A	C4'-C3'-O3'	-5.42	101.27	109.40
1	X	1769	U	C3'-C2'-O2'	5.42	118.83	110.70
10	H	24	VAL	N-CA-C	-5.42	100.67	108.53
18	P	86	LEU	N-CA-C	5.42	117.35	108.52
1	X	1152	C	C2'-C3'-O3'	5.42	117.63	109.50
1	X	1776	A	O3'-P-O5'	-5.42	95.87	104.00
22	T	14	ARG	CA-C-N	5.42	131.89	121.54
22	T	14	ARG	C-N-CA	5.42	131.89	121.54
1	X	1632	A	O4'-C4'-C3'	-5.42	100.68	106.10
1	X	1983	G	C3'-C2'-O2'	5.42	118.83	110.70
12	J	21	ASP	CA-C-N	5.42	129.38	121.31
12	J	21	ASP	C-N-CA	5.42	129.38	121.31
1	X	2548	G	O4'-C1'-C2'	-5.42	102.19	107.60
12	J	46	ASN	N-CA-C	-5.41	106.81	113.41
24	V	24	GLU	CA-C-N	5.41	127.79	120.38
24	V	24	GLU	C-N-CA	5.41	127.79	120.38
1	X	2694	G	C4'-C3'-C2'	-5.41	97.19	102.60
1	X	1036	G	O4'-C1'-C2'	5.41	111.21	105.80
1	X	2045	A	C2'-C3'-O3'	5.41	117.61	109.50
1	X	358	C	P-O5'-C5'	5.41	129.01	120.90
1	X	2544	A	C4'-C3'-O3'	-5.41	104.89	113.00
11	I	41	SER	N-CA-C	5.41	122.31	110.80
1	X	2655	C	C3'-C2'-O2'	5.40	118.81	110.70
13	K	94	TYR	CA-C-N	5.40	131.86	121.54
13	K	94	TYR	C-N-CA	5.40	131.86	121.54
1	X	1690	U	P-O5'-C5'	-5.40	112.80	120.90
1	X	181	A	C4'-C3'-O3'	5.39	117.49	109.40
15	M	31	ASP	N-CA-C	5.39	122.29	110.80
1	X	1152	C	P-O5'-C5'	5.39	128.99	120.90
17	O	34	GLU	CA-C-N	5.39	127.82	120.54
17	O	34	GLU	C-N-CA	5.39	127.82	120.54
1	X	560	G	C4'-C3'-C2'	5.39	107.99	102.60
1	X	1971	C	P-O5'-C5'	-5.39	112.81	120.90
1	X	1965	U	C5'-C4'-C3'	-5.39	107.92	116.00
1	X	2010	G	C4'-C3'-C2'	-5.38	97.22	102.60
21	S	108	VAL	CA-C-N	5.38	128.03	120.28
21	S	108	VAL	C-N-CA	5.38	128.03	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2527	G	P-O5'-C5'	-5.38	112.83	120.90
15	M	36	ASP	CA-C-N	5.38	130.05	122.09
15	M	36	ASP	C-N-CA	5.38	130.05	122.09
1	X	512	A	C3'-C2'-O2'	5.38	118.77	110.70
5	C	164	VAL	CA-C-N	5.38	131.81	121.54
5	C	164	VAL	C-N-CA	5.38	131.81	121.54
1	X	112	U	N1-C1'-C2'	5.38	120.06	112.00
1	X	1143	A	C5'-C4'-O4'	5.38	117.86	109.80
1	X	1711	C	C1'-O4'-C4'	-5.38	104.32	109.70
1	X	2477	C	C1'-C2'-O2'	5.38	116.46	108.40
11	I	77	LEU	CA-C-N	5.38	127.74	120.38
11	I	77	LEU	C-N-CA	5.38	127.74	120.38
1	X	2509	A	P-O3'-C3'	5.37	128.26	120.20
1	X	2051	U	O3'-P-O5'	-5.37	95.94	104.00
14	L	60	LYS	CA-C-N	5.37	131.80	121.54
14	L	60	LYS	C-N-CA	5.37	131.80	121.54
1	X	1811	A	C4'-C3'-C2'	5.37	107.97	102.60
1	X	636	G	C5'-C4'-C3'	-5.37	107.95	116.00
1	X	2497	A	O4'-C4'-C3'	-5.37	100.73	106.10
1	X	2780	A	P-O5'-C5'	5.36	128.94	120.90
1	X	518	A	P-O5'-C5'	5.36	128.94	120.90
2	Y	77	G	P-O5'-C5'	5.36	128.94	120.90
4	B	90	SER	CA-C-N	5.36	130.30	122.69
4	B	90	SER	C-N-CA	5.36	130.30	122.69
13	K	94	TYR	N-CA-CB	5.36	118.51	109.94
3	A	270	ILE	CA-C-N	5.36	131.61	121.97
3	A	270	ILE	C-N-CA	5.36	131.61	121.97
1	X	1128	G	P-O5'-C5'	5.35	128.93	120.90
1	X	2032	G	C3'-C2'-O2'	5.35	118.73	110.70
20	R	88	THR	CA-C-N	5.35	125.77	120.31
20	R	88	THR	C-N-CA	5.35	125.77	120.31
1	X	2338	C	P-O3'-C3'	5.35	128.23	120.20
1	X	342	G	C4'-C3'-O3'	5.35	117.42	109.40
1	X	455	A	P-O3'-C3'	5.35	128.22	120.20
1	X	1785	A	P-O5'-C5'	-5.35	112.87	120.90
1	X	59	G	P-O3'-C3'	5.35	128.22	120.20
1	X	534	U	P-O5'-C5'	5.35	128.92	120.90
1	X	2705	A	P-O3'-C3'	5.35	128.22	120.20
26	Z	14	SER	CA-C-N	5.35	127.76	120.54
26	Z	14	SER	C-N-CA	5.35	127.76	120.54
7	E	109	TYR	CA-C-N	5.34	127.70	120.38
7	E	109	TYR	C-N-CA	5.34	127.70	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1652	G	P-O3'-C3'	5.34	128.21	120.20
12	J	128	ILE	N-CA-C	5.34	115.34	108.82
1	X	1308	C	C3'-C2'-C1'	-5.34	95.96	101.30
2	Y	10	U	C3'-C2'-O2'	5.34	118.71	110.70
26	Z	48	ASN	N-CA-C	5.34	116.78	111.07
1	X	1692	C	C3'-C2'-C1'	5.34	106.64	101.30
1	X	797	A	C4'-C3'-O3'	-5.33	105.01	113.00
1	X	1142	G	O3'-P-O5'	-5.33	96.01	104.00
2	Y	11	G	O4'-C4'-C3'	-5.33	98.67	104.00
17	O	52	GLY	CA-C-N	5.33	127.42	120.28
17	O	52	GLY	C-N-CA	5.33	127.42	120.28
1	X	1938	U	O4'-C1'-C2'	5.32	111.12	105.80
1	X	2699	G	P-O3'-C3'	5.32	128.18	120.20
1	X	83	A	C1'-O4'-C4'	-5.32	104.38	109.70
1	X	1409	U	C1'-O4'-C4'	-5.32	104.38	109.70
4	B	19	ARG	N-CA-C	5.32	117.64	109.07
1	X	1441	A	C2'-C3'-O3'	5.32	117.48	109.50
1	X	232	A	P-O5'-C5'	5.32	128.87	120.90
1	X	559	C	C1'-O4'-C4'	-5.32	104.58	109.90
1	X	1711	C	P-O5'-C5'	5.32	128.87	120.90
12	J	86	LYS	N-CA-C	5.31	117.62	109.07
1	X	994	A	O4'-C4'-C3'	5.31	109.31	104.00
1	X	2498	U	P-O3'-C3'	5.31	128.17	120.20
1	X	539	A	N9-C1'-C2'	5.31	121.97	114.00
1	X	689	A	C1'-O4'-C4'	-5.31	104.59	109.90
1	X	859	U	N1-C1'-C2'	5.31	121.96	114.00
1	X	1397	A	C4'-C3'-O3'	-5.31	105.04	113.00
1	X	1680	U	O3'-P-O5'	-5.30	96.04	104.00
19	Q	68	PHE	CA-C-N	5.30	131.52	121.97
19	Q	68	PHE	C-N-CA	5.30	131.52	121.97
1	X	2721	A	C3'-C2'-O2'	5.30	118.65	110.70
1	X	1307	U	P-O5'-C5'	5.30	128.85	120.90
1	X	685	U	N1-C1'-C2'	5.30	119.94	112.00
1	X	2018	G	C2'-C3'-O3'	5.29	117.44	109.50
1	X	2217	G	C1'-O4'-C4'	-5.29	104.41	109.70
1	X	1885	C	C4'-C3'-C2'	-5.29	97.31	102.60
1	X	1749	G	C3'-C2'-C1'	-5.29	96.21	101.50
1	X	1201	G	P-O3'-C3'	5.29	128.13	120.20
24	V	44	ARG	CA-C-N	5.28	127.31	120.44
24	V	44	ARG	C-N-CA	5.28	127.31	120.44
1	X	475	U	C3'-C2'-O2'	5.28	118.62	110.70
1	X	1522	C	C3'-C2'-C1'	-5.28	96.02	101.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	124	A	C4'-C3'-O3'	-5.28	105.09	113.00
1	X	1882	G	C3'-C2'-O2'	5.28	118.61	110.70
12	J	77	LYS	N-CA-C	5.28	117.27	108.99
1	X	1686	A	N9-C1'-C2'	5.27	119.91	112.00
1	X	308	C	P-O5'-C5'	5.27	128.81	120.90
22	T	19	LYS	N-CA-C	5.27	122.03	110.80
1	X	2588	U	C2'-C3'-O3'	5.27	117.41	109.50
1	X	2689	C	C4'-C3'-O3'	-5.27	105.10	113.00
1	X	1825	C	O4'-C1'-C2'	-5.27	102.33	107.60
1	X	1291	G	C3'-C2'-O2'	5.26	118.60	110.70
1	X	2628	C	O4'-C4'-C3'	-5.26	98.74	104.00
1	X	1409	U	N1-C1'-C2'	5.26	121.89	114.00
1	X	522	G	C2'-C3'-O3'	5.26	117.39	109.50
1	X	801	A	P-O3'-C3'	5.26	128.09	120.20
1	X	2553	G	P-O5'-C5'	5.26	128.79	120.90
1	X	1249	G	N9-C1'-C2'	5.26	121.89	114.00
1	X	1629	G	C3'-C2'-O2'	5.26	118.58	110.70
23	U	68	ARG	N-CA-C	-5.26	105.20	111.03
1	X	1754	G	P-O3'-C3'	5.25	128.08	120.20
1	X	2393	G	P-O3'-C3'	-5.25	112.32	120.20
2	Y	90	C	C3'-C2'-C1'	-5.25	96.05	101.30
1	X	608	G	C3'-C2'-O2'	5.25	118.58	110.70
1	X	1433	A	C1'-O4'-C4'	-5.25	104.45	109.70
1	X	1798	G	O3'-P-O5'	-5.25	96.12	104.00
1	X	2005	U	P-O5'-C5'	5.25	128.78	120.90
21	S	29	ASN	CA-C-N	5.25	128.12	120.98
21	S	29	ASN	C-N-CA	5.25	128.12	120.98
1	X	539	A	P-O5'-C5'	5.25	128.78	120.90
1	X	1820	G	C4'-C3'-C2'	5.25	107.85	102.60
1	X	809	C	O4'-C1'-N1	5.25	116.37	108.50
1	X	2566	A	O3'-P-O5'	-5.25	96.13	104.00
16	N	38	THR	CA-C-N	5.25	127.74	120.29
16	N	38	THR	C-N-CA	5.25	127.74	120.29
9	G	74	MET	N-CA-C	5.24	116.25	108.86
1	X	2406	C	P-O3'-C3'	5.24	128.06	120.20
19	Q	7	LEU	CA-C-N	5.24	127.30	120.28
19	Q	7	LEU	C-N-CA	5.24	127.30	120.28
1	X	1094	C	P-O5'-C5'	5.24	128.75	120.90
1	X	933	G	P-O3'-C3'	-5.23	112.35	120.20
1	X	1233	A	P-O5'-C5'	5.23	128.75	120.90
10	H	115	ALA	CA-C-N	5.23	127.81	120.28
10	H	115	ALA	C-N-CA	5.23	127.81	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	T	15	ASP	CA-C-N	5.23	131.53	121.54
22	T	15	ASP	C-N-CA	5.23	131.53	121.54
1	X	1022	A	O5'-C5'-C4'	-5.23	103.66	111.50
10	H	78	SER	N-CA-C	-5.23	105.64	112.23
22	T	39	ARG	N-CA-C	-5.23	100.72	109.24
1	X	2399	C	C3'-C2'-O2'	5.23	118.54	110.70
1	X	1442	C	C2'-C3'-O3'	5.22	117.34	109.50
1	X	2298	U	C4'-C3'-O3'	5.22	117.24	109.40
1	X	1482	U	N1-C1'-C2'	5.22	121.83	114.00
1	X	2795	A	C4'-C3'-O3'	-5.22	105.17	113.00
1	X	1458	A	P-O3'-C3'	5.22	128.03	120.20
1	X	1763	G	P-O5'-C5'	-5.22	113.07	120.90
1	X	559	C	O4'-C1'-C2'	-5.22	102.38	107.60
1	X	2696	A	C4'-C3'-C2'	-5.22	97.38	102.60
2	Y	117	G	C2'-C3'-O3'	5.22	121.53	113.70
1	X	1882	G	C3'-C2'-C1'	5.21	106.52	101.30
1	X	2223	U	P-O3'-C3'	-5.21	112.38	120.20
1	X	1140	A	C5'-C4'-C3'	-5.21	108.19	116.00
23	U	19	ILE	N-CA-C	5.21	120.18	109.34
1	X	1574	A	P-O5'-C5'	5.21	128.71	120.90
1	X	2228	U	C3'-C2'-C1'	5.21	106.71	101.50
1	X	2266	A	C2'-C3'-O3'	5.21	117.31	109.50
1	X	2551	A	P-O3'-C3'	5.21	128.01	120.20
18	P	12	LYS	CA-C-N	5.21	127.52	120.65
18	P	12	LYS	C-N-CA	5.21	127.52	120.65
1	X	1801	C	P-O3'-C3'	5.21	128.01	120.20
1	X	2246	A	N9-C1'-C2'	5.21	119.81	112.00
1	X	501	G	C3'-C2'-O2'	5.20	118.50	110.70
9	G	78	ASP	CA-CB-CG	5.20	117.80	112.60
13	K	5	LYS	CA-C-N	5.20	131.48	121.54
13	K	5	LYS	C-N-CA	5.20	131.48	121.54
1	X	574	C	C3'-C2'-O2'	5.20	118.50	110.70
9	G	34	PRO	CA-C-N	5.20	131.47	121.54
9	G	34	PRO	C-N-CA	5.20	131.47	121.54
20	R	81	VAL	CA-C-N	5.20	131.47	121.54
20	R	81	VAL	C-N-CA	5.20	131.47	121.54
1	X	2788	C	C2'-C3'-O3'	-5.20	105.91	113.70
1	X	1992	G	C3'-C2'-O2'	5.19	118.49	110.70
1	X	800	U	O3'-P-O5'	-5.19	96.21	104.00
1	X	2794	G	P-O3'-C3'	5.19	127.99	120.20
3	A	69	ARG	CA-C-N	5.19	128.61	120.82
3	A	69	ARG	C-N-CA	5.19	128.61	120.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	886	A	C3'-C2'-C1'	-5.19	96.11	101.30
2	Y	107	C	P-O3'-C3'	5.19	127.99	120.20
3	A	203	ASN	CA-C-N	5.19	128.19	122.22
3	A	203	ASN	C-N-CA	5.19	128.19	122.22
1	X	95	G	P-O3'-C3'	5.19	127.98	120.20
1	X	2414	A	C4'-C3'-O3'	-5.19	105.22	113.00
1	X	2507	U	C3'-C2'-O2'	5.19	118.48	110.70
1	X	1497	C	C5'-C4'-C3'	-5.18	108.22	116.00
20	R	77	HIS	CA-C-N	5.18	130.08	121.99
20	R	77	HIS	C-N-CA	5.18	130.08	121.99
20	R	80	LYS	CA-C-N	-5.18	116.35	123.14
20	R	80	LYS	C-N-CA	-5.18	116.35	123.14
1	X	418	C	C1'-O4'-C4'	-5.18	104.72	109.90
1	X	1986	G	P-O3'-C3'	-5.18	112.43	120.20
5	C	105	ALA	CA-C-N	5.18	127.22	120.28
5	C	105	ALA	C-N-CA	5.18	127.22	120.28
1	X	203	G	N9-C1'-C2'	5.18	119.77	112.00
5	C	195	ILE	N-CA-CB	5.18	119.77	111.23
17	O	93	ILE	N-CA-C	5.18	115.51	107.28
1	X	826	U	P-O5'-C5'	5.18	128.66	120.90
22	T	18	PRO	CA-C-N	5.18	131.43	121.54
22	T	18	PRO	C-N-CA	5.18	131.43	121.54
1	X	1628	C	P-O5'-C5'	-5.17	113.14	120.90
1	X	26	G	N9-C1'-C2'	5.17	119.76	112.00
1	X	1021	A	P-O5'-C5'	5.17	128.66	120.90
12	J	20	GLY	CA-C-N	5.17	131.42	121.54
12	J	20	GLY	C-N-CA	5.17	131.42	121.54
1	X	953	G	C3'-C2'-O2'	5.17	118.45	110.70
1	X	1279	G	O3'-P-O5'	-5.17	96.24	104.00
1	X	2413	A	O3'-P-O5'	-5.17	96.25	104.00
1	X	1032	A	C4'-C3'-O3'	5.17	120.75	113.00
1	X	2487	G	C3'-C2'-O2'	5.17	118.45	110.70
9	G	108	GLY	N-CA-C	-5.17	100.94	113.18
1	X	247	A	P-O3'-C3'	5.16	127.94	120.20
8	F	137	THR	N-CA-C	5.16	117.37	110.35
1	X	967	G	P-O5'-C5'	5.16	128.64	120.90
1	X	1000	G	O4'-C1'-C2'	-5.16	100.64	105.80
1	X	955	G	C3'-C2'-O2'	5.16	118.44	110.70
2	Y	74	A	P-O3'-C3'	5.16	127.94	120.20
10	H	94	ASN	CA-CB-CG	5.16	117.76	112.60
12	J	43	ILE	CA-C-N	5.16	128.54	120.75
12	J	43	ILE	C-N-CA	5.16	128.54	120.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	411	C	O3'-P-O5'	-5.16	96.27	104.00
1	X	1683	G	C3'-C2'-O2'	5.16	118.43	110.70
1	X	922	A	C4'-C3'-O3'	-5.15	105.27	113.00
1	X	126	C	O5'-C5'-C4'	-5.15	103.77	111.50
1	X	812	G	O3'-P-O5'	-5.15	96.28	104.00
1	X	843	G	P-O5'-C5'	5.15	128.62	120.90
1	X	1001	A	N9-C1'-C2'	5.15	119.72	112.00
1	X	1015	U	O3'-P-O5'	-5.15	96.28	104.00
1	X	2290	A	P-O5'-C5'	5.15	128.62	120.90
1	X	1790	G	C2'-C3'-O3'	5.14	117.22	109.50
1	X	2512	A	P-O5'-C5'	5.14	128.61	120.90
1	X	1795	C	P-O5'-C5'	5.14	128.61	120.90
1	X	2044	G	C1'-C2'-O2'	5.14	119.51	111.80
1	X	2659	C	P-O3'-C3'	-5.14	112.49	120.20
5	C	63	GLY	CA-C-N	5.14	128.90	120.63
5	C	63	GLY	C-N-CA	5.14	128.90	120.63
13	K	56	LYS	CA-C-N	5.14	125.80	119.99
13	K	56	LYS	C-N-CA	5.14	125.80	119.99
1	X	1601	U	C2'-C3'-O3'	5.14	117.21	109.50
1	X	1602	G	P-O3'-C3'	5.14	127.91	120.20
1	X	1758	C	C1'-C2'-O2'	5.14	116.10	108.40
1	X	2028	C	O4'-C4'-C3'	-5.14	98.86	104.00
1	X	2044	G	C2'-C3'-O3'	5.14	117.20	109.50
1	X	2418	A	P-O3'-C3'	5.14	127.91	120.20
1	X	2650	G	C5'-C4'-C3'	-5.14	108.29	116.00
1	X	2803	C	C1'-C2'-O2'	5.14	116.11	108.40
17	O	25	LEU	CA-C-N	5.13	128.14	120.90
17	O	25	LEU	C-N-CA	5.13	128.14	120.90
5	C	59	TYR	CA-C-N	5.13	131.47	121.41
5	C	59	TYR	C-N-CA	5.13	131.47	121.41
1	X	1958	G	C3'-C2'-O2'	5.13	118.39	110.70
1	X	710	C	C4'-C3'-O3'	-5.13	105.31	113.00
1	X	1290	A	C3'-C2'-O2'	5.13	118.39	110.70
1	X	585	U	C1'-C2'-O2'	5.12	116.09	108.40
1	X	808	C	O3'-P-O5'	-5.12	96.31	104.00
1	X	2245	A	P-O3'-C3'	5.12	127.89	120.20
1	X	1335	A	P-O3'-C3'	-5.12	112.53	120.20
1	X	1469	U	P-O3'-C3'	5.12	127.88	120.20
1	X	1963	G	P-O3'-C3'	5.12	127.87	120.20
1	X	991	A	N9-C1'-C2'	5.11	119.67	112.00
1	X	97	U	C5'-C4'-C3'	-5.11	108.33	116.00
5	C	123	PHE	CA-C-N	5.11	130.26	122.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	123	PHE	C-N-CA	5.11	130.26	122.29
1	X	730	C	N1-C1'-C2'	5.11	119.67	112.00
1	X	2015	G	N9-C1'-C2'	5.11	121.67	114.00
1	X	2314	A	P-O5'-C5'	5.11	128.56	120.90
3	A	55	GLY	N-CA-C	5.11	125.28	113.18
1	X	848	A	C3'-C2'-O2'	5.10	118.35	110.70
1	X	2392	G	P-O5'-C5'	5.10	128.55	120.90
2	Y	46	G	C3'-C2'-C1'	5.10	106.40	101.30
3	A	264	LYS	CA-C-N	5.10	127.63	120.28
3	A	264	LYS	C-N-CA	5.10	127.63	120.28
1	X	2241	U	P-O5'-C5'	-5.10	113.25	120.90
1	X	2545	A	P-O5'-C5'	5.10	128.55	120.90
3	A	252	LYS	N-CA-C	5.10	121.08	109.81
1	X	167	A	P-O5'-C5'	5.10	128.54	120.90
1	X	1732	U	C4'-C3'-O3'	5.10	117.04	109.40
1	X	2230	G	C5'-C4'-O4'	-5.09	102.16	109.80
1	X	2339	A	P-O5'-C5'	5.09	128.54	120.90
1	X	2585	C	C3'-C2'-C1'	-5.09	96.21	101.30
1	X	666	U	O4'-C1'-N1	5.09	116.13	108.50
1	X	2504	G	C5'-C4'-C3'	-5.09	108.37	116.00
5	C	58	MET	N-CA-C	5.09	121.63	110.80
1	X	2837	G	P-O3'-C3'	-5.08	112.57	120.20
2	Y	92	G	P-O5'-C5'	5.08	128.53	120.90
1	X	99	U	C4'-C3'-O3'	5.08	117.03	109.40
1	X	674	U	C1'-C2'-O2'	5.08	116.02	108.40
1	X	317	U	O3'-P-O5'	-5.08	96.38	104.00
1	X	742	G	C4'-C3'-O3'	-5.08	105.38	113.00
2	Y	86	A	C1'-O4'-C4'	-5.08	104.82	109.90
1	X	1755	G	O4'-C1'-C2'	-5.08	102.52	107.60
1	X	1635	G	C1'-C2'-O2'	5.08	116.01	108.40
2	Y	107	C	C2'-C3'-O3'	5.08	121.31	113.70
10	H	12	ASP	CA-CB-CG	5.08	117.67	112.60
1	X	759	C	N1-C1'-C2'	5.07	119.61	112.00
9	G	116	ARG	N-CA-C	5.07	116.89	111.36
23	U	57	VAL	N-CA-C	5.07	115.98	108.23
2	Y	17	A	P-O3'-C3'	5.07	127.80	120.20
2	Y	91	A	O3'-P-O5'	5.07	111.60	104.00
1	X	2261	G	C4'-C3'-C2'	5.07	107.67	102.60
20	R	76	LEU	N-CA-C	5.07	117.55	109.65
9	G	62	ILE	N-CA-C	5.06	117.42	111.09
14	L	94	TYR	CA-C-N	5.06	131.21	121.54
14	L	94	TYR	C-N-CA	5.06	131.21	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2189	A	O4'-C1'-C2'	-5.06	102.54	107.60
1	X	2568	A	O4'-C4'-C3'	-5.06	98.94	104.00
1	X	1684	G	O3'-P-O5'	-5.06	96.41	104.00
1	X	2362	G	C4'-C3'-O3'	-5.06	105.41	113.00
16	N	30	LYS	N-CA-C	5.06	119.72	113.50
1	X	1170	U	C3'-C2'-O2'	5.06	118.28	110.70
13	K	3	HIS	CA-CB-CG	5.06	118.86	113.80
13	K	104	ARG	N-CA-C	5.05	121.57	110.80
3	A	203	ASN	CB-CA-C	5.05	120.47	110.42
20	R	6	ALA	N-CA-C	5.05	121.55	110.80
1	X	410	A	O3'-P-O5'	-5.05	96.43	104.00
1	X	522	G	N9-C1'-C2'	5.05	121.57	114.00
1	X	968	C	O4'-C4'-C3'	-5.05	101.05	106.10
1	X	998	C	C4'-C3'-C2'	-5.05	97.55	102.60
1	X	2262	C	C3'-C2'-O2'	5.05	118.27	110.70
1	X	2368	G	C4'-C3'-O3'	-5.05	105.43	113.00
1	X	418	C	N1-C1'-C2'	5.05	119.57	112.00
2	Y	53	G	N9-C1'-C2'	5.05	119.57	112.00
1	X	2506	C	C3'-C2'-O2'	5.04	118.27	110.70
1	X	799	C	C3'-C2'-O2'	5.04	118.27	110.70
1	X	2024	U	C4'-C3'-O3'	-5.04	105.44	113.00
1	X	2527	G	O3'-P-O5'	-5.04	96.44	104.00
12	J	81	GLU	CA-C-N	5.04	131.17	121.54
12	J	81	GLU	C-N-CA	5.04	131.17	121.54
14	L	36	LYS	CA-C-N	5.04	131.31	121.63
14	L	36	LYS	C-N-CA	5.04	131.31	121.63
1	X	598	U	O4'-C4'-C3'	-5.04	98.96	104.00
1	X	655	A	O4'-C1'-N9	5.04	116.06	108.50
1	X	1337	G	C4'-C3'-C2'	5.04	107.64	102.60
1	X	1441	A	C4'-C3'-O3'	5.04	116.96	109.40
1	X	1467	U	C1'-C2'-O2'	5.04	115.96	108.40
1	X	1477	C	C3'-C2'-O2'	5.04	118.26	110.70
1	X	2375	G	C3'-C2'-O2'	5.04	118.26	110.70
12	J	42	TRP	CA-C-N	-5.04	116.33	122.93
12	J	42	TRP	C-N-CA	-5.04	116.33	122.93
2	Y	88	C	C1'-O4'-C4'	-5.04	104.86	109.90
11	I	35	LYS	CA-C-N	5.04	131.29	121.41
11	I	35	LYS	C-N-CA	5.04	131.29	121.41
1	X	517	A	C3'-C2'-O2'	5.04	118.26	110.70
1	X	887	G	C3'-C2'-O2'	5.04	118.26	110.70
1	X	1162	A	C4'-C3'-C2'	-5.04	97.56	102.60
1	X	90	G	N9-C1'-C2'	5.04	119.56	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	S	77	ALA	N-CA-C	5.04	116.73	109.48
1	X	575	U	P-O3'-C3'	5.04	127.75	120.20
1	X	824	U	C1'-O4'-C4'	-5.04	104.67	109.70
1	X	1087	C	P-O5'-C5'	5.04	128.45	120.90
3	A	197	GLY	CA-C-N	5.04	129.56	122.46
3	A	197	GLY	C-N-CA	5.04	129.56	122.46
15	M	101	ARG	CA-C-N	5.04	127.53	120.28
15	M	101	ARG	C-N-CA	5.04	127.53	120.28
19	Q	44	GLN	CA-C-N	5.03	127.28	120.38
19	Q	44	GLN	C-N-CA	5.03	127.28	120.38
1	X	921	A	O3'-P-O5'	-5.03	96.45	104.00
1	X	1632	A	P-O3'-C3'	5.03	127.75	120.20
1	X	1792	C	P-O3'-C3'	5.03	127.75	120.20
1	X	1184	G	P-O3'-C3'	5.03	127.74	120.20
5	C	133	PHE	N-CA-C	-5.03	105.88	111.36
26	Z	36	CYS	N-CA-C	5.03	121.51	110.80
1	X	487	G	P-O5'-C5'	5.03	128.44	120.90
17	O	77	GLY	CA-C-N	5.03	131.02	121.97
17	O	77	GLY	C-N-CA	5.03	131.02	121.97
24	V	15	ALA	CA-C-N	5.02	127.01	120.28
24	V	15	ALA	C-N-CA	5.02	127.01	120.28
1	X	1787	U	C3'-C2'-O2'	5.02	118.23	110.70
3	A	214	TRP	CA-C-N	5.02	131.13	121.54
3	A	214	TRP	C-N-CA	5.02	131.13	121.54
1	X	1763	G	C1'-C2'-O2'	5.02	115.93	108.40
1	X	699	G	P-O3'-C3'	5.02	127.73	120.20
1	X	2454	C	N1-C1'-C2'	5.02	119.53	112.00
16	N	103	PRO	CA-C-N	5.02	126.97	120.44
16	N	103	PRO	C-N-CA	5.02	126.97	120.44
1	X	40	U	C3'-C2'-O2'	5.02	118.22	110.70
1	X	1273	G	C1'-C2'-O2'	5.02	115.93	108.40
1	X	1663	C	P-O3'-C3'	5.02	127.73	120.20
1	X	1979	C	P-O3'-C3'	5.02	127.73	120.20
1	X	2808	U	C1'-O4'-C4'	-5.02	104.68	109.70
11	I	5	ASP	CA-C-N	5.01	127.89	120.82
11	I	5	ASP	C-N-CA	5.01	127.89	120.82
19	Q	73	ASN	CA-C-N	5.01	131.12	121.54
19	Q	73	ASN	C-N-CA	5.01	131.12	121.54
1	X	562	G	C3'-C2'-C1'	-5.01	96.29	101.30
1	X	941	U	C4'-C3'-C2'	-5.01	97.59	102.60
1	X	968	C	C5'-C4'-O4'	5.01	116.61	109.10
1	X	1489	C	O4'-C1'-N1	5.01	115.71	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	J	121	LEU	CA-C-N	5.01	127.24	120.38
12	J	121	LEU	C-N-CA	5.01	127.24	120.38
1	X	1830	C	C1'-O4'-C4'	-5.01	104.69	109.70
1	X	1668	G	C1'-C2'-O2'	5.00	115.91	108.40
1	X	2009	U	P-O3'-C3'	-5.00	112.69	120.20
1	X	2641	A	C1'-C2'-O2'	5.00	115.90	108.40
15	M	104	LEU	N-CA-C	5.00	121.45	110.80
23	U	32	ARG	CA-C-N	5.00	130.22	121.52
23	U	32	ARG	C-N-CA	5.00	130.22	121.52

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	1251	G	Sidechain
1	X	699	G	Sidechain
1	X	967	G	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	57651	0	29049	540	0
2	Y	2598	0	1328	22	0
3	A	1826	0	1885	87	0
4	B	1539	0	1600	60	0
5	C	1506	0	1525	58	0
6	D	1400	0	1481	20	0
7	E	1286	0	1336	10	0
8	F	503	0	520	6	0
9	G	1114	0	1144	49	0
10	H	997	0	1046	30	0
11	I	1067	0	1103	40	0
12	J	1090	0	1125	35	0
13	K	878	0	930	24	0
14	L	779	0	820	20	0
15	M	871	0	894	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	N	978	0	1020	33	0
17	O	741	0	756	24	0
18	P	1014	0	1096	26	0
19	Q	726	0	753	11	0
20	R	825	0	881	27	0
21	S	1345	0	1372	32	0
22	T	625	0	655	11	0
23	U	552	0	604	31	0
24	V	533	0	558	7	0
25	W	424	0	470	17	0
26	Z	457	0	462	20	0
27	1	53	0	0	0	0
28	2	46	0	0	1	0
29	3	63	0	0	0	0
30	4	297	0	330	4	0
31	M	1	0	0	0	0
31	X	28	0	0	0	0
31	Y	6	0	0	0	0
32	X	58	0	67	19	0
All	All	83877	0	54810	1108	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 8.

All (1108) 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)
4:B:117:MET:SD	4:B:117:MET:CE	2.02	1.47
9:G:100:TYR:HB2	9:G:116:ARG:NH1	1.69	1.08
9:G:33:ILE:HB	9:G:34:PRO:HD3	1.38	1.03
1:X:558:G:H4'	1:X:559:C:H5'	1.40	1.02
1:X:1448:A:H61	1:X:1574:A:H61	1.09	1.00
5:C:43:ALA:HB1	5:C:86:PRO:HB2	1.46	0.96
4:B:152:LYS:HB2	9:G:106:TYR:HB3	1.49	0.95
1:X:1542:G:H22	1:X:1562:G:H1	1.13	0.94
1:X:1007:A:H4'	16:N:93:LYS:HB3	1.46	0.94
1:X:1919:A:H2	1:X:1926:U:H3	1.09	0.94
4:B:116:VAL:HG22	4:B:136:ARG:HE	1.31	0.93
11:I:62:LYS:HE2	11:I:64:GLY:HA3	1.53	0.91
32:X:2929:1F4:H59	32:X:2929:1F4:H60	1.51	0.90
11:I:30:ALA:HB3	11:I:34:HIS:CE1	2.07	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:77:C:H42	1:X:106:G:H1	1.21	0.88
15:M:79:ARG:HG3	15:M:79:ARG:HH11	1.36	0.88
1:X:1770:U:H5	1:X:1775:A:N7	1.70	0.88
14:L:38:ILE:HG13	14:L:39:TYR:H	1.39	0.88
4:B:116:VAL:HG22	4:B:136:ARG:NE	1.88	0.87
21:S:71:MET:HA	21:S:78:PRO:HA	1.58	0.85
4:B:131:SER:HB3	4:B:134:TRP:CD1	2.11	0.85
3:A:252:LYS:HD2	3:A:253:PRO:HD3	1.59	0.84
1:X:1817:U:H4'	3:A:252:LYS:HE2	1.59	0.83
1:X:1266:G:N7	11:I:32:ARG:NH1	2.25	0.83
13:K:10:LEU:HD21	13:K:17:ARG:HB2	1.61	0.82
3:A:248:THR:HB	3:A:249:PRO:HD3	1.60	0.82
1:X:2371:A:H2	1:X:2403:C:H42	1.28	0.82
3:A:218:LYS:HE3	3:A:221:GLN:HB2	1.62	0.82
1:X:38:G:H1	1:X:453:U:H3	1.25	0.81
1:X:1278:A:H2	1:X:1997:A:H62	1.26	0.80
9:G:33:ILE:HB	9:G:34:PRO:CD	2.11	0.80
1:X:2387:U:H2'	1:X:2388:G:H8	1.45	0.80
9:G:100:TYR:HB2	9:G:116:ARG:HH11	1.47	0.79
4:B:134:TRP:CD1	4:B:134:TRP:H	2.02	0.78
1:X:1342:U:H5''	1:X:1343:C:H5	1.48	0.78
1:X:559:C:H2'	1:X:560:G:O4'	1.84	0.78
3:A:43:ARG:N	3:A:43:ARG:HD2	1.99	0.78
1:X:823:U:OP1	11:I:32:ARG:NH1	2.17	0.78
32:X:2929:1F4:H3	32:X:2929:1F4:C39	2.13	0.78
9:G:68:PRO:HD2	9:G:76:GLN:HB3	1.66	0.78
16:N:66:ASN:HB3	16:N:76:TYR:H	1.50	0.77
1:X:640:C:H4'	1:X:660:G:H21	1.49	0.77
15:M:59:GLY:HA3	15:M:64:LYS:HA	1.65	0.77
3:A:172:TYR:HA	3:A:186:HIS:HA	1.66	0.76
1:X:224:G:OP2	1:X:226:C:N4	2.17	0.76
5:C:29:GLU:HB2	11:I:18:ARG:HH12	1.50	0.76
1:X:673:G:H5'	5:C:93:TYR:CE1	2.20	0.76
1:X:689:A:H8	1:X:2052:G:H21	1.33	0.76
14:L:33:ARG:HD2	14:L:38:ILE:HD13	1.66	0.76
26:Z:35:GLN:O	26:Z:37:HIS:N	2.19	0.76
21:S:6:LYS:H	21:S:7:PRO:HD3	1.48	0.75
1:X:1007:A:H1'	17:O:6:GLN:HG2	1.67	0.75
26:Z:4:HIS:HB3	26:Z:5:PRO:HD3	1.69	0.75
13:K:10:LEU:CD2	13:K:17:ARG:HB2	2.15	0.75
2:Y:45:C:H2'	6:D:92:ARG:HH11	1.52	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:134:TRP:H	4:B:134:TRP:HD1	1.32	0.75
15:M:79:ARG:HH11	15:M:79:ARG:CG	2.00	0.75
3:A:243:GLY:C	3:A:244:ARG:HD3	2.11	0.75
10:H:25:LEU:HD11	10:H:52:VAL:HG23	1.70	0.73
25:W:12:ARG:HG2	25:W:12:ARG:HH11	1.52	0.73
1:X:1329:U:H2'	1:X:1330:G:H8	1.52	0.73
1:X:1919:A:H2	1:X:1926:U:N3	1.84	0.73
1:X:652:C:H42	1:X:657:A:H61	1.35	0.73
17:O:73:LYS:HB2	17:O:82:ARG:HB2	1.70	0.73
15:M:79:ARG:HG3	15:M:79:ARG:NH1	2.02	0.73
9:G:100:TYR:HB2	9:G:116:ARG:HH12	1.51	0.72
17:O:57:GLN:H	17:O:97:GLY:HA3	1.53	0.72
1:X:2387:U:H2'	1:X:2388:G:C8	2.23	0.72
1:X:1329:U:H2'	1:X:1330:G:C8	2.25	0.72
11:I:62:LYS:CE	11:I:64:GLY:HA3	2.19	0.72
4:B:152:LYS:CB	9:G:106:TYR:HB3	2.20	0.71
5:C:48:ARG:HB2	5:C:51:VAL:HG22	1.70	0.71
11:I:62:LYS:HE2	11:I:64:GLY:CA	2.20	0.71
1:X:2241:U:H5	22:T:17:ASN:OD1	1.72	0.71
1:X:617:U:H5	1:X:632:A:H2	1.38	0.70
3:A:231:HIS:HD2	3:A:233:HIS:H	1.38	0.70
5:C:137:ALA:HB1	5:C:142:LEU:HB2	1.73	0.70
1:X:617:U:C5	1:X:632:A:C2	2.80	0.70
1:X:1673:C:H2'	1:X:1674:C:H6	1.55	0.70
4:B:110:GLY:O	13:K:3:HIS:CD2	2.45	0.70
1:X:2039:G:N2	26:Z:4:HIS:O	2.22	0.69
4:B:14:ILE:HG22	4:B:21:ILE:HB	1.74	0.69
1:X:1561:A:H3'	1:X:1562:G:C8	2.27	0.69
13:K:79:VAL:HA	13:K:83:VAL:HG13	1.73	0.69
23:U:48:LYS:CG	23:U:49:LYS:H	2.04	0.69
1:X:1832:G:H1	1:X:1885:C:H42	1.37	0.69
1:X:2063:A:H4'	23:U:39:LYS:HG2	1.73	0.69
3:A:231:HIS:CD2	3:A:233:HIS:H	2.11	0.69
14:L:33:ARG:NH1	14:L:38:ILE:HB	2.08	0.68
1:X:1466:C:H2'	1:X:1467:U:O4'	1.93	0.68
5:C:48:ARG:C	5:C:50:GLN:H	2.00	0.68
1:X:1278:A:N6	1:X:1996:A:H5''	2.08	0.68
1:X:501:G:H2'	1:X:502:A:C8	2.28	0.68
1:X:577:U:H2'	1:X:579:G:OP2	1.94	0.68
1:X:2770:A:H4'	1:X:2771:C:H5'	1.74	0.67
9:G:61:ARG:NH1	9:G:66:HIS:H	1.90	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1882:G:N2	1:X:1885:C:H41	1.92	0.67
1:X:1278:A:H61	1:X:1996:A:H5''	1.60	0.67
1:X:2767:C:H1'	4:B:62:PRO:HG3	1.77	0.67
25:W:12:ARG:HH11	25:W:12:ARG:CG	2.06	0.67
3:A:210:GLY:HA2	3:A:213:ARG:HB2	1.76	0.67
9:G:132:PHE:CZ	9:G:145:HIS:HB2	2.30	0.67
9:G:67:ARG:HG2	9:G:70:PHE:HA	1.76	0.67
13:K:11:ASN:OD1	13:K:17:ARG:NH2	2.27	0.67
3:A:43:ARG:HE	3:A:55:GLY:HA2	1.60	0.67
9:G:104:THR:OG1	9:G:110:LEU:HB3	1.95	0.67
20:R:7:GLY:HA3	20:R:42:ARG:O	1.94	0.67
1:X:168:A:H2'	1:X:169:C:C6	2.30	0.66
1:X:1885:C:C4'	3:A:244:ARG:HD2	2.24	0.66
1:X:1342:U:H5''	1:X:1343:C:C5	2.31	0.66
32:X:2929:1F4:H3	32:X:2929:1F4:H51	1.76	0.66
32:X:2929:1F4:H60	32:X:2929:1F4:C50	2.23	0.66
1:X:617:U:H5	1:X:632:A:C2	2.14	0.66
12:J:15:ARG:HD2	12:J:74:PRO:HD2	1.77	0.66
25:W:4:LYS:HG2	25:W:52:GLU:HB3	1.78	0.65
1:X:1673:C:C5'	4:B:136:ARG:HD3	2.26	0.65
2:Y:45:C:H2'	6:D:92:ARG:NH1	2.10	0.65
4:B:194:GLY:HA2	15:M:2:GLN:HB3	1.77	0.65
1:X:1810:U:H2'	3:A:157:ARG:HD3	1.78	0.65
1:X:2266:A:H62	1:X:2323:U:H3	1.43	0.65
1:X:2551:A:N7	4:B:145:LYS:HB2	2.10	0.65
1:X:320:A:N3	1:X:340:G:O2'	2.29	0.65
1:X:1811:A:H5''	3:A:161:THR:HG21	1.78	0.65
1:X:797:A:C5	3:A:229:VAL:HG21	2.31	0.64
1:X:1673:C:H2'	1:X:1674:C:C6	2.31	0.64
11:I:17:LYS:O	11:I:18:ARG:HB2	1.97	0.64
20:R:25:LEU:H	20:R:80:LYS:HA	1.62	0.64
24:V:25:LEU:HD21	24:V:47:ARG:HG2	1.78	0.64
12:J:48:ILE:HD12	12:J:71:PRO:HG3	1.80	0.64
1:X:1744:G:OP1	15:M:100:ARG:HD2	1.97	0.64
1:X:482:A:H2'	1:X:483:A:O4'	1.96	0.64
1:X:742:G:C6	3:A:208:LYS:HB3	2.33	0.64
1:X:1609:G:H2'	1:X:1610:A:C8	2.32	0.64
12:J:28:VAL:HG23	12:J:137:VAL:HB	1.80	0.64
16:N:66:ASN:HB2	16:N:70:ARG:NH1	2.13	0.64
1:X:1582:A:OP1	3:A:211:ARG:NH2	2.31	0.63
1:X:1745:C:P	15:M:101:ARG:HH22	2.20	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:28:VAL:HG12	12:J:29:ALA:H	1.63	0.63
1:X:841:G:H2'	1:X:842:A:C8	2.33	0.63
1:X:764:A:H5'	18:P:111:ARG:HA	1.79	0.63
1:X:2653:A:O2'	10:H:41:ASN:ND2	2.32	0.63
1:X:800:U:H5''	1:X:801:A:H5'	1.81	0.63
1:X:1674:C:H2'	1:X:1675:C:C6	2.34	0.63
1:X:451:A:H2'	1:X:452:G:C8	2.34	0.62
15:M:60:SER:HB3	15:M:63:ARG:HH22	1.64	0.62
3:A:67:PHE:HB3	3:A:153:ALA:H	1.64	0.62
18:P:32:ARG:HA	18:P:121:THR:HG22	1.81	0.62
4:B:152:LYS:H	9:G:106:TYR:HB3	1.64	0.62
5:C:176:ASN:HB3	5:C:179:ASP:HB2	1.81	0.62
11:I:108:LEU:HD23	11:I:129:ALA:HB1	1.82	0.62
4:B:152:LYS:HB2	9:G:106:TYR:CB	2.27	0.62
23:U:32:ARG:HG2	23:U:33:LYS:N	2.13	0.62
21:S:3:LEU:HD11	21:S:56:VAL:HG13	1.80	0.62
1:X:797:A:N7	3:A:229:VAL:HG21	2.15	0.62
6:D:143:TYR:HA	6:D:146:VAL:HG22	1.82	0.62
24:V:28:LEU:HD12	24:V:43:VAL:HG22	1.81	0.62
1:X:1753:A:O5'	1:X:1753:A:H8	1.82	0.61
11:I:28:LYS:NZ	11:I:36:GLY:HA2	2.16	0.61
13:K:3:HIS:HB3	13:K:5:LYS:HD2	1.81	0.61
10:H:124:MET:O	10:H:127:VAL:HG12	2.00	0.61
2:Y:28:A:H8	2:Y:29:C:C5	2.17	0.61
1:X:670:U:H2'	1:X:671:A:C8	2.35	0.61
23:U:51:ILE:HA	23:U:59:THR:O	2.01	0.61
1:X:2083:G:H1	1:X:2172:U:H3	1.48	0.61
1:X:746:G:N7	1:X:774:A:C6	2.69	0.61
1:X:341:A:O2'	1:X:342:G:H8	1.83	0.61
1:X:564:U:H2'	1:X:565:A:C8	2.36	0.61
25:W:7:ARG:HB2	25:W:50:LEU:HA	1.82	0.61
1:X:1574:A:O2'	1:X:1575:C:H3'	2.00	0.61
1:X:226:C:OP2	1:X:2373:C:O2'	2.19	0.60
1:X:450:C:H2'	1:X:451:A:C8	2.35	0.60
23:U:52:ARG:NE	23:U:79:GLU:HA	2.16	0.60
1:X:1437:A:H2'	1:X:1438:G:H8	1.64	0.60
1:X:1745:C:OP1	15:M:101:ARG:NH2	2.33	0.60
15:M:17:GLU:O	15:M:21:THR:OG1	2.17	0.60
3:A:223:GLY:HA2	3:A:226:MET:SD	2.40	0.60
16:N:66:ASN:HB3	16:N:76:TYR:HB2	1.83	0.60
1:X:512:A:H4'	18:P:15:LYS:HB3	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2543:A:H5'	1:X:2627:G:H4'	1.82	0.60
5:C:47:THR:HA	5:C:82:VAL:HB	1.83	0.60
12:J:62:GLY:HA3	12:J:64:LYS:HE3	1.84	0.60
1:X:960:U:H2'	1:X:961:G:C8	2.37	0.60
5:C:176:ASN:HD22	5:C:179:ASP:H	1.48	0.60
1:X:504:G:H4'	18:P:27:VAL:HG12	1.84	0.60
1:X:412:U:H5''	23:U:68:ARG:HH22	1.67	0.60
1:X:168:A:H2'	1:X:169:C:H6	1.67	0.59
1:X:2484:G:H22	32:X:2929:1F4:H56	1.67	0.59
5:C:34:GLN:HB3	5:C:38:ARG:HH11	1.66	0.59
8:F:74:MET:HE1	8:F:127:VAL:HA	1.83	0.59
1:X:954:U:OP2	11:I:38:LYS:HG2	2.01	0.59
1:X:2528:G:H2'	1:X:2529:G:H8	1.66	0.59
5:C:54:THR:HG21	5:C:72:ARG:HB3	1.84	0.59
1:X:38:G:H21	5:C:42:THR:HG21	1.66	0.59
1:X:530:G:H2'	1:X:531:G:C8	2.37	0.59
1:X:1782:A:N6	1:X:1820:G:O2'	2.35	0.59
4:B:50:GLY:HA3	4:B:75:THR:HG21	1.85	0.59
16:N:66:ASN:HB2	16:N:70:ARG:HH11	1.67	0.59
18:P:27:VAL:HG23	18:P:125:THR:HG22	1.85	0.59
20:R:45:LYS:HA	20:R:76:LEU:O	2.02	0.59
18:P:40:LEU:HB3	26:Z:25:LEU:HD13	1.84	0.59
21:S:93:GLU:HB3	21:S:121:GLN:HG3	1.83	0.59
1:X:187:U:H2'	1:X:188:G:C8	2.37	0.59
10:H:78:SER:HA	10:H:91:PHE:O	2.03	0.59
1:X:1885:C:H4'	3:A:244:ARG:HD2	1.83	0.58
17:O:36:LYS:HE2	17:O:56:VAL:HG22	1.85	0.58
22:T:45:PHE:HD2	22:T:77:ARG:HB3	1.67	0.58
1:X:689:A:H2	1:X:815:A:H61	1.51	0.58
3:A:252:LYS:CD	3:A:253:PRO:HD3	2.32	0.58
13:K:3:HIS:CE1	13:K:5:LYS:HZ2	2.21	0.58
16:N:66:ASN:CB	16:N:76:TYR:H	2.17	0.58
1:X:165:G:H2'	1:X:166:G:O4'	2.04	0.58
1:X:501:G:H2'	1:X:502:A:H8	1.65	0.58
5:C:38:ARG:HH12	5:C:176:ASN:HD21	1.51	0.58
12:J:40:PRO:HB3	12:J:99:LYS:HD2	1.86	0.58
5:C:48:ARG:C	5:C:50:GLN:N	2.61	0.58
1:X:1999:U:O2'	26:Z:7:PRO:O	2.21	0.58
4:B:4:ILE:HG22	4:B:96:PHE:HE1	1.67	0.58
15:M:82:PRO:HG2	15:M:85:SER:HB2	1.85	0.58
1:X:553:C:H42	1:X:559:C:H42	1.49	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1656:U:H4'	1:X:2678:C:H4'	1.84	0.58
1:X:405:C:H2'	1:X:406:G:H8	1.69	0.58
1:X:742:G:H2'	1:X:1766:U:H1'	1.85	0.58
1:X:1584:G:N3	3:A:58:HIS:CE1	2.72	0.58
4:B:26:VAL:HG11	4:B:198:LEU:HD11	1.85	0.58
6:D:123:ASP:HB3	6:D:127:ASN:HB2	1.83	0.58
1:X:114:C:O2'	1:X:124:A:N3	2.37	0.57
1:X:1468:A:H5'	1:X:1472:C:N4	2.19	0.57
1:X:1071:U:H4'	1:X:1072:U:H3'	1.85	0.57
20:R:48:VAL:HG12	20:R:50:GLY:H	1.69	0.57
23:U:48:LYS:HG2	23:U:49:LYS:H	1.68	0.57
5:C:58:MET:HB2	5:C:70:GLY:O	2.04	0.57
5:C:119:ALA:H	5:C:189:ASP:HA	1.69	0.57
9:G:105:GLY:O	9:G:106:TYR:C	2.46	0.57
1:X:482:A:O5'	1:X:482:A:H8	1.88	0.57
1:X:1040:A:H5''	12:J:129:GLN:HE22	1.69	0.57
3:A:45:ASN:CG	3:A:46:ARG:H	2.12	0.57
23:U:56:GLN:HE21	23:U:57:VAL:HG23	1.70	0.57
1:X:1437:A:H2'	1:X:1438:G:C8	2.40	0.57
7:E:127:GLU:HG3	7:E:130:ARG:HB2	1.87	0.57
12:J:25:GLY:HA3	12:J:102:ARG:HA	1.87	0.57
23:U:48:LYS:CG	23:U:49:LYS:N	2.68	0.57
25:W:12:ARG:HG3	25:W:50:LEU:HD21	1.85	0.57
1:X:712:A:H2'	1:X:713:G:O4'	2.05	0.57
1:X:2081:U:H3	1:X:2174:G:H1	1.53	0.57
5:C:43:ALA:CB	5:C:86:PRO:HB2	2.29	0.57
10:H:13:ASN:HD21	10:H:109:ARG:HG2	1.70	0.57
1:X:1845:A:H2'	1:X:1846:A:C8	2.40	0.56
19:Q:68:PHE:O	19:Q:70:GLY:N	2.38	0.56
1:X:1699:A:H61	1:X:1723:U:H3	1.51	0.56
1:X:1787:U:H2'	1:X:1788:C:C6	2.41	0.56
1:X:829:C:H2'	1:X:830:C:C6	2.40	0.56
1:X:1982:C:H5''	1:X:2703:C:O2'	2.05	0.56
3:A:36:ALA:HB1	3:A:62:TYR:O	2.04	0.56
1:X:1033:G:H22	1:X:1153:A:H2	1.53	0.56
1:X:559:C:H2'	1:X:560:G:C1'	2.35	0.56
1:X:1173:G:H4'	17:O:22:VAL:HG23	1.86	0.56
14:L:27:LEU:HD23	14:L:44:ASP:HA	1.87	0.56
23:U:14:VAL:O	23:U:15:VAL:HG22	2.06	0.56
1:X:530:G:H2'	1:X:531:G:H8	1.69	0.56
5:C:149:LEU:HD11	5:C:170:LEU:HD13	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1268:U:C2	5:C:66:ASN:HA	2.41	0.56
1:X:215:G:H21	1:X:632:A:H8	1.52	0.56
1:X:2653:A:H2'	10:H:41:ASN:ND2	2.21	0.56
20:R:22:VAL:HG11	20:R:80:LYS:HD2	1.88	0.56
1:X:1348:C:H2'	1:X:1349:A:C8	2.40	0.56
1:X:2266:A:N6	1:X:2323:U:H3	2.04	0.56
1:X:1505:U:HO2'	1:X:1506:C:H6	1.53	0.55
1:X:2516:U:H2'	1:X:2517:C:C6	2.40	0.55
32:X:2929:1F4:O18	32:X:2929:1F4:H9	2.06	0.55
11:I:97:ARG:O	11:I:98:LEU:HB2	2.06	0.55
16:N:66:ASN:HB3	16:N:76:TYR:CB	2.35	0.55
1:X:187:U:H2'	1:X:188:G:H8	1.70	0.55
1:X:1454:U:H2'	1:X:1455:C:C6	2.41	0.55
1:X:1468:A:H5'	1:X:1472:C:H41	1.71	0.55
3:A:38:PRO:HA	3:A:61:LEU:HD23	1.88	0.55
1:X:1348:C:H2'	1:X:1349:A:H8	1.71	0.55
1:X:1770:U:C5	1:X:1775:A:N7	2.62	0.55
1:X:1882:G:H21	1:X:1885:C:H41	1.53	0.55
1:X:1948:C:H5''	1:X:1949:A:H2'	1.89	0.55
20:R:52:ASN:HD21	20:R:71:GLN:HE21	1.55	0.55
1:X:1595:A:H2'	1:X:1596:A:O4'	2.07	0.55
1:X:2212:U:H2'	1:X:2213:G:C8	2.41	0.55
16:N:84:LYS:HG3	16:N:92:ARG:HH22	1.70	0.55
22:T:41:ARG:HE	22:T:41:ARG:HA	1.72	0.55
1:X:1030:U:HO2'	1:X:1032:A:H2	1.54	0.55
6:D:104:ILE:HA	6:D:108:LEU:HD12	1.88	0.55
1:X:559:C:C2'	1:X:560:G:O4'	2.54	0.54
1:X:774:A:O5'	1:X:774:A:H8	1.90	0.54
5:C:136:TRP:O	5:C:140:ASN:ND2	2.40	0.54
9:G:106:TYR:O	9:G:110:LEU:HG	2.06	0.54
18:P:97:VAL:HG22	18:P:124:ILE:HG23	1.87	0.54
1:X:75:C:H5''	24:V:48:ARG:HG3	1.89	0.54
1:X:1032:A:C8	1:X:1032:A:H3'	2.42	0.54
1:X:2484:G:N2	32:X:2929:1F4:H56	2.22	0.54
5:C:164:VAL:C	5:C:166:TRP:H	2.15	0.54
16:N:37:GLN:HA	16:N:40:LEU:HD12	1.90	0.54
1:X:333:A:H2'	5:C:162:ARG:HH12	1.72	0.54
1:X:1135:C:H2'	1:X:1136:G:O4'	2.06	0.54
1:X:1264:C:OP1	16:N:10:ARG:HG3	2.08	0.54
21:S:127:PRO:C	21:S:129:ARG:H	2.16	0.54
1:X:2659:C:H5'	4:B:189:PRO:HA	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:219:G:N2	1:X:231:G:H2'	2.22	0.54
32:X:2929:1F4:H18	32:X:2929:1F4:C54	2.38	0.54
3:A:60:ARG:HD3	3:A:86:PRO:O	2.06	0.54
5:C:95:LEU:HD23	5:C:96:PRO:HD2	1.90	0.54
8:F:79:ARG:HG2	8:F:84:ILE:HB	1.90	0.54
1:X:2196:U:H5'	1:X:2197:U:OP2	2.08	0.54
21:S:91:PRO:HG2	21:S:125:PRO:HD2	1.90	0.54
1:X:29:U:H5''	16:N:7:GLY:HA2	1.90	0.54
1:X:356:A:H2'	1:X:357:A:C8	2.43	0.54
5:C:148:VAL:HG13	5:C:185:ARG:HB2	1.90	0.54
9:G:67:ARG:CG	9:G:70:PHE:HA	2.37	0.54
1:X:2627:G:H2'	1:X:2628:C:O4'	2.08	0.54
6:D:80:ARG:HD3	6:D:83:MET:HB2	1.91	0.53
1:X:760:U:O2	1:X:1997:A:H1'	2.08	0.53
32:X:2929:1F4:C39	32:X:2929:1F4:H9	2.38	0.53
9:G:140:GLN:HG2	9:G:144:MET:HE3	1.91	0.53
10:H:77:THR:HA	10:H:94:ASN:HB3	1.89	0.53
16:N:6:THR:O	16:N:9:VAL:HG23	2.08	0.53
21:S:123:VAL:HG23	21:S:161:ALA:HB2	1.90	0.53
1:X:171:G:H2'	1:X:172:A:O4'	2.08	0.53
1:X:2482:A:H4'	1:X:2483:U:OP1	2.08	0.53
1:X:1134:C:H2'	1:X:1135:C:H6	1.74	0.53
1:X:2459:C:H2'	1:X:2459:C:O2	2.08	0.53
3:A:182:LEU:HD12	3:A:269:PHE:HB2	1.90	0.53
13:K:87:TYR:CE1	13:K:94:TYR:HD2	2.27	0.53
15:M:29:PRO:HB2	15:M:99:VAL:HG21	1.90	0.53
21:S:95:SER:HB3	21:S:119:ASN:HD22	1.74	0.53
1:X:1223:G:H5'	1:X:1225:G:O4'	2.08	0.53
1:X:1673:C:H5'	4:B:136:ARG:HD3	1.91	0.53
9:G:132:PHE:HB2	9:G:145:HIS:CE1	2.44	0.53
1:X:732:G:H2'	1:X:733:G:C8	2.43	0.53
1:X:1076:U:H3	1:X:1080:A:H2'	1.74	0.53
2:Y:9:G:H1	2:Y:116:C:H42	1.56	0.53
4:B:5:LEU:HG	4:B:195:LEU:HD11	1.91	0.53
10:H:83:ARG:CZ	10:H:89:ILE:HD11	2.38	0.53
14:L:38:ILE:HG13	14:L:39:TYR:N	2.17	0.53
20:R:26:SER:H	20:R:30:LYS:HG3	1.73	0.53
21:S:6:LYS:N	21:S:7:PRO:HD3	2.20	0.53
1:X:555:U:H5'	1:X:556:A:C8	2.43	0.53
1:X:761:G:OP2	18:P:109:ARG:HG3	2.08	0.53
11:I:102:LYS:O	11:I:104:ARG:N	2.35	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:62:ARG:HE	26:Z:25:LEU:HD11	1.74	0.53
1:X:2041:A:H61	32:X:2929:1F4:H46	1.73	0.53
23:U:32:ARG:HG2	23:U:33:LYS:H	1.72	0.53
1:X:633:G:H2'	1:X:634:G:H8	1.73	0.53
1:X:941:U:H1'	25:W:43:MET:HE1	1.91	0.53
1:X:577:U:H5''	1:X:956:A:N6	2.23	0.52
1:X:1287:A:H2'	1:X:1288:A:H5''	1.91	0.52
1:X:1468:A:O5'	1:X:1468:A:C8	2.62	0.52
1:X:2225:G:H2'	1:X:2226:A:C8	2.43	0.52
1:X:2270:U:H2'	1:X:2271:C:C6	2.43	0.52
1:X:2518:C:H1'	30:4:1:MET:HE3	1.90	0.52
25:W:3:ILE:HG23	25:W:51:LEU:HD22	1.92	0.52
1:X:796:A:H8	1:X:797:A:H4'	1.74	0.52
10:H:70:VAL:CG2	10:H:98:ILE:HG23	2.38	0.52
1:X:1378:A:H1'	23:U:16:ASN:HD21	1.74	0.52
1:X:1998:A:O5'	1:X:1998:A:H8	1.92	0.52
3:A:79:VAL:HG21	3:A:111:LEU:HD22	1.91	0.52
4:B:131:SER:O	4:B:132:LYS:HG2	2.10	0.52
1:X:1039:A:N6	1:X:1136:G:H2'	2.24	0.52
1:X:2505:G:H1	1:X:2516:U:H3	1.58	0.52
3:A:245:VAL:HG12	3:A:250:TRP:O	2.09	0.52
1:X:110:U:H3'	1:X:111:G:C8	2.44	0.52
1:X:760:U:C5	26:Z:3:LYS:HG3	2.44	0.52
1:X:768:U:H2'	1:X:769:C:O4'	2.09	0.52
1:X:1609:G:H2'	1:X:1610:A:H8	1.73	0.52
4:B:31:CYS:HB3	4:B:49:ILE:HG23	1.90	0.52
12:J:37:ALA:O	12:J:100:PRO:HA	2.09	0.52
1:X:2860:C:H2'	1:X:2861:A:O4'	2.09	0.52
1:X:83:A:H2	1:X:97:U:O2	1.92	0.52
1:X:568:G:H2'	1:X:569:C:O4'	2.09	0.52
1:X:1859:A:H2'	1:X:1860:A:C8	2.45	0.52
1:X:2372:A:H5''	11:I:61:PRO:HB3	1.92	0.52
2:Y:46:G:H5'	6:D:92:ARG:HH12	1.73	0.52
8:F:117:ALA:HB1	8:F:122:ALA:HB1	1.92	0.52
13:K:17:ARG:HH11	13:K:20:LEU:CD2	2.23	0.52
14:L:8:ARG:HG3	14:L:9:ARG:H	1.74	0.52
23:U:51:ILE:HG23	23:U:59:THR:HA	1.92	0.52
23:U:51:ILE:HG12	23:U:59:THR:HB	1.92	0.52
1:X:465:C:O2'	1:X:483:A:N6	2.42	0.52
1:X:1465:G:N2	1:X:1477:C:O2	2.41	0.52
1:X:1856:U:OP1	1:X:2389:G:O2'	2.26	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:152:LYS:H	9:G:106:TYR:CB	2.22	0.52
10:H:27:SER:HA	10:H:50:ILE:HD12	1.90	0.52
13:K:28:LEU:HD12	13:K:48:VAL:HG21	1.92	0.52
17:O:40:VAL:HG12	17:O:43:GLU:HA	1.91	0.52
1:X:504:G:H21	18:P:78:ASN:HD21	1.57	0.52
1:X:1673:C:H5''	4:B:136:ARG:HD3	1.91	0.52
1:X:2528:G:C8	1:X:2528:G:H5''	2.45	0.52
1:X:2594:U:C2	26:Z:7:PRO:HA	2.45	0.52
3:A:208:LYS:C	3:A:209:ALA:O	2.53	0.52
14:L:36:LYS:HB3	14:L:64:LYS:HB2	1.92	0.52
1:X:216:U:H2'	1:X:217:U:O4'	2.10	0.52
1:X:450:C:H2'	1:X:451:A:H8	1.73	0.52
1:X:1623:C:H4'	1:X:1624:A:O5'	2.10	0.52
4:B:16:LYS:HB2	4:B:21:ILE:HD11	1.92	0.52
4:B:116:VAL:CG2	4:B:136:ARG:HE	2.15	0.51
1:X:400:U:H5	23:U:21:ARG:HH12	1.57	0.51
1:X:1804:U:H2'	1:X:1805:G:H8	1.73	0.51
1:X:2797:G:OP2	13:K:3:HIS:NE2	2.42	0.51
2:Y:43:G:H5'	2:Y:44:C:H5''	1.91	0.51
3:A:43:ARG:HB3	3:A:54:ILE:HG12	1.91	0.51
1:X:413:G:O5'	1:X:413:G:H8	1.93	0.51
1:X:611:C:H6	1:X:611:C:H5''	1.75	0.51
1:X:627:A:H2'	1:X:628:A:C8	2.46	0.51
1:X:1586:A:H5'	3:A:38:PRO:HG3	1.93	0.51
9:G:93:LYS:HB3	9:G:96:ASP:HB3	1.92	0.51
15:M:69:ARG:HG3	15:M:78:GLU:HG3	1.93	0.51
20:R:59:LYS:HG2	20:R:62:MET:HB3	1.93	0.51
21:S:117:VAL:HG22	21:S:168:VAL:HA	1.91	0.51
1:X:388:G:H2'	1:X:389:G:H8	1.75	0.51
1:X:451:A:H2'	1:X:452:G:H8	1.74	0.51
1:X:1016:C:O2'	9:G:56:THR:HG21	2.11	0.51
32:X:2929:1F4:C23	32:X:2929:1F4:C41	2.88	0.51
5:C:24:SER:HA	5:C:27:LEU:HD12	1.93	0.51
1:X:2042:A:OP1	5:C:66:ASN:ND2	2.44	0.51
1:X:2545:A:H61	10:H:40:GLY:HA3	1.74	0.51
4:B:117:MET:HE2	4:B:136:ARG:HB2	1.92	0.51
6:D:4:LEU:HG	6:D:5:LYS:H	1.74	0.51
6:D:114:PHE:HZ	6:D:176:PRO:HG2	1.74	0.51
1:X:699:G:H5'	1:X:699:G:C8	2.46	0.51
7:E:6:LYS:HB3	7:E:69:ARG:HD3	1.93	0.51
1:X:840:U:O2	1:X:2225:G:H4'	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2289:A:H3'	1:X:2290:A:H8	1.75	0.51
4:B:146:THR:OG1	4:B:147:PRO:HD3	2.11	0.51
17:O:8:GLY:H	17:O:20:ILE:HD13	1.75	0.51
1:X:334:G:OP1	1:X:349:G:N2	2.44	0.51
1:X:1542:G:N2	1:X:1562:G:H1	1.94	0.51
15:M:44:ARG:HE	15:M:46:ARG:HH21	1.58	0.51
1:X:1736:C:H2'	1:X:1737:G:C8	2.46	0.50
3:A:58:HIS:O	3:A:58:HIS:ND1	2.44	0.50
20:R:105:ARG:HH22	20:R:112:LYS:HA	1.76	0.50
1:X:935:C:H2'	1:X:936:A:C8	2.45	0.50
1:X:1584:G:H4'	3:A:59:LYS:HG2	1.94	0.50
5:C:22:VAL:HG22	5:C:106:MET:HG3	1.92	0.50
6:D:93:GLY:H	6:D:96:MET:HE2	1.76	0.50
1:X:1454:U:H2'	1:X:1455:C:H6	1.76	0.50
6:D:152:MET:HE2	6:D:154:ILE:HD11	1.93	0.50
17:O:15:SER:HA	17:O:95:ILE:O	2.11	0.50
21:S:3:LEU:HD13	21:S:32:PHE:HB3	1.93	0.50
1:X:1834:G:H1	1:X:1881:U:H3	1.59	0.50
1:X:2271:C:P	14:L:18:ARG:HH21	2.35	0.50
32:X:2929:1F4:C50	32:X:2929:1F4:C52	2.90	0.50
4:B:4:ILE:HG12	4:B:28:ALA:HB1	1.94	0.50
4:B:61:LYS:HB3	4:B:62:PRO:HD3	1.93	0.50
12:J:26:ASP:HB3	12:J:68:ARG:HH22	1.76	0.50
23:U:52:ARG:HD3	23:U:70:LEU:HD22	1.92	0.50
1:X:620:G:N2	1:X:630:G:H1'	2.26	0.50
1:X:1142:G:C1'	9:G:103:TYR:HD2	2.25	0.50
1:X:1656:U:H2'	1:X:1657:A:H5''	1.94	0.50
1:X:2002:A:N7	26:Z:9:LYS:HD2	2.26	0.50
4:B:35:GLN:HB2	4:B:48:GLN:HB3	1.93	0.50
13:K:17:ARG:HH11	13:K:20:LEU:HD22	1.76	0.50
16:N:24:PHE:O	16:N:29:SER:HB3	2.11	0.50
1:X:969:U:H5''	12:J:17:ARG:HH11	1.77	0.50
1:X:1685:A:H5''	10:H:5:GLN:HG2	1.93	0.50
3:A:182:LEU:HB2	3:A:268:ARG:O	2.11	0.50
3:A:246:PRO:HD2	3:A:249:PRO:O	2.12	0.50
5:C:148:VAL:HB	5:C:167:VAL:HG12	1.93	0.50
9:G:132:PHE:CE2	9:G:145:HIS:HB2	2.47	0.50
14:L:66:ASP:C	14:L:68:ALA:H	2.19	0.50
1:X:884:C:H2'	1:X:885:A:H8	1.77	0.50
15:M:33:VAL:HG22	15:M:51:GLU:HB2	1.93	0.50
17:O:48:GLY:C	17:O:50:ASP:H	2.20	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:92:THR:HB	20:R:95:ARG:HH22	1.75	0.50
21:S:51:LEU:HB3	21:S:65:LEU:HD12	1.94	0.50
1:X:2056:C:H4'	3:A:228:PRO:HB2	1.93	0.49
26:Z:30:LEU:HD22	26:Z:39:LYS:HB3	1.94	0.49
1:X:2861:A:O2'	26:Z:31:THR:HG23	2.12	0.49
9:G:154:GLU:C	9:G:157:PRO:HD2	2.36	0.49
23:U:48:LYS:HG2	23:U:49:LYS:N	2.27	0.49
1:X:504:G:H4'	18:P:27:VAL:CG1	2.42	0.49
9:G:34:PRO:HA	9:G:69:ASP:CG	2.37	0.49
1:X:1326:U:H2'	1:X:1626:A:C2	2.48	0.49
1:X:1448:A:H61	1:X:1574:A:N6	1.93	0.49
1:X:1632:A:H8	1:X:1632:A:H5'	1.77	0.49
1:X:1979:C:H4'	1:X:1980:A:OP1	2.13	0.49
1:X:2597:G:H21	4:B:150:VAL:HG11	1.77	0.49
5:C:4:ILE:HG22	5:C:13:ARG:HH21	1.77	0.49
8:F:112:MET:HA	8:F:115:LEU:HD12	1.94	0.49
14:L:15:ARG:HD2	14:L:91:ARG:HD2	1.95	0.49
26:Z:45:ILE:HG21	26:Z:57:VAL:HG23	1.94	0.49
1:X:1089:C:H5'	8:F:132:ARG:HH12	1.77	0.49
1:X:2546:G:H2'	1:X:2547:C:C6	2.48	0.49
1:X:2653:A:C2'	10:H:41:ASN:ND2	2.75	0.49
3:A:66:ASP:HB3	3:A:105:ILE:HD12	1.93	0.49
10:H:113:PRO:HB3	10:H:134:LEU:HD12	1.94	0.49
13:K:11:ASN:HD21	13:K:17:ARG:NH1	2.09	0.49
1:X:347:C:H4'	20:R:15:HIS:CD2	2.48	0.49
1:X:1750:A:H1'	1:X:2690:A:C2	2.47	0.49
1:X:2039:G:N3	1:X:2039:G:H2'	2.28	0.49
2:Y:50:U:OP1	14:L:94:TYR:HA	2.13	0.49
9:G:90:LEU:HD23	9:G:94:LYS:HA	1.94	0.49
21:S:5:ALA:HB1	21:S:7:PRO:HD3	1.94	0.49
21:S:56:VAL:HG12	21:S:57:GLU:H	1.78	0.49
3:A:58:HIS:O	3:A:59:LYS:HB3	2.11	0.49
2:Y:92:G:H8	2:Y:92:G:OP2	1.95	0.49
16:N:74:MET:HG2	16:N:78:THR:HG22	1.94	0.49
1:X:1030:U:H3	1:X:1153:A:H62	1.61	0.49
1:X:1478:U:H2'	1:X:1479:G:H8	1.78	0.49
1:X:2035:G:H4'	4:B:143:GLN:O	2.13	0.49
3:A:164:GLN:HB3	3:A:176:ARG:HB3	1.94	0.49
10:H:112:GLY:O	10:H:131:PRO:HD2	2.13	0.49
16:N:66:ASN:HD22	16:N:70:ARG:HH12	1.60	0.49
1:X:229:G:OP1	11:I:49:PHE:HE1	1.96	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1509:A:H8	1:X:1510:A:C8	2.30	0.49
13:K:87:TYR:HE1	13:K:94:TYR:HD2	1.59	0.49
16:N:75:ASN:ND2	16:N:78:THR:H	2.10	0.49
1:X:1469:U:P	1:X:1471:G:OP2	2.71	0.48
1:X:2779:C:H2'	1:X:2780:A:C8	2.48	0.48
3:A:209:ALA:C	3:A:211:ARG:H	2.21	0.48
4:B:27:LEU:HD23	4:B:51:TYR:OH	2.12	0.48
17:O:71:ILE:HD11	17:O:86:HIS:HB2	1.94	0.48
1:X:463:C:H42	1:X:467:U:H5	1.60	0.48
1:X:643:A:H4'	11:I:67:ASN:HB3	1.95	0.48
1:X:793:G:H21	1:X:796:A:H62	1.61	0.48
1:X:1333:G:N2	1:X:1344:C:N4	2.61	0.48
32:X:2929:1F4:H3	32:X:2929:1F4:O18	2.12	0.48
6:D:60:ILE:HD12	6:D:61:THR:HG23	1.95	0.48
1:X:611:C:H4'	5:C:98:GLN:HE22	1.79	0.48
3:A:37:LEU:HD13	3:A:38:PRO:HD2	1.95	0.48
18:P:102:THR:HG21	18:P:118:LYS:HB3	1.95	0.48
1:X:1608:U:H2'	1:X:1609:G:C8	2.48	0.48
1:X:2230:G:OP1	12:J:84:MET:HE3	2.13	0.48
1:X:2857:C:H5'	13:K:96:ARG:HG3	1.94	0.48
1:X:1478:U:H2'	1:X:1479:G:C8	2.48	0.48
1:X:1515:U:H2'	1:X:1516:A:H8	1.79	0.48
3:A:165:VAL:HA	3:A:175:VAL:HG12	1.94	0.48
11:I:30:ALA:HB3	11:I:34:HIS:HE1	1.70	0.48
16:N:50:ARG:O	16:N:53:LYS:HG2	2.13	0.48
25:W:4:LYS:CG	25:W:52:GLU:HB3	2.43	0.48
1:X:654:A:H2	1:X:655:A:H3'	1.78	0.48
1:X:794:A:H5'	3:A:218:LYS:NZ	2.29	0.48
1:X:958:G:H2'	1:X:959:C:C6	2.49	0.48
1:X:1202:U:H2'	1:X:1203:A:H8	1.78	0.48
1:X:2821:G:H2'	1:X:2822:U:C6	2.49	0.48
11:I:32:ARG:HD2	17:O:79:GLN:NE2	2.29	0.48
12:J:73:LYS:H	12:J:94:TRP:CD1	2.31	0.48
23:U:48:LYS:HG3	23:U:49:LYS:H	1.79	0.48
1:X:82:G:N1	1:X:100:G:H2'	2.29	0.48
1:X:503:G:H2'	1:X:504:G:O4'	2.14	0.48
1:X:1093:U:H5'	8:F:117:ALA:HA	1.96	0.48
17:O:10:LYS:HG3	17:O:11:GLN:HG2	1.96	0.48
20:R:38:LEU:HB3	20:R:47:VAL:HB	1.95	0.48
1:X:527:C:OP1	26:Z:16:ARG:NH2	2.46	0.48
1:X:1167:A:H61	16:N:48:ARG:HG2	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:118:ASN:HD22	3:A:119:ALA:N	2.12	0.48
14:L:31:VAL:HG21	14:L:100:VAL:HG23	1.96	0.48
20:R:23:ILE:HG22	20:R:33:THR:HB	1.95	0.48
1:X:621:U:H2'	1:X:622:U:C6	2.49	0.48
1:X:1918:G:H1'	1:X:1947:G:N2	2.28	0.48
1:X:2045:A:O5'	1:X:2045:A:H8	1.96	0.48
10:H:26:ASN:CB	10:H:38:GLY:H	2.26	0.48
11:I:130:ILE:HG22	11:I:140:VAL:HG21	1.96	0.48
18:P:25:PHE:C	18:P:25:PHE:CD2	2.90	0.48
23:U:65:ASN:HA	23:U:68:ARG:HD3	1.96	0.48
1:X:881:U:H2'	1:X:882:C:C6	2.49	0.47
1:X:1497:C:C6	1:X:1497:C:H5''	2.50	0.47
1:X:1687:C:OP2	1:X:2529:G:OP1	2.32	0.47
1:X:1736:C:H2'	1:X:1737:G:H8	1.79	0.47
6:D:8:TYR:O	6:D:12:VAL:HB	2.14	0.47
1:X:1515:U:H2'	1:X:1516:A:C8	2.49	0.47
2:Y:21:C:H2'	2:Y:22:U:O4'	2.13	0.47
3:A:45:ASN:CG	3:A:46:ARG:N	2.72	0.47
23:U:52:ARG:HE	23:U:79:GLU:HA	1.77	0.47
24:V:42:ARG:NH1	24:V:45:GLN:OE1	2.47	0.47
1:X:1406:A:N6	19:Q:15:LYS:HG2	2.29	0.47
1:X:1674:C:H2'	1:X:1675:C:H6	1.76	0.47
32:X:2929:1F4:C41	32:X:2929:1F4:H11	2.44	0.47
10:H:116:ARG:HH11	15:M:38:LYS:HD3	1.79	0.47
18:P:57:LEU:HD13	18:P:69:ALA:HA	1.96	0.47
3:A:118:ASN:HD22	3:A:119:ALA:H	1.61	0.47
7:E:67:LEU:O	7:E:71:LEU:HG	2.15	0.47
9:G:67:ARG:HE	9:G:70:PHE:HA	1.78	0.47
11:I:62:LYS:NZ	11:I:64:GLY:HA3	2.28	0.47
20:R:22:VAL:HG13	20:R:81:VAL:O	2.14	0.47
25:W:1:MET:HB3	25:W:34:VAL:HG12	1.96	0.47
1:X:1673:C:H5'	4:B:136:ARG:HH11	1.78	0.47
1:X:1937:G:O2'	1:X:1939:U:O4	2.28	0.47
1:X:2362:G:H2'	1:X:2363:G:C8	2.49	0.47
4:B:133:LYS:HG2	4:B:137:ARG:HB3	1.96	0.47
1:X:588:G:H2'	1:X:589:C:H6	1.78	0.47
1:X:1168:G:O2'	25:W:28:ILE:HG12	2.15	0.47
1:X:1507:A:H2'	1:X:1508:G:H8	1.79	0.47
1:X:2394:G:H4'	11:I:65:PHE:HB3	1.96	0.47
3:A:186:HIS:HB2	3:A:188:GLU:CG	2.44	0.47
10:H:90:ARG:HG2	15:M:78:GLU:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:32:ARG:HD2	17:O:79:GLN:HE22	1.80	0.47
1:X:388:G:H2'	1:X:389:G:C8	2.50	0.47
1:X:2014:A:C6	1:X:2477:C:H1'	2.49	0.47
3:A:208:LYS:O	3:A:209:ALA:O	2.32	0.47
4:B:149:ARG:NH1	9:G:106:TYR:HB2	2.29	0.47
4:B:149:ARG:CZ	9:G:106:TYR:HD1	2.28	0.47
9:G:61:ARG:HH11	9:G:66:HIS:H	1.61	0.47
11:I:58:ALA:O	11:I:59:ARG:CB	2.62	0.47
21:S:23:ALA:HA	21:S:83:PHE:O	2.14	0.47
21:S:131:PRO:HG3	21:S:155:PRO:HG2	1.97	0.47
1:X:7:G:H2'	1:X:8:A:C8	2.50	0.47
1:X:203:G:H21	1:X:205:A:H62	1.63	0.47
1:X:588:G:H2'	1:X:589:C:C6	2.49	0.47
1:X:2048:C:H1'	1:X:2428:U:O2	2.14	0.47
1:X:2493:U:H2'	1:X:2494:C:C6	2.50	0.47
3:A:202:LYS:C	3:A:204:ILE:H	2.22	0.47
4:B:5:LEU:HD12	4:B:197:VAL:HG22	1.97	0.47
13:K:97:ILE:HA	13:K:112:LEU:O	2.14	0.47
17:O:38:LEU:HD23	17:O:47:PHE:HB3	1.96	0.47
1:X:1255:A:H2'	1:X:1256:C:C6	2.50	0.47
1:X:1584:G:N3	3:A:58:HIS:HE1	2.10	0.47
6:D:40:LEU:HD21	6:D:87:ILE:HD12	1.96	0.47
19:Q:61:LYS:H	19:Q:72:ARG:HA	1.79	0.47
1:X:745:C:H2'	1:X:746:G:O4'	2.14	0.47
6:D:63:GLN:HG3	6:D:95:ARG:HH21	1.79	0.47
16:N:49:ASP:HA	16:N:52:ASN:HB2	1.97	0.47
1:X:609:U:H4'	11:I:18:ARG:HE	1.80	0.46
1:X:2653:A:H4'	10:H:42:LYS:HB2	1.97	0.46
19:Q:12:ILE:HD13	19:Q:12:ILE:H	1.80	0.46
2:Y:94:G:H5'	21:S:74:ARG:HH12	1.79	0.46
9:G:61:ARG:HG2	9:G:65:LYS:HE3	1.96	0.46
9:G:157:PRO:C	9:G:159:SER:H	2.23	0.46
12:J:28:VAL:HG13	12:J:135:ARG:HG2	1.98	0.46
16:N:88:ILE:CG1	17:O:49:GLU:HB2	2.45	0.46
1:X:2604:G:H2'	1:X:2605:C:O4'	2.15	0.46
9:G:116:ARG:HA	9:G:119:LEU:HD12	1.98	0.46
1:X:1329:U:H5'	1:X:1405:A:H1'	1.97	0.46
1:X:1996:A:H5'	18:P:118:LYS:HZ1	1.79	0.46
1:X:2286:G:C2	1:X:2287:G:H1'	2.50	0.46
3:A:244:ARG:HD3	3:A:244:ARG:N	2.30	0.46
5:C:122:GLY:C	5:C:124:ASP:H	2.22	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:45:PHE:CD2	22:T:77:ARG:HB3	2.47	0.46
1:X:118:U:H4'	1:X:119:G:H5''	1.97	0.46
1:X:876:A:H2'	1:X:877:G:C8	2.50	0.46
1:X:1148:G:H2'	1:X:1149:G:O4'	2.14	0.46
9:G:66:HIS:HA	16:N:67:ALA:HB1	1.98	0.46
15:M:13:LEU:HD12	15:M:13:LEU:HA	1.70	0.46
20:R:35:LYS:HE3	20:R:37:LEU:HB3	1.98	0.46
21:S:19:ILE:HD12	21:S:79:ILE:HA	1.97	0.46
22:T:48:GLY:HA3	22:T:79:ILE:O	2.15	0.46
25:W:47:VAL:HB	25:W:50:LEU:HD12	1.98	0.46
1:X:2574:G:N2	1:X:2577:A:C8	2.82	0.46
4:B:117:MET:HG3	4:B:136:ARG:HG3	1.98	0.46
11:I:32:ARG:HB3	17:O:79:GLN:NE2	2.31	0.46
12:J:109:GLY:HA3	21:S:112:LEU:HD21	1.97	0.46
16:N:72:HIS:HB2	16:N:110:VAL:HG11	1.96	0.46
18:P:85:MET:HE2	18:P:130:GLU:HG3	1.96	0.46
1:X:547:U:H2'	1:X:548:G:C8	2.50	0.46
1:X:649:G:H22	1:X:661:C:H1'	1.80	0.46
1:X:1169:C:H4'	25:W:28:ILE:O	2.16	0.46
1:X:1333:G:N2	1:X:1344:C:H41	2.14	0.46
1:X:1675:C:OP1	4:B:134:TRP:CE2	2.69	0.46
1:X:2522:G:H2'	1:X:2523:G:C8	2.50	0.46
14:L:63:ASN:HB3	14:L:66:ASP:HB2	1.96	0.46
19:Q:20:MET:HG2	19:Q:92:ALA:O	2.16	0.46
1:X:1505:U:O2'	1:X:1506:C:H6	1.98	0.46
1:X:2691:C:O2'	1:X:2693:U:H5'	2.16	0.46
1:X:2784:A:C6	1:X:2866:A:C8	3.04	0.46
11:I:77:LEU:HD13	11:I:110:ALA:HA	1.98	0.46
11:I:121:HIS:HA	11:I:141:VAL:HB	1.98	0.46
26:Z:33:CYS:HB2	26:Z:46:CYS:SG	2.56	0.46
1:X:333:A:H2'	5:C:162:ARG:NH1	2.30	0.46
1:X:540:G:H1'	1:X:2004:U:O2'	2.16	0.46
1:X:609:U:H5'	11:I:18:ARG:HD3	1.97	0.46
1:X:636:G:C8	1:X:636:G:H5''	2.51	0.46
19:Q:66:GLY:O	19:Q:68:PHE:N	2.34	0.46
22:T:71:ASN:HD21	22:T:74:LYS:HG2	1.81	0.46
1:X:784:U:H2'	1:X:785:U:C6	2.51	0.45
1:X:1032:A:H3'	1:X:1032:A:H8	1.78	0.45
1:X:2062:U:H2'	1:X:2063:A:C8	2.52	0.45
1:X:2352:A:H2'	1:X:2353:G:H8	1.81	0.45
17:O:25:LEU:HB2	17:O:32:LYS:HE2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:172:A:H61	1:X:175:C:H3'	1.81	0.45
1:X:240:U:H2'	1:X:241:C:O4'	2.16	0.45
4:B:32:PRO:HA	4:B:89:ASP:HB3	1.98	0.45
20:R:90:LYS:HB2	20:R:108:VAL:HG21	1.98	0.45
6:D:106:ILE:HG21	6:D:139:PRO:HB3	1.98	0.45
12:J:21:ASP:HA	12:J:99:LYS:HE2	1.97	0.45
12:J:42:TRP:CD1	12:J:97:VAL:HG12	2.51	0.45
1:X:313:U:H2'	1:X:314:G:H8	1.81	0.45
1:X:523:A:O2'	16:N:11:ARG:HD2	2.16	0.45
1:X:673:G:H5'	5:C:93:TYR:CD1	2.52	0.45
1:X:1805:G:N3	3:A:50:THR:CG2	2.80	0.45
1:X:2210:C:OP1	23:U:45:ASN:HA	2.17	0.45
1:X:2371:A:H1'	11:I:59:ARG:HG3	1.97	0.45
1:X:2843:A:C8	1:X:2843:A:H5''	2.51	0.45
5:C:5:ASN:HB3	5:C:10:ASN:HA	1.99	0.45
25:W:19:THR:HG21	25:W:46:THR:HG22	1.98	0.45
1:X:322:A:N6	1:X:339:U:H2'	2.31	0.45
1:X:428:A:H2'	1:X:429:C:O4'	2.17	0.45
1:X:631:G:H1	5:C:97:ARG:NH1	2.14	0.45
1:X:674:U:H2'	1:X:675:C:O4'	2.17	0.45
1:X:1673:C:H5'	4:B:136:ARG:NH1	2.31	0.45
1:X:1845:A:N1	1:X:2070:G:H1'	2.31	0.45
1:X:635:C:O2'	1:X:670:U:H5''	2.17	0.45
1:X:710:C:H2'	1:X:711:C:C6	2.52	0.45
1:X:1234:C:H2'	1:X:1235:C:H6	1.82	0.45
1:X:1805:G:N3	3:A:50:THR:HG22	2.31	0.45
2:Y:28:A:C8	2:Y:29:C:C5	3.02	0.45
1:X:1832:G:H1	1:X:1885:C:N4	2.09	0.45
1:X:1981:A:H2'	1:X:1982:C:O4'	2.16	0.45
1:X:1997:A:H2'	1:X:1998:A:C8	2.51	0.45
2:Y:46:G:H4'	6:D:92:ARG:HH12	1.82	0.45
3:A:83:GLU:N	3:A:92:ILE:O	2.46	0.45
7:E:11:VAL:HG11	7:E:50:LEU:HD13	1.98	0.45
12:J:31:GLY:HA2	12:J:108:ALA:HB2	1.99	0.45
18:P:85:MET:HE1	18:P:129:ALA:HA	1.99	0.45
18:P:105:ARG:HE	18:P:105:ARG:HB3	1.64	0.45
20:R:105:ARG:NH2	20:R:112:LYS:HA	2.32	0.45
23:U:19:ILE:HA	23:U:42:GLN:HA	1.98	0.45
1:X:1573:G:H3'	1:X:1574:A:O4'	2.17	0.45
3:A:134:ARG:HG3	3:A:135:PHE:HD2	1.81	0.45
5:C:74:VAL:HG23	5:C:76:THR:H	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:11:ALA:O	10:H:110:VAL:HA	2.17	0.45
12:J:42:TRP:CG	12:J:95:VAL:HG11	2.52	0.45
12:J:104:MET:HE1	12:J:130:THR:HG22	1.98	0.45
1:X:1164:C:H5'	16:N:76:TYR:CE2	2.52	0.45
1:X:2222:U:H2'	1:X:2223:U:C6	2.52	0.45
1:X:2579:A:H2'	1:X:2580:C:C6	2.52	0.45
1:X:2661:G:O6	1:X:2708:U:H1'	2.17	0.45
6:D:8:TYR:HB2	6:D:173:MET:HE1	1.99	0.45
1:X:593:C:N4	1:X:594:G:C6	2.85	0.45
1:X:640:C:C4'	1:X:660:G:H21	2.23	0.45
15:M:79:ARG:CG	15:M:79:ARG:NH1	2.68	0.45
23:U:22:GLY:HA3	23:U:39:LYS:HD2	1.98	0.45
1:X:636:G:O2'	1:X:669:G:H4'	2.17	0.44
1:X:1045:G:N2	1:X:1133:G:H1'	2.31	0.44
1:X:1367:A:H2'	1:X:1368:G:O4'	2.17	0.44
4:B:119:ARG:HG2	4:B:120:TRP:CE2	2.52	0.44
9:G:70:PHE:HB2	16:N:64:ARG:HE	1.83	0.44
20:R:97:GLN:HB2	20:R:101:GLY:HA2	1.99	0.44
1:X:1494:G:H2'	1:X:1495:G:O4'	2.17	0.44
1:X:1769:U:H2'	1:X:1775:A:N6	2.31	0.44
1:X:2252:A:H2'	1:X:2253:A:C8	2.52	0.44
3:A:79:VAL:HG21	3:A:111:LEU:CD2	2.47	0.44
3:A:227:ASN:O	3:A:228:PRO:C	2.60	0.44
1:X:1117:G:H2'	1:X:1118:G:H8	1.80	0.44
1:X:1202:U:H5'	17:O:78:VAL:HG22	1.98	0.44
1:X:1373:G:N2	1:X:2192:U:H3	2.15	0.44
1:X:2195:C:H6	1:X:2195:C:H5''	1.82	0.44
2:Y:72:C:H2'	2:Y:73:C:H6	1.82	0.44
3:A:147:LEU:HD22	3:A:183:ARG:HH22	1.82	0.44
3:A:202:LYS:C	3:A:204:ILE:N	2.75	0.44
3:A:208:LYS:HE3	3:A:208:LYS:HA	2.00	0.44
12:J:73:LYS:H	12:J:94:TRP:HD1	1.65	0.44
20:R:25:LEU:N	20:R:80:LYS:HA	2.30	0.44
1:X:224:G:H4'	1:X:399:G:C5	2.52	0.44
1:X:339:U:O4	1:X:343:A:C8	2.70	0.44
1:X:796:A:H4'	1:X:2567:G:H4'	1.99	0.44
1:X:956:A:C4	1:X:2427:A:C2	3.06	0.44
1:X:1834:G:H1'	3:A:244:ARG:HH22	1.82	0.44
9:G:70:PHE:HB2	16:N:64:ARG:HG2	1.98	0.44
10:H:70:VAL:HG21	10:H:98:ILE:HG23	1.98	0.44
18:P:41:VAL:HG22	18:P:60:ILE:HG21	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:358:C:H6	1:X:358:C:O5'	2.01	0.44
1:X:1833:U:H2'	1:X:1834:G:C8	2.53	0.44
2:Y:89:G:N2	2:Y:92:G:C8	2.86	0.44
3:A:42:GLY:H	3:A:43:ARG:NH1	2.15	0.44
3:A:231:HIS:ND1	3:A:247:VAL:HA	2.31	0.44
5:C:46:ARG:HD2	5:C:51:VAL:HB	1.99	0.44
12:J:98:VAL:HG11	12:J:104:MET:HG2	2.00	0.44
1:X:819:C:OP2	11:I:41:SER:HA	2.17	0.44
1:X:1524:C:H3'	1:X:1525:A:H8	1.82	0.44
1:X:1819:U:OP2	3:A:222:ARG:NH2	2.50	0.44
1:X:1978:U:H1'	10:H:3:MET:HE1	1.99	0.44
1:X:2056:C:H5'	3:A:229:VAL:HG22	2.00	0.44
1:X:2609:G:H2'	1:X:2610:G:C8	2.52	0.44
4:B:5:LEU:HD22	4:B:49:ILE:HG22	1.99	0.44
4:B:54:LYS:HD3	4:B:59:VAL:HG22	1.99	0.44
12:J:77:LYS:O	12:J:88:LYS:HD2	2.18	0.44
22:T:40:GLN:HE21	22:T:57:HIS:HB3	1.83	0.44
1:X:490:A:N3	1:X:492:G:H5''	2.33	0.44
1:X:1223:G:H5''	1:X:1224:A:H3'	2.00	0.44
1:X:1725:C:H42	1:X:1741:G:H1	1.64	0.44
1:X:2002:A:N1	1:X:2018:G:O6	2.51	0.44
3:A:67:PHE:HB3	3:A:153:ALA:N	2.31	0.44
7:E:164:PHE:O	7:E:166:GLY:N	2.51	0.44
12:J:44:LYS:HB3	12:J:46:ASN:ND2	2.33	0.44
13:K:76:VAL:HA	13:K:79:VAL:HG12	2.00	0.44
1:X:940:G:H21	25:W:43:MET:HE2	1.83	0.44
3:A:43:ARG:HG3	3:A:54:ILE:O	2.18	0.44
10:H:24:VAL:HG13	10:H:45:ALA:HB2	1.99	0.44
12:J:78:LYS:HE2	12:J:81:GLU:HA	2.00	0.44
18:P:72:LEU:HD12	18:P:126:ILE:HD13	2.00	0.44
11:I:8:PRO:HB2	11:I:14:LYS:NZ	2.32	0.44
14:L:8:ARG:CG	14:L:9:ARG:H	2.31	0.44
19:Q:51:ILE:HD11	19:Q:81:ARG:HD3	2.00	0.44
21:S:3:LEU:HB3	21:S:34:LEU:HB3	1.99	0.44
1:X:1101:U:H2'	1:X:1102:G:C8	2.53	0.43
1:X:2506:C:H5'	30:4:33:LYS:HD2	2.00	0.43
1:X:2506:C:H5''	30:4:30:VAL:HB	2.00	0.43
5:C:107:ALA:HB1	5:C:180:ILE:HD11	2.00	0.43
19:Q:39:LYS:HG2	19:Q:43:GLN:HE21	1.83	0.43
1:X:760:U:C6	26:Z:3:LYS:HG3	2.53	0.43
1:X:1230:C:H2'	1:X:1231:A:H8	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1333:G:N7	1:X:1342:U:H5'	2.32	0.43
1:X:2324:G:H5''	1:X:2326:C:O4'	2.18	0.43
3:A:247:VAL:CG2	3:A:248:THR:N	2.81	0.43
5:C:95:LEU:CD2	5:C:96:PRO:HD2	2.48	0.43
5:C:150:LEU:HA	5:C:187:VAL:HB	2.00	0.43
9:G:43:VAL:HB	9:G:167:LYS:HG2	1.99	0.43
13:K:34:ILE:HG13	13:K:113:ILE:HG23	2.01	0.43
21:S:117:VAL:HG23	21:S:168:VAL:HG13	2.00	0.43
1:X:114:C:H2'	1:X:115:G:C8	2.53	0.43
1:X:2551:A:O5'	1:X:2553:G:H4'	2.18	0.43
3:A:145:LEU:HB3	3:A:155:LEU:HD12	2.00	0.43
4:B:134:TRP:CD1	4:B:134:TRP:N	2.76	0.43
6:D:117:ILE:HD13	6:D:130:LEU:HD11	2.00	0.43
11:I:54:SER:HA	11:I:58:ALA:HB3	2.00	0.43
1:X:342:G:O3'	1:X:343:A:C8	2.71	0.43
1:X:695:G:N2	1:X:808:C:O2	2.44	0.43
5:C:127:ASP:HB2	5:C:128:ALA:H	1.64	0.43
26:Z:4:HIS:HB3	26:Z:5:PRO:CD	2.45	0.43
1:X:84:G:N3	1:X:101:A:C2	2.86	0.43
1:X:314:G:H2'	1:X:315:G:C8	2.53	0.43
1:X:457:C:O2'	1:X:461:A:N3	2.51	0.43
1:X:538:A:H5''	9:G:139:ARG:HE	1.83	0.43
1:X:1577:G:H2'	1:X:1578:U:O4'	2.19	0.43
1:X:1996:A:H5'	18:P:118:LYS:NZ	2.33	0.43
1:X:2594:U:H2'	1:X:2595:C:H6	1.83	0.43
32:X:2929:1F4:C41	32:X:2929:1F4:C16	2.97	0.43
2:Y:91:A:H2'	2:Y:92:G:C8	2.54	0.43
5:C:30:VAL:HG11	5:C:177:VAL:HG21	2.00	0.43
5:C:133:PHE:HB2	5:C:160:ALA:HB1	2.00	0.43
12:J:62:GLY:H	21:S:175:ARG:N	2.16	0.43
1:X:339:U:H4'	20:R:77:HIS:ND1	2.34	0.43
1:X:1539:U:H2'	1:X:1540:C:C6	2.54	0.43
1:X:1782:A:O3'	3:A:206:LEU:HB2	2.18	0.43
1:X:2006:G:H4'	1:X:2596:C:O3'	2.19	0.43
1:X:2066:G:N2	1:X:2216:G:H1'	2.34	0.43
1:X:2170:C:H2'	1:X:2171:U:H4'	2.01	0.43
1:X:2277:A:H2'	1:X:2278:A:O4'	2.18	0.43
3:A:245:VAL:N	3:A:252:LYS:HE3	2.34	0.43
5:C:74:VAL:O	5:C:77:PHE:HB2	2.18	0.43
5:C:170:LEU:HA	5:C:171:PRO:HD3	1.95	0.43
10:H:22:ILE:HD11	10:H:54:SER:HB2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:69:ILE:HG22	17:O:86:HIS:HB3	2.00	0.43
30:4:19:ARG:HD2	30:4:24:LEU:HD22	2.01	0.43
1:X:1919:A:C2	1:X:1926:U:N3	2.74	0.43
1:X:2825:A:H2'	1:X:2826:C:C6	2.54	0.43
3:A:63:ARG:O	3:A:65:ILE:HD12	2.18	0.43
12:J:61:ARG:HD3	21:S:174:PRO:HB2	1.99	0.43
1:X:742:G:N1	3:A:208:LYS:HD3	2.33	0.43
1:X:1148:G:O2'	9:G:134:MET:HG3	2.18	0.43
1:X:1283:C:H5''	1:X:1284:G:O5'	2.19	0.43
10:H:19:ILE:HG22	10:H:55:VAL:HA	2.01	0.43
10:H:27:SER:OG	10:H:49:ASP:HA	2.19	0.43
15:M:22:ARG:HD2	15:M:83:PHE:O	2.19	0.43
1:X:205:A:H3'	1:X:205:A:C8	2.54	0.43
1:X:551:A:H2'	1:X:552:C:O4'	2.19	0.43
1:X:1469:U:OP1	1:X:1471:G:OP2	2.36	0.43
1:X:1643:A:H61	1:X:1656:U:H3	1.67	0.43
1:X:2320:G:H2'	1:X:2321:C:O4'	2.19	0.43
32:X:2929:1F4:H9	32:X:2929:1F4:H53	2.00	0.43
4:B:11:MET:HA	4:B:23:VAL:O	2.19	0.43
5:C:148:VAL:O	5:C:167:VAL:HA	2.19	0.43
10:H:10:VAL:HG11	10:H:98:ILE:HD12	2.00	0.43
13:K:33:ARG:HD3	13:K:112:LEU:HD22	2.01	0.43
16:N:66:ASN:HB3	16:N:76:TYR:N	2.27	0.43
20:R:24:VAL:HB	20:R:29:HIS:O	2.19	0.43
1:X:504:G:N2	18:P:78:ASN:HD21	2.17	0.43
1:X:882:C:H2'	1:X:883:A:O4'	2.19	0.43
1:X:1268:U:H5	5:C:68:ARG:HB2	1.84	0.43
1:X:1497:C:H5''	1:X:1497:C:H6	1.84	0.43
2:Y:32:C:H1'	2:Y:59:A:H61	1.84	0.43
2:Y:107:C:H2'	2:Y:108:G:O4'	2.19	0.43
20:R:18:LYS:H	20:R:18:LYS:HD3	1.84	0.43
25:W:27:LYS:O	25:W:30:ASP:HB2	2.19	0.43
1:X:487:G:H4'	1:X:512:A:N1	2.34	0.42
1:X:1373:G:H22	1:X:2192:U:H3	1.67	0.42
1:X:1978:U:H3'	1:X:1979:C:H2'	2.01	0.42
1:X:2235:G:N2	1:X:2254:C:C4	2.87	0.42
3:A:201:HIS:CD2	3:A:204:ILE:HD12	2.54	0.42
5:C:130:THR:HG23	5:C:160:ALA:HA	2.00	0.42
7:E:33:LEU:HD13	7:E:136:ILE:HG22	2.01	0.42
9:G:45:ASP:HA	9:G:83:ILE:HG13	2.01	0.42
13:K:90:ARG:HA	13:K:91:PRO:HD3	1.89	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:149:ALA:HB3	21:S:164:PRO:HA	1.99	0.42
1:X:322:A:H3'	1:X:323:G:H8	1.83	0.42
1:X:636:G:H5''	1:X:636:G:H8	1.84	0.42
1:X:719:A:H2'	1:X:720:A:O4'	2.19	0.42
1:X:1337:G:OP2	18:P:105:ARG:NH1	2.52	0.42
7:E:6:LYS:H	7:E:65:HIS:HE1	1.66	0.42
25:W:12:ARG:CG	25:W:12:ARG:NH1	2.76	0.42
26:Z:6:VAL:HG22	26:Z:7:PRO:HD2	2.00	0.42
1:X:5:A:H2'	1:X:6:A:C8	2.54	0.42
1:X:812:G:H3'	1:X:813:A:H2'	2.01	0.42
1:X:1371:G:H8	1:X:1371:G:O5'	2.02	0.42
1:X:2011:U:H2'	1:X:2012:A:O4'	2.19	0.42
1:X:2024:U:H2'	1:X:2025:A:O4'	2.20	0.42
1:X:2220:A:H2'	1:X:2221:G:C8	2.54	0.42
1:X:2489:C:C4	1:X:2490:U:C5	3.08	0.42
7:E:126:PRO:HG2	7:E:130:ARG:HH22	1.85	0.42
18:P:46:ARG:HG3	18:P:95:ALA:HB3	2.01	0.42
20:R:93:ARG:HG2	20:R:108:VAL:HA	2.01	0.42
1:X:346:C:O2	1:X:347:C:C5	2.72	0.42
1:X:441:A:H3'	1:X:442:A:H8	1.84	0.42
1:X:638:A:C8	11:I:74:VAL:HG11	2.55	0.42
2:Y:108:G:H4'	21:S:26:LYS:HB3	2.02	0.42
10:H:64:VAL:HG22	10:H:106:ARG:NH1	2.35	0.42
15:M:34:ARG:HH22	15:M:90:GLN:N	2.17	0.42
1:X:877:G:H2'	1:X:878:C:C6	2.55	0.42
1:X:958:G:H2'	1:X:959:C:H6	1.84	0.42
1:X:1656:U:C2'	1:X:1657:A:H5''	2.50	0.42
1:X:2200:G:H2'	1:X:2201:G:C8	2.55	0.42
1:X:2519:C:O2'	1:X:2720:A:N3	2.44	0.42
2:Y:91:A:H8	2:Y:91:A:OP2	2.03	0.42
3:A:213:ARG:C	3:A:215:LEU:H	2.27	0.42
5:C:117:LEU:HD23	5:C:187:VAL:HG22	2.01	0.42
14:L:44:ASP:HB2	14:L:51:LEU:HD13	2.01	0.42
1:X:50:G:H4'	1:X:51:A:H5'	2.02	0.42
1:X:700:C:H2'	1:X:701:U:O4'	2.20	0.42
1:X:1332:G:C6	1:X:1333:G:N1	2.88	0.42
1:X:2683:C:H2'	1:X:2684:A:O4'	2.19	0.42
3:A:43:ARG:HD2	3:A:43:ARG:H	1.78	0.42
4:B:16:LYS:HB2	4:B:21:ILE:CD1	2.49	0.42
11:I:119:THR:HG23	11:I:139:ARG:HB3	2.02	0.42
21:S:71:MET:H	21:S:71:MET:HE2	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:205:A:H3'	1:X:205:A:H8	1.84	0.42
1:X:810:U:H2'	1:X:811:G:O4'	2.20	0.42
1:X:1737:G:H2'	1:X:1738:U:C6	2.55	0.42
1:X:2545:A:H61	10:H:40:GLY:CA	2.32	0.42
1:X:2658:A:H4'	4:B:165:VAL:HG11	2.02	0.42
2:Y:89:G:H5''	2:Y:90:C:OP2	2.19	0.42
2:Y:102:A:H2'	2:Y:103:A:C8	2.54	0.42
3:A:219:PRO:O	3:A:220:HIS:C	2.62	0.42
4:B:131:SER:HB3	4:B:134:TRP:HD1	1.79	0.42
4:B:152:LYS:N	9:G:106:TYR:HB3	2.33	0.42
12:J:137:VAL:HG13	21:S:71:MET:HE1	2.02	0.42
16:N:13:ARG:HA	16:N:16:LYS:HE2	2.02	0.42
17:O:12:TYR:HB2	17:O:40:VAL:H	1.84	0.42
17:O:88:GLN:HE21	17:O:88:GLN:HA	1.85	0.42
1:X:590:C:H2'	1:X:591:G:C8	2.55	0.42
1:X:1279:G:O2'	1:X:1995:G:O6	2.26	0.42
1:X:1381:G:O5'	1:X:1381:G:H8	2.03	0.42
1:X:2241:U:C5	22:T:17:ASN:OD1	2.63	0.42
1:X:2352:A:H2'	1:X:2353:G:C8	2.54	0.42
1:X:2528:G:H2'	1:X:2529:G:C8	2.49	0.42
1:X:2687:G:H2'	1:X:2688:G:H8	1.85	0.42
3:A:173:VAL:HG23	3:A:187:SER:HB3	2.02	0.42
11:I:82:ASP:H	11:I:114:ILE:HG21	1.84	0.42
14:L:68:ALA:HB1	14:L:102:ALA:HB3	2.01	0.42
19:Q:62:ARG:O	19:Q:70:GLY:HA3	2.19	0.42
23:U:22:GLY:HA3	23:U:39:LYS:CD	2.49	0.42
1:X:631:G:H4'	1:X:632:A:H5'	2.02	0.42
1:X:666:U:O2'	1:X:667:U:H5''	2.20	0.42
1:X:688:A:N3	1:X:2422:C:O2'	2.46	0.42
1:X:708:G:OP1	1:X:1393:G:O2'	2.37	0.42
1:X:1035:G:C8	1:X:1036:G:H2'	2.55	0.42
1:X:1100:G:H21	1:X:1113:C:H42	1.67	0.42
1:X:1314:A:H2	1:X:1642:G:N3	2.17	0.42
1:X:1620:C:O2'	1:X:1626:A:N1	2.46	0.42
1:X:1765:C:H6	1:X:1765:C:O5'	2.03	0.42
1:X:1774:A:C6	1:X:2566:A:C2	3.08	0.42
1:X:1804:U:H2'	1:X:1805:G:C8	2.54	0.42
4:B:133:LYS:O	4:B:134:TRP:C	2.62	0.42
4:B:193:GLY:O	15:M:2:GLN:N	2.53	0.42
5:C:33:TRP:CE3	5:C:95:LEU:HD12	2.54	0.42
5:C:194:GLU:O	5:C:195:ILE:HG12	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:31:GLY:HA2	23:U:32:ARG:HH11	1.85	0.42
1:X:1929:U:H2'	1:X:1930:C:C6	2.54	0.42
5:C:180:ILE:HG13	5:C:181:LEU:N	2.35	0.42
9:G:170:PRO:HB2	9:G:171:LEU:H	1.75	0.42
15:M:38:LYS:HB3	15:M:46:ARG:HB3	2.01	0.42
1:X:149:A:H2'	1:X:150:A:H8	1.84	0.41
1:X:554:U:H4'	1:X:555:U:OP2	2.20	0.41
1:X:1017:C:O2'	9:G:134:MET:O	2.37	0.41
1:X:1167:A:C5	16:N:51:ARG:HD3	2.55	0.41
1:X:1302:C:H2'	1:X:1303:U:H6	1.85	0.41
5:C:94:THR:HG22	5:C:100:ARG:HH12	1.84	0.41
9:G:132:PHE:HZ	9:G:142:ARG:HA	1.85	0.41
10:H:132:GLU:HG2	10:H:134:LEU:HG	2.02	0.41
11:I:28:LYS:HZ1	11:I:36:GLY:HA2	1.83	0.41
13:K:8:ARG:O	13:K:9:LYS:HB3	2.20	0.41
13:K:76:VAL:O	13:K:80:MET:HB2	2.20	0.41
20:R:29:HIS:CD2	20:R:51:VAL:HG22	2.55	0.41
1:X:54:G:C2	1:X:114:C:C2	3.08	0.41
1:X:224:G:H4'	1:X:399:G:C4	2.55	0.41
1:X:622:U:H2'	1:X:623:G:O4'	2.21	0.41
1:X:1975:G:N2	1:X:1979:C:O2'	2.52	0.41
1:X:2053:G:H2'	1:X:2054:A:C8	2.54	0.41
1:X:2796:A:H2'	1:X:2797:G:C8	2.55	0.41
32:X:2929:1F4:H18	32:X:2929:1F4:C53	2.50	0.41
24:V:32:ALA:HB2	24:V:37:LEU:HG	2.02	0.41
1:X:692:C:H2'	1:X:693:A:C8	2.55	0.41
1:X:1032:A:C8	1:X:1032:A:C3'	3.03	0.41
1:X:1249:G:O2'	1:X:1250:A:H8	2.03	0.41
1:X:1287:A:H2	1:X:1661:C:O2	2.03	0.41
1:X:1385:C:H2'	1:X:1386:A:O4'	2.20	0.41
1:X:1973:C:H2'	1:X:1974:U:O4'	2.21	0.41
1:X:2859:U:N3	26:Z:52:TYR:CE1	2.88	0.41
11:I:102:LYS:C	11:I:104:ARG:H	2.24	0.41
12:J:6:LYS:O	12:J:71:PRO:HD2	2.20	0.41
23:U:47:HIS:HB2	23:U:48:LYS:H	1.71	0.41
1:X:237:G:H1'	1:X:632:A:H1'	2.02	0.41
1:X:649:G:H2'	1:X:650:U:C6	2.55	0.41
1:X:934:G:H1'	22:T:26:PHE:CD1	2.55	0.41
1:X:960:U:H2'	1:X:961:G:H8	1.82	0.41
1:X:1266:G:C8	11:I:32:ARG:NH1	2.85	0.41
1:X:1811:A:H3'	3:A:178:PRO:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2209:G:H4'	23:U:46:LEU:HB2	2.02	0.41
3:A:42:GLY:C	3:A:43:ARG:HH11	2.28	0.41
11:I:60:LEU:HD12	11:I:60:LEU:HA	1.89	0.41
12:J:64:LYS:HG2	21:S:112:LEU:HD22	2.02	0.41
25:W:4:LYS:HE3	25:W:52:GLU:O	2.20	0.41
1:X:1224:A:H4'	1:X:1225:G:OP2	2.20	0.41
1:X:1381:G:H2'	1:X:1799:A:H61	1.86	0.41
1:X:1687:C:O5'	1:X:1687:C:H6	2.02	0.41
5:C:58:MET:HE1	5:C:69:HIS:CB	2.50	0.41
6:D:75:SER:HB2	6:D:79:LEU:HB2	2.03	0.41
12:J:6:LYS:HE3	12:J:7:ARG:HE	1.86	0.41
12:J:36:ILE:HG13	12:J:103:VAL:HA	2.03	0.41
1:X:1792:C:N4	1:X:2185:U:H5'	2.36	0.41
1:X:2225:G:H2'	1:X:2226:A:H8	1.85	0.41
1:X:2556:A:H5''	1:X:2557:G:H5'	2.02	0.41
1:X:2590:U:O4'	32:X:2929:1F4:H32	2.21	0.41
4:B:104:ALA:HB3	4:B:170:LEU:HD12	2.02	0.41
11:I:28:LYS:HZ3	11:I:36:GLY:HA2	1.86	0.41
13:K:96:ARG:O	13:K:113:ILE:HA	2.20	0.41
1:X:1:G:N3	1:X:1:G:H2'	2.36	0.41
1:X:946:U:H2'	1:X:947:C:C6	2.56	0.41
1:X:1117:G:H2'	1:X:1118:G:C8	2.55	0.41
1:X:2633:A:N1	1:X:2644:A:H5''	2.35	0.41
3:A:213:ARG:HD2	3:A:213:ARG:HA	1.97	0.41
5:C:171:PRO:O	5:C:173:ALA:N	2.54	0.41
9:G:62:ILE:HG23	9:G:135:LEU:HD21	2.02	0.41
15:M:34:ARG:NH1	15:M:91:VAL:HB	2.36	0.41
21:S:141:MET:SD	21:S:147:ILE:HG12	2.61	0.41
1:X:654:A:C2	1:X:655:A:H3'	2.56	0.41
1:X:1132:C:H6	1:X:1132:C:O5'	2.03	0.41
1:X:2395:C:H2'	1:X:2396:C:H5''	2.02	0.41
9:G:53:ARG:HH22	9:G:171:LEU:HD12	1.85	0.41
12:J:14:PHE:CE1	12:J:90:ALA:HB2	2.56	0.41
1:X:95:G:H4'	24:V:41:HIS:ND1	2.35	0.41
1:X:322:A:H3'	1:X:323:G:C8	2.55	0.41
1:X:494:A:C8	20:R:56:LYS:HD2	2.56	0.41
1:X:762:A:H4'	1:X:1284:G:N3	2.36	0.41
1:X:1009:C:H2'	1:X:1010:U:O4'	2.21	0.41
1:X:1106:A:H2'	1:X:1107:A:H8	1.86	0.41
1:X:2791:C:O2	1:X:2858:A:O2'	2.39	0.41
4:B:55:ALA:HB3	4:B:58:LYS:HD2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:105:THR:HB	4:B:166:THR:HG23	2.03	0.41
7:E:24:PHE:HB2	7:E:37:TYR:HD1	1.85	0.41
12:J:27:TYR:HB2	12:J:137:VAL:HG21	2.02	0.41
14:L:31:VAL:HG23	14:L:38:ILE:HD11	2.01	0.41
16:N:68:GLY:HA2	16:N:71:LEU:HD23	2.02	0.41
20:R:22:VAL:HG22	20:R:83:LEU:H	1.85	0.41
21:S:107:GLU:HG3	21:S:112:LEU:HA	2.02	0.41
23:U:14:VAL:HB	23:U:15:VAL:H	1.75	0.41
23:U:65:ASN:OD1	23:U:65:ASN:N	2.54	0.41
1:X:98:U:H1'	1:X:100:G:C4	2.56	0.41
1:X:188:G:H2'	1:X:189:A:C8	2.56	0.41
1:X:657:A:C8	1:X:657:A:H3'	2.56	0.41
1:X:874:A:H2'	1:X:875:G:O4'	2.21	0.41
1:X:1467:U:H6	1:X:1467:U:H3'	1.85	0.41
1:X:1469:U:H5'	1:X:1470:G:N7	2.36	0.41
1:X:1533:G:H2'	1:X:1534:A:H8	1.86	0.41
1:X:1615:C:OP2	19:Q:35:LYS:HD2	2.20	0.41
1:X:2357:A:H1'	14:L:88:VAL:HG11	2.02	0.41
5:C:176:ASN:ND2	5:C:179:ASP:H	2.16	0.41
14:L:66:ASP:C	14:L:68:ALA:N	2.78	0.41
14:L:76:ALA:HB2	14:L:107:ALA:HA	2.02	0.41
17:O:19:VAL:HG13	17:O:90:PHE:CD1	2.56	0.41
22:T:38:VAL:CG1	22:T:59:LEU:HD12	2.50	0.41
1:X:99:U:H5''	1:X:100:G:C8	2.57	0.40
1:X:956:A:C5	1:X:2427:A:C2	3.09	0.40
1:X:1835:C:H2'	1:X:1836:C:C6	2.56	0.40
1:X:2526:U:H2'	1:X:2527:G:C8	2.57	0.40
5:C:30:VAL:HA	5:C:95:LEU:HD11	2.02	0.40
16:N:88:ILE:HG13	17:O:49:GLU:HB2	2.03	0.40
18:P:19:LYS:HB3	18:P:19:LYS:HE2	1.76	0.40
24:V:2:LYS:H	24:V:3:PRO:CD	2.33	0.40
28:2:14:LYS:CA	28:2:15:THR:CA	2.98	0.40
1:X:957:G:H2'	1:X:958:G:H8	1.86	0.40
1:X:1248:G:O5'	1:X:1248:G:H8	2.04	0.40
1:X:1835:C:O2'	3:A:254:THR:HB	2.21	0.40
1:X:2796:A:OP2	13:K:5:LYS:NZ	2.55	0.40
3:A:147:LEU:HD22	3:A:183:ARG:NH2	2.35	0.40
19:Q:56:MET:SD	19:Q:57:ASN:N	2.91	0.40
21:S:53:ASP:HA	21:S:63:PRO:HA	2.03	0.40
22:T:41:ARG:HA	22:T:41:ARG:NE	2.34	0.40
23:U:43:ARG:HH21	23:U:43:ARG:HB2	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:649:G:N2	1:X:660:G:N2	2.69	0.40
1:X:651:C:H2'	1:X:652:C:H6	1.86	0.40
1:X:2064:U:H2'	1:X:2065:A:C8	2.56	0.40
1:X:2419:C:N3	1:X:2420:C:H1'	2.37	0.40
32:X:2929:1F4:H7	32:X:2929:1F4:O46	2.22	0.40
2:Y:22:U:H3	2:Y:65:A:H61	1.68	0.40
3:A:166:GLN:HB2	3:A:174:ILE:HG22	2.03	0.40
12:J:70:PHE:HA	12:J:71:PRO:HD3	1.95	0.40
16:N:42:ALA:O	16:N:46:GLU:N	2.51	0.40
23:U:20:ARG:HB2	23:U:43:ARG:HD2	2.02	0.40
26:Z:36:CYS:HB3	26:Z:49:CYS:HB3	1.94	0.40
26:Z:42:SER:O	26:Z:44:HIS:HD2	2.03	0.40
1:X:506:G:H4'	18:P:21:ARG:HH21	1.85	0.40
1:X:877:G:H2'	1:X:878:C:H6	1.86	0.40
1:X:1519:G:H2'	1:X:1520:G:H8	1.86	0.40
1:X:1796:A:N3	3:A:50:THR:HG23	2.36	0.40
9:G:35:LYS:C	9:G:37:ASP:H	2.28	0.40
21:S:36:ARG:O	21:S:40:ASP:HB2	2.22	0.40
1:X:1255:A:H2'	1:X:1256:C:H6	1.86	0.40
1:X:1467:U:C6	1:X:1467:U:H5''	2.57	0.40
1:X:2042:A:O3'	5:C:63:GLY:HA2	2.21	0.40
1:X:2422:C:H2'	1:X:2423:G:C8	2.56	0.40
4:B:181:LEU:HD21	15:M:12:LEU:CD2	2.51	0.40
7:E:140:LEU:O	7:E:144:VAL:HG23	2.22	0.40
9:G:103:TYR:HB3	9:G:107:GLN:HE21	1.85	0.40
16:N:95:LEU:HA	16:N:98:ILE:HD12	2.04	0.40
17:O:10:LYS:HE3	17:O:11:GLN:HG2	2.03	0.40
20:R:16:PHE:HE2	20:R:80:LYS:HZ3	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	238/274 (87%)	173 (73%)	47 (20%)	18 (8%)	1	9
4	B	203/211 (96%)	173 (85%)	25 (12%)	5 (2%)	4	28
5	C	195/205 (95%)	127 (65%)	40 (20%)	28 (14%)	0	3
6	D	175/180 (97%)	142 (81%)	26 (15%)	7 (4%)	2	20
7	E	169/185 (91%)	134 (79%)	26 (15%)	9 (5%)	1	14
8	F	69/144 (48%)	57 (83%)	9 (13%)	3 (4%)	2	18
9	G	140/174 (80%)	99 (71%)	26 (19%)	15 (11%)	0	5
10	H	132/134 (98%)	117 (89%)	12 (9%)	3 (2%)	5	30
11	I	139/156 (89%)	81 (58%)	39 (28%)	19 (14%)	0	3
12	J	134/141 (95%)	98 (73%)	24 (18%)	12 (9%)	0	6
13	K	111/116 (96%)	92 (83%)	13 (12%)	6 (5%)	1	14
14	L	102/114 (90%)	75 (74%)	15 (15%)	12 (12%)	0	4
15	M	106/166 (64%)	90 (85%)	10 (9%)	6 (6%)	1	13
16	N	115/118 (98%)	91 (79%)	17 (15%)	7 (6%)	1	13
17	O	92/100 (92%)	66 (72%)	13 (14%)	13 (14%)	0	3
18	P	125/134 (93%)	104 (83%)	17 (14%)	4 (3%)	3	24
19	Q	91/95 (96%)	63 (69%)	16 (18%)	12 (13%)	0	3
20	R	108/115 (94%)	65 (60%)	26 (24%)	17 (16%)	0	2
21	S	173/237 (73%)	135 (78%)	27 (16%)	11 (6%)	1	12
22	T	82/91 (90%)	65 (79%)	12 (15%)	5 (6%)	1	13
23	U	70/81 (86%)	41 (59%)	15 (21%)	14 (20%)	0	1
24	V	64/67 (96%)	57 (89%)	5 (8%)	2 (3%)	3	25
25	W	53/55 (96%)	47 (89%)	5 (9%)	1 (2%)	6	33
26	Z	56/60 (93%)	45 (80%)	6 (11%)	5 (9%)	0	7
30	4	35/37 (95%)	23 (66%)	11 (31%)	1 (3%)	3	26
All	All	2977/3390 (88%)	2260 (76%)	482 (16%)	235 (8%)	1	8

All (235) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	45	ASN
3	A	209	ALA
3	A	217	ARG
3	A	248	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	249	PRO
3	A	250	TRP
3	A	271	VAL
5	C	4	ILE
5	C	20	PRO
5	C	60	GLY
5	C	66	ASN
5	C	129	LYS
5	C	164	VAL
5	C	165	SER
5	C	172	VAL
5	C	195	ILE
6	D	10	ASP
6	D	81	GLN
6	D	122	PHE
7	E	165	VAL
9	G	33	ILE
9	G	67	ARG
9	G	92	GLY
9	G	97	ASP
9	G	104	THR
9	G	170	PRO
10	H	27	SER
11	I	18	ARG
11	I	47	ALA
11	I	49	PHE
11	I	64	GLY
11	I	98	LEU
11	I	99	VAL
11	I	103	ASN
12	J	80	ALA
12	J	82	THR
12	J	88	LYS
13	K	6	ALA
13	K	92	GLY
14	L	21	THR
14	L	61	SER
14	L	68	ALA
14	L	95	LYS
15	M	29	PRO
16	N	8	ILE
16	N	95	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	O	7	THR
17	O	10	LYS
17	O	22	VAL
17	O	48	GLY
19	Q	6	ILE
19	Q	61	LYS
19	Q	63	LYS
19	Q	67	ARG
19	Q	69	ILE
20	R	11	ASN
20	R	15	HIS
20	R	60	PRO
20	R	82	ALA
20	R	107	ALA
21	S	6	LYS
21	S	26	LYS
21	S	56	VAL
21	S	91	PRO
21	S	156	GLU
22	T	19	LYS
23	U	15	VAL
23	U	19	ILE
23	U	32	ARG
23	U	34	THR
23	U	56	GLN
23	U	60	VAL
26	Z	4	HIS
26	Z	36	CYS
26	Z	53	ASP
3	A	35	GLU
3	A	58	HIS
3	A	220	HIS
4	B	132	LYS
5	C	22	VAL
5	C	83	ALA
5	C	121	ASP
5	C	190	ALA
5	C	196	VAL
6	D	124	GLY
7	E	59	GLN
7	E	173	ALA
9	G	37	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	G	105	GLY
9	G	107	GLN
9	G	158	HIS
10	H	5	GLN
10	H	29	ILE
11	I	36	GLY
11	I	54	SER
11	I	62	LYS
11	I	68	VAL
12	J	11	ARG
12	J	83	ARG
12	J	87	GLY
12	J	91	VAL
13	K	4	GLY
13	K	9	LYS
14	L	31	VAL
14	L	40	ALA
14	L	94	TYR
15	M	26	ASP
15	M	31	ASP
15	M	39	VAL
15	M	57	ILE
16	N	7	GLY
16	N	87	ASN
17	O	8	GLY
17	O	9	GLY
17	O	14	VAL
18	P	9	ARG
18	P	85	MET
19	Q	12	ILE
19	Q	84	GLU
20	R	85	ASP
20	R	98	ILE
22	T	11	LYS
23	U	29	GLY
23	U	41	VAL
23	U	76	LYS
24	V	2	LYS
24	V	36	GLN
30	4	3	VAL
3	A	254	THR
3	A	269	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	B	129	HIS
4	B	146	THR
5	C	9	GLN
5	C	10	ASN
5	C	15	ILE
5	C	67	ALA
5	C	113	GLU
5	C	114	GLY
5	C	163	ASN
5	C	189	ASP
6	D	71	LYS
6	D	119	PRO
9	G	34	PRO
11	I	91	ASP
12	J	81	GLU
14	L	33	ARG
14	L	52	ALA
15	M	74	GLY
16	N	92	ARG
16	N	94	VAL
17	O	11	GLN
17	O	49	GLU
18	P	132	GLY
19	Q	62	ARG
19	Q	74	ASP
19	Q	89	GLU
20	R	14	LEU
20	R	83	LEU
20	R	87	GLU
20	R	96	LYS
21	S	88	TYR
21	S	128	ARG
22	T	74	LYS
23	U	27	ASP
26	Z	24	ALA
26	Z	37	HIS
3	A	54	ILE
3	A	55	GLY
5	C	13	ARG
5	C	18	PRO
5	C	194	GLU
6	D	40	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	E	19	ALA
7	E	65	HIS
8	F	118	GLY
9	G	159	SER
11	I	59	ARG
11	I	65	PHE
11	I	90	ARG
12	J	17	ARG
12	J	29	ALA
13	K	95	THR
14	L	60	LYS
17	O	31	ASP
17	O	36	LYS
17	O	78	VAL
19	Q	87	SER
20	R	63	THR
21	S	33	ALA
21	S	74	ARG
22	T	13	GLY
22	T	27	GLY
3	A	247	VAL
3	A	255	LYS
4	B	90	SER
5	C	55	GLY
5	C	68	ARG
7	E	7	GLN
7	E	55	PRO
7	E	92	VAL
11	I	37	GLN
11	I	115	SER
12	J	21	ASP
14	L	53	ALA
17	O	30	GLY
20	R	6	ALA
20	R	108	VAL
23	U	26	ALA
23	U	47	HIS
25	W	14	GLY
3	A	187	SER
4	B	137	ARG
5	C	126	ALA
9	G	165	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	I	86	THR
13	K	93	GLY
14	L	39	TYR
16	N	65	ILE
18	P	20	LEU
20	R	50	GLY
21	S	125	PRO
23	U	12	ASN
9	G	68	PRO
12	J	28	VAL
20	R	51	VAL
7	E	126	PRO
8	F	96	VAL
11	I	9	THR
21	S	174	PRO
8	F	120	VAL
20	R	111	GLY
3	A	270	ILE
9	G	138	GLY
19	Q	66	GLY
23	U	14	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	185/215 (86%)	146 (79%)	39 (21%)	1	7
4	B	155/157 (99%)	118 (76%)	37 (24%)	1	5
5	C	157/163 (96%)	108 (69%)	49 (31%)	0	2
6	D	153/156 (98%)	127 (83%)	26 (17%)	2	13
7	E	136/144 (94%)	115 (85%)	21 (15%)	2	16
8	F	51/107 (48%)	45 (88%)	6 (12%)	5	24
9	G	118/146 (81%)	86 (73%)	32 (27%)	0	3
10	H	103/103 (100%)	83 (81%)	20 (19%)	1	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	I	108/121 (89%)	74 (68%)	34 (32%)	0	2
12	J	110/115 (96%)	90 (82%)	20 (18%)	2	11
13	K	90/93 (97%)	72 (80%)	18 (20%)	1	8
14	L	74/82 (90%)	53 (72%)	21 (28%)	0	3
15	M	94/134 (70%)	69 (73%)	25 (27%)	0	3
16	N	96/97 (99%)	74 (77%)	22 (23%)	1	6
17	O	75/79 (95%)	53 (71%)	22 (29%)	0	2
18	P	109/115 (95%)	89 (82%)	20 (18%)	2	11
19	Q	75/76 (99%)	59 (79%)	16 (21%)	1	7
20	R	91/96 (95%)	70 (77%)	21 (23%)	1	6
21	S	149/192 (78%)	113 (76%)	36 (24%)	1	5
22	T	62/67 (92%)	54 (87%)	8 (13%)	4	22
23	U	57/66 (86%)	33 (58%)	24 (42%)	0	0
24	V	54/55 (98%)	43 (80%)	11 (20%)	1	8
25	W	48/48 (100%)	35 (73%)	13 (27%)	0	3
26	Z	51/53 (96%)	39 (76%)	12 (24%)	1	5
30	4	35/35 (100%)	28 (80%)	7 (20%)	1	8
All	All	2436/2715 (90%)	1876 (77%)	560 (23%)	1	6

All (560) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	37	LEU
3	A	39	LYS
3	A	40	THR
3	A	43	ARG
3	A	44	ASN
3	A	46	ARG
3	A	48	ARG
3	A	49	ILE
3	A	52	ARG
3	A	63	ARG
3	A	68	LYS
3	A	82	ILE
3	A	88	ARG
3	A	105	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	111	LEU
3	A	118	ASN
3	A	145	LEU
3	A	157	ARG
3	A	162	SER
3	A	163	VAL
3	A	169	GLU
3	A	183	ARG
3	A	186	HIS
3	A	188	GLU
3	A	196	VAL
3	A	203	ASN
3	A	208	LYS
3	A	212	SER
3	A	218	LYS
3	A	222	ARG
3	A	226	MET
3	A	240	THR
3	A	245	VAL
3	A	247	VAL
3	A	248	THR
3	A	252	LYS
3	A	254	THR
3	A	259	THR
3	A	270	ILE
4	B	2	LYS
4	B	4	ILE
4	B	5	LEU
4	B	14	ILE
4	B	27	LEU
4	B	34	VAL
4	B	35	GLN
4	B	41	THR
4	B	49	ILE
4	B	69	LYS
4	B	72	VAL
4	B	75	THR
4	B	82	ARG
4	B	103	ASP
4	B	107	THR
4	B	113	THR
4	B	118	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	B	119	ARG
4	B	131	SER
4	B	133	LYS
4	B	134	TRP
4	B	136	ARG
4	B	137	ARG
4	B	140	SER
4	B	141	ILE
4	B	145	LYS
4	B	149	ARG
4	B	150	VAL
4	B	152	LYS
4	B	154	LYS
4	B	162	MET
4	B	165	VAL
4	B	192	ASN
4	B	198	LEU
4	B	199	ARG
4	B	200	SER
4	B	203	LYS
5	C	3	GLN
5	C	7	ILE
5	C	10	ASN
5	C	13	ARG
5	C	14	THR
5	C	15	ILE
5	C	45	THR
5	C	48	ARG
5	C	51	VAL
5	C	52	SER
5	C	53	LYS
5	C	58	MET
5	C	59	TYR
5	C	62	LYS
5	C	64	THR
5	C	66	ASN
5	C	71	ASP
5	C	72	ARG
5	C	74	VAL
5	C	76	THR
5	C	89	ARG
5	C	91	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	C	94	THR
5	C	95	LEU
5	C	97	ARG
5	C	102	LEU
5	C	118	VAL
5	C	121	ASP
5	C	124	ASP
5	C	127	ASP
5	C	130	THR
5	C	132	ASN
5	C	134	ILE
5	C	136	TRP
5	C	138	LYS
5	C	140	ASN
5	C	143	ASP
5	C	148	VAL
5	C	150	LEU
5	C	151	VAL
5	C	153	ASP
5	C	154	ASP
5	C	164	VAL
5	C	166	TRP
5	C	175	VAL
5	C	180	ILE
5	C	181	LEU
5	C	188	ILE
5	C	194	GLU
6	D	11	GLN
6	D	33	LYS
6	D	40	LEU
6	D	45	GLU
6	D	57	LEU
6	D	60	ILE
6	D	67	ILE
6	D	71	LYS
6	D	79	LEU
6	D	80	ARG
6	D	89	VAL
6	D	95	ARG
6	D	112	ARG
6	D	115	ARG
6	D	117	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	D	125	ARG
6	D	130	LEU
6	D	134	GLU
6	D	136	LEU
6	D	142	THR
6	D	145	MET
6	D	150	ARG
6	D	153	ASP
6	D	164	GLU
6	D	171	GLN
6	D	175	LEU
7	E	15	VAL
7	E	21	ASP
7	E	35	VAL
7	E	40	GLU
7	E	50	LEU
7	E	59	GLN
7	E	67	LEU
7	E	69	ARG
7	E	72	VAL
7	E	84	THR
7	E	86	ASN
7	E	98	LEU
7	E	114	ILE
7	E	121	VAL
7	E	122	THR
7	E	130	ARG
7	E	133	VAL
7	E	139	GLN
7	E	140	LEU
7	E	141	VAL
7	E	155	ASP
8	F	78	ILE
8	F	84	ILE
8	F	96	VAL
8	F	110	THR
8	F	111	LYS
8	F	136	VAL
9	G	31	THR
9	G	33	ILE
9	G	38	GLU
9	G	41	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	G	56	THR
9	G	61	ARG
9	G	62	ILE
9	G	63	ARG
9	G	70	PHE
9	G	75	ILE
9	G	78	ASP
9	G	91	THR
9	G	95	LEU
9	G	98	LYS
9	G	101	THR
9	G	102	ARG
9	G	104	THR
9	G	112	THR
9	G	113	GLU
9	G	114	THR
9	G	117	GLU
9	G	119	LEU
9	G	122	HIS
9	G	127	ILE
9	G	132	PHE
9	G	135	LEU
9	G	137	LYS
9	G	145	HIS
9	G	150	VAL
9	G	154	GLU
9	G	165	VAL
9	G	168	THR
10	H	1	MET
10	H	7	ARG
10	H	9	ASP
10	H	10	VAL
10	H	19	ILE
10	H	23	ARG
10	H	29	ILE
10	H	41	ASN
10	H	83	ARG
10	H	85	ASP
10	H	88	THR
10	H	89	ILE
10	H	90	ARG
10	H	94	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	H	102	GLN
10	H	106	ARG
10	H	117	GLU
10	H	124	MET
10	H	126	ILE
10	H	127	VAL
11	I	4	HIS
11	I	6	LEU
11	I	13	ARG
11	I	18	ARG
11	I	21	ARG
11	I	26	THR
11	I	29	THR
11	I	39	SER
11	I	40	ARG
11	I	45	LYS
11	I	50	GLU
11	I	53	ARG
11	I	56	LEU
11	I	57	ILE
11	I	60	LEU
11	I	62	LYS
11	I	65	PHE
11	I	76	LYS
11	I	77	LEU
11	I	78	SER
11	I	79	GLN
11	I	83	LEU
11	I	85	ASP
11	I	86	THR
11	I	87	THR
11	I	90	ARG
11	I	93	LEU
11	I	98	LEU
11	I	99	VAL
11	I	101	ARG
11	I	108	LEU
11	I	113	GLU
11	I	114	ILE
11	I	142	LEU
12	J	7	ARG
12	J	8	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	J	11	ARG
12	J	17	ARG
12	J	32	ASP
12	J	43	ILE
12	J	44	LYS
12	J	52	ARG
12	J	54	VAL
12	J	64	LYS
12	J	67	ILE
12	J	73	LYS
12	J	93	TYR
12	J	95	VAL
12	J	103	VAL
12	J	126	LEU
12	J	129	GLN
12	J	131	LYS
12	J	134	LYS
12	J	140	GLU
13	K	8	ARG
13	K	10	LEU
13	K	11	ASN
13	K	12	ARG
13	K	17	ARG
13	K	26	THR
13	K	28	LEU
13	K	45	ARG
13	K	51	LEU
13	K	53	THR
13	K	60	LEU
13	K	73	LYS
13	K	83	VAL
13	K	94	TYR
13	K	95	THR
13	K	99	ARG
13	K	109	THR
13	K	115	LEU
14	L	11	LEU
14	L	13	THR
14	L	18	ARG
14	L	31	VAL
14	L	33	ARG
14	L	36	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	L	37	HIS
14	L	43	ILE
14	L	64	LYS
14	L	66	ASP
14	L	67	THR
14	L	87	VAL
14	L	88	VAL
14	L	89	PHE
14	L	90	ASP
14	L	91	ARG
14	L	93	SER
14	L	94	TYR
14	L	95	LYS
14	L	99	ARG
14	L	108	ARG
15	M	5	ILE
15	M	6	LYS
15	M	7	ILE
15	M	12	LEU
15	M	13	LEU
15	M	14	ARG
15	M	31	ASP
15	M	34	ARG
15	M	35	VAL
15	M	40	ARG
15	M	54	VAL
15	M	57	ILE
15	M	58	ASN
15	M	63	ARG
15	M	68	VAL
15	M	77	VAL
15	M	78	GLU
15	M	79	ARG
15	M	88	VAL
15	M	89	ASN
15	M	93	ILE
15	M	95	GLU
15	M	98	LYS
15	M	99	VAL
15	M	100	ARG
16	N	5	LYS
16	N	8	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	N	9	VAL
16	N	13	ARG
16	N	18	LEU
16	N	19	LYS
16	N	22	LYS
16	N	30	LYS
16	N	40	LEU
16	N	51	ARG
16	N	52	ASN
16	N	58	ARG
16	N	60	LEU
16	N	71	LEU
16	N	81	ASN
16	N	83	LEU
16	N	88	ILE
16	N	90	LEU
16	N	92	ARG
16	N	93	LYS
16	N	95	LEU
16	N	102	GLU
17	O	13	ARG
17	O	18	ASP
17	O	19	VAL
17	O	20	ILE
17	O	21	ARG
17	O	22	VAL
17	O	25	LEU
17	O	26	GLN
17	O	28	GLU
17	O	38	LEU
17	O	39	PHE
17	O	40	VAL
17	O	46	VAL
17	O	50	ASP
17	O	56	VAL
17	O	62	GLU
17	O	69	ILE
17	O	71	ILE
17	O	78	VAL
17	O	88	GLN
17	O	93	ILE
17	O	96	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	P	11	LYS
18	P	19	LYS
18	P	20	LEU
18	P	32	ARG
18	P	45	ILE
18	P	60	ILE
18	P	62	ARG
18	P	71	VAL
18	P	72	LEU
18	P	84	GLU
18	P	86	LEU
18	P	87	GLU
18	P	102	THR
18	P	103	LEU
18	P	109	ARG
18	P	113	SER
18	P	118	LYS
18	P	124	ILE
18	P	125	THR
18	P	126	ILE
19	Q	7	LEU
19	Q	8	GLN
19	Q	12	ILE
19	Q	14	GLU
19	Q	26	SER
19	Q	29	VAL
19	Q	38	ILE
19	Q	40	ASP
19	Q	42	ILE
19	Q	56	MET
19	Q	58	VAL
19	Q	63	LYS
19	Q	65	VAL
19	Q	67	ARG
19	Q	82	LEU
19	Q	84	GLU
20	R	11	ASN
20	R	13	LYS
20	R	18	LYS
20	R	23	ILE
20	R	25	LEU
20	R	26	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	R	46	VAL
20	R	48	VAL
20	R	62	MET
20	R	66	GLN
20	R	73	GLU
20	R	80	LYS
20	R	81	VAL
20	R	87	GLU
20	R	88	THR
20	R	98	ILE
20	R	104	VAL
20	R	105	ARG
20	R	106	VAL
20	R	108	VAL
20	R	113	THR
21	S	2	GLU
21	S	13	LYS
21	S	14	LEU
21	S	15	ASP
21	S	22	VAL
21	S	26	LYS
21	S	41	ARG
21	S	44	ARG
21	S	48	THR
21	S	51	LEU
21	S	53	ASP
21	S	54	ILE
21	S	61	THR
21	S	65	LEU
21	S	66	VAL
21	S	67	LYS
21	S	71	MET
21	S	73	LYS
21	S	76	ARG
21	S	79	ILE
21	S	94	VAL
21	S	95	SER
21	S	100	THR
21	S	101	THR
21	S	113	VAL
21	S	120	LEU
21	S	128	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	S	130	ILE
21	S	132	GLN
21	S	133	GLU
21	S	134	LEU
21	S	139	THR
21	S	152	ILE
21	S	160	LEU
21	S	163	ASP
21	S	166	LEU
22	T	16	SER
22	T	17	ASN
22	T	41	ARG
22	T	46	LYS
22	T	49	GLN
22	T	62	LEU
22	T	66	LYS
22	T	79	ILE
23	U	8	THR
23	U	10	LYS
23	U	11	LYS
23	U	13	LEU
23	U	14	VAL
23	U	17	SER
23	U	19	ILE
23	U	23	LYS
23	U	30	VAL
23	U	32	ARG
23	U	34	THR
23	U	37	ILE
23	U	42	GLN
23	U	43	ARG
23	U	47	HIS
23	U	52	ARG
23	U	57	VAL
23	U	62	LEU
23	U	63	SER
23	U	65	ASN
23	U	70	LEU
23	U	75	TYR
23	U	78	ILE
23	U	79	GLU
24	V	6	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	V	7	ARG
24	V	13	ASP
24	V	14	PHE
24	V	21	ARG
24	V	25	LEU
24	V	28	LEU
24	V	37	LEU
24	V	53	LEU
24	V	60	LEU
24	V	65	GLU
25	W	4	LYS
25	W	6	VAL
25	W	9	VAL
25	W	10	ILE
25	W	12	ARG
25	W	26	ARG
25	W	32	ARG
25	W	34	VAL
25	W	36	ASP
25	W	37	THR
25	W	40	VAL
25	W	45	LYS
25	W	46	THR
26	Z	3	LYS
26	Z	4	HIS
26	Z	6	VAL
26	Z	8	LYS
26	Z	9	LYS
26	Z	14	SER
26	Z	18	MET
26	Z	25	LEU
26	Z	35	GLN
26	Z	40	LYS
26	Z	41	LEU
26	Z	57	VAL
30	4	2	LYS
30	4	4	ARG
30	4	9	LYS
30	4	14	CYS
30	4	17	VAL
30	4	25	VAL
30	4	30	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	76	ASN
3	A	118	ASN
3	A	201	HIS
3	A	231	HIS
4	B	35	GLN
4	B	48	GLN
4	B	129	HIS
4	B	180	ASN
4	B	192	ASN
5	C	10	ASN
5	C	28	HIS
5	C	61	GLN
5	C	66	ASN
5	C	98	GLN
5	C	176	ASN
6	D	19	GLN
6	D	37	ASN
6	D	63	GLN
6	D	118	ASN
6	D	120	ASN
7	E	18	ASN
7	E	86	ASN
7	E	106	ASN
9	G	36	ASN
9	G	76	GLN
9	G	87	GLN
9	G	161	GLN
10	H	41	ASN
10	H	94	ASN
10	H	102	GLN
11	I	34	HIS
11	I	37	GLN
11	I	66	ASN
12	J	13	GLN
12	J	46	ASN
12	J	58	HIS
12	J	129	GLN
13	K	13	ASN
13	K	50	GLN
14	L	49	GLN
15	M	90	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	N	31	GLN
16	N	66	ASN
16	N	75	ASN
17	O	6	GLN
17	O	57	GLN
17	O	79	GLN
17	O	88	GLN
18	P	73	ASN
18	P	78	ASN
18	P	81	HIS
18	P	115	ASN
18	P	133	ASN
19	Q	8	GLN
19	Q	43	GLN
19	Q	57	ASN
20	R	15	HIS
20	R	29	HIS
20	R	32	GLN
20	R	44	GLN
20	R	71	GLN
21	S	70	GLN
21	S	80	HIS
21	S	105	GLN
21	S	119	ASN
22	T	3	HIS
22	T	17	ASN
22	T	35	ASN
22	T	49	GLN
22	T	57	HIS
22	T	71	ASN
23	U	16	ASN
23	U	42	GLN
23	U	56	GLN
25	W	54	GLN
26	Z	43	HIS
26	Z	44	HIS
26	Z	48	ASN

5.3.3 RNA ⓘ

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
-----	-------	----------	-------------------	-----------------

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2683/2880 (93%)	739 (27%)	250 (9%)
2	Y	121/123 (98%)	43 (35%)	12 (9%)
All	All	2804/3003 (93%)	782 (27%)	262 (9%)

All (782) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	7	G
1	X	13	A
1	X	14	A
1	X	15	G
1	X	23	G
1	X	34	U
1	X	35	G
1	X	45	C
1	X	48	A
1	X	49	U
1	X	50	G
1	X	54	G
1	X	62	U
1	X	63	A
1	X	69	G
1	X	70	A
1	X	71	A
1	X	72	A
1	X	73	A
1	X	74	G
1	X	82	G
1	X	83	A
1	X	84	G
1	X	89	A
1	X	90	G
1	X	91	A
1	X	97	U
1	X	99	U
1	X	100	G
1	X	101	A
1	X	107	G
1	X	108	G
1	X	111	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	112	U
1	X	116	A
1	X	117	A
1	X	118	U
1	X	123	A
1	X	127	C
1	X	129	A
1	X	136	A
1	X	137	A
1	X	138	G
1	X	143	A
1	X	147	G
1	X	154	U
1	X	157	G
1	X	158	A
1	X	173	A
1	X	174	A
1	X	176	A
1	X	177	U
1	X	181	A
1	X	182	G
1	X	191	G
1	X	192	G
1	X	193	A
1	X	198	A
1	X	199	A
1	X	203	G
1	X	204	A
1	X	205	A
1	X	206	U
1	X	207	U
1	X	209	G
1	X	219	G
1	X	225	G
1	X	227	G
1	X	228	A
1	X	229	G
1	X	238	G
1	X	239	A
1	X	241	C
1	X	242	A
1	X	243	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	245	C
1	X	246	C
1	X	248	A
1	X	310	A
1	X	312	G
1	X	313	U
1	X	319	G
1	X	321	A
1	X	322	A
1	X	323	G
1	X	332	C
1	X	333	A
1	X	334	G
1	X	335	A
1	X	338	G
1	X	340	G
1	X	342	G
1	X	343	A
1	X	344	G
1	X	349	G
1	X	358	C
1	X	360	A
1	X	361	G
1	X	388	G
1	X	396	U
1	X	397	U
1	X	399	G
1	X	400	U
1	X	409	G
1	X	411	C
1	X	414	A
1	X	416	U
1	X	417	C
1	X	418	C
1	X	419	G
1	X	424	G
1	X	425	A
1	X	433	G
1	X	441	A
1	X	455	A
1	X	456	C
1	X	458	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	459	A
1	X	461	A
1	X	463	C
1	X	466	A
1	X	467	U
1	X	468	A
1	X	469	G
1	X	470	U
1	X	484	G
1	X	490	A
1	X	492	G
1	X	495	C
1	X	504	G
1	X	506	G
1	X	513	A
1	X	514	G
1	X	515	A
1	X	518	A
1	X	519	C
1	X	520	C
1	X	522	G
1	X	523	A
1	X	534	U
1	X	539	A
1	X	540	G
1	X	541	C
1	X	542	A
1	X	543	G
1	X	554	U
1	X	555	U
1	X	557	U
1	X	558	G
1	X	559	C
1	X	560	G
1	X	572	G
1	X	580	A
1	X	581	A
1	X	582	G
1	X	583	C
1	X	584	A
1	X	595	A
1	X	596	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	597	U
1	X	601	A
1	X	602	C
1	X	613	A
1	X	614	G
1	X	623	G
1	X	625	A
1	X	627	A
1	X	631	G
1	X	632	A
1	X	633	G
1	X	636	G
1	X	645	G
1	X	648	A
1	X	649	G
1	X	652	C
1	X	654	A
1	X	655	A
1	X	657	A
1	X	658	G
1	X	664	C
1	X	665	A
1	X	667	U
1	X	668	A
1	X	677	G
1	X	681	A
1	X	683	A
1	X	684	C
1	X	690	A
1	X	695	G
1	X	697	G
1	X	698	A
1	X	699	G
1	X	700	C
1	X	703	A
1	X	717	G
1	X	718	A
1	X	723	C
1	X	725	C
1	X	727	U
1	X	728	G
1	X	729	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	730	C
1	X	731	A
1	X	732	G
1	X	739	G
1	X	742	G
1	X	743	A
1	X	751	G
1	X	753	U
1	X	754	G
1	X	760	U
1	X	777	A
1	X	778	G
1	X	788	G
1	X	789	G
1	X	790	A
1	X	795	A
1	X	797	A
1	X	798	G
1	X	801	A
1	X	802	A
1	X	803	C
1	X	804	C
1	X	805	G
1	X	806	A
1	X	807	A
1	X	814	G
1	X	815	A
1	X	816	U
1	X	818	G
1	X	824	U
1	X	825	C
1	X	832	A
1	X	840	U
1	X	841	G
1	X	842	A
1	X	843	G
1	X	858	G
1	X	859	U
1	X	860	U
1	X	872	G
1	X	879	A
1	X	883	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	886	A
1	X	891	A
1	X	919	U
1	X	922	A
1	X	926	C
1	X	931	G
1	X	938	G
1	X	939	C
1	X	940	G
1	X	941	U
1	X	943	U
1	X	944	A
1	X	952	A
1	X	956	A
1	X	957	G
1	X	967	G
1	X	968	C
1	X	969	U
1	X	970	A
1	X	971	A
1	X	972	C
1	X	973	U
1	X	979	A
1	X	984	A
1	X	985	G
1	X	994	A
1	X	995	A
1	X	996	C
1	X	998	C
1	X	1000	G
1	X	1001	A
1	X	1002	C
1	X	1006	C
1	X	1007	A
1	X	1010	U
1	X	1014	G
1	X	1016	C
1	X	1019	U
1	X	1020	A
1	X	1022	A
1	X	1023	U
1	X	1024	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1028	G
1	X	1033	G
1	X	1034	U
1	X	1036	G
1	X	1037	U
1	X	1044	U
1	X	1053	G
1	X	1054	C
1	X	1055	A
1	X	1056	U
1	X	1057	A
1	X	1058	G
1	X	1068	A
1	X	1069	G
1	X	1072	U
1	X	1073	G
1	X	1077	U
1	X	1081	A
1	X	1082	G
1	X	1086	C
1	X	1087	C
1	X	1090	C
1	X	1094	C
1	X	1097	A
1	X	1098	G
1	X	1099	A
1	X	1100	G
1	X	1101	U
1	X	1108	U
1	X	1121	G
1	X	1122	A
1	X	1123	G
1	X	1125	G
1	X	1127	C
1	X	1128	G
1	X	1129	A
1	X	1130	U
1	X	1141	U
1	X	1143	A
1	X	1145	C
1	X	1146	G
1	X	1152	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1153	A
1	X	1161	U
1	X	1168	G
1	X	1182	U
1	X	1184	G
1	X	1185	C
1	X	1186	G
1	X	1187	A
1	X	1189	G
1	X	1191	G
1	X	1192	A
1	X	1194	U
1	X	1209	G
1	X	1223	G
1	X	1224	A
1	X	1233	A
1	X	1250	A
1	X	1251	G
1	X	1261	G
1	X	1262	U
1	X	1263	G
1	X	1264	C
1	X	1266	G
1	X	1269	G
1	X	1282	A
1	X	1284	G
1	X	1285	A
1	X	1288	A
1	X	1289	A
1	X	1302	C
1	X	1313	U
1	X	1314	A
1	X	1315	A
1	X	1319	C
1	X	1325	U
1	X	1326	U
1	X	1334	A
1	X	1342	U
1	X	1345	G
1	X	1346	C
1	X	1353	A
1	X	1354	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1357	U
1	X	1358	C
1	X	1359	G
1	X	1365	U
1	X	1372	A
1	X	1378	A
1	X	1379	A
1	X	1381	G
1	X	1392	U
1	X	1399	C
1	X	1404	C
1	X	1409	U
1	X	1410	U
1	X	1412	C
1	X	1413	U
1	X	1428	G
1	X	1429	A
1	X	1430	G
1	X	1432	G
1	X	1433	A
1	X	1434	U
1	X	1439	G
1	X	1440	G
1	X	1441	A
1	X	1442	C
1	X	1443	G
1	X	1460	G
1	X	1465	G
1	X	1467	U
1	X	1468	A
1	X	1469	U
1	X	1470	G
1	X	1474	A
1	X	1475	U
1	X	1476	G
1	X	1489	C
1	X	1490	U
1	X	1496	G
1	X	1497	C
1	X	1498	G
1	X	1505	U
1	X	1506	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1508	G
1	X	1513	U
1	X	1514	C
1	X	1523	A
1	X	1524	C
1	X	1525	A
1	X	1528	C
1	X	1529	C
1	X	1531	C
1	X	1533	G
1	X	1545	G
1	X	1548	U
1	X	1551	U
1	X	1552	C
1	X	1553	G
1	X	1554	G
1	X	1562	G
1	X	1563	U
1	X	1570	C
1	X	1571	G
1	X	1574	A
1	X	1575	C
1	X	1576	G
1	X	1582	A
1	X	1585	A
1	X	1594	U
1	X	1600	U
1	X	1601	U
1	X	1602	G
1	X	1603	A
1	X	1607	A
1	X	1608	U
1	X	1609	G
1	X	1613	G
1	X	1614	C
1	X	1618	U
1	X	1619	A
1	X	1624	A
1	X	1625	A
1	X	1626	A
1	X	1631	C
1	X	1632	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1634	A
1	X	1635	G
1	X	1648	C
1	X	1651	U
1	X	1656	U
1	X	1657	A
1	X	1665	C
1	X	1668	G
1	X	1685	A
1	X	1686	A
1	X	1691	G
1	X	1695	U
1	X	1699	A
1	X	1710	U
1	X	1711	C
1	X	1712	G
1	X	1713	G
1	X	1714	A
1	X	1717	A
1	X	1732	U
1	X	1733	U
1	X	1734	C
1	X	1746	A
1	X	1749	G
1	X	1750	A
1	X	1754	G
1	X	1755	G
1	X	1764	A
1	X	1773	C
1	X	1776	A
1	X	1777	A
1	X	1778	U
1	X	1782	A
1	X	1790	G
1	X	1791	C
1	X	1792	C
1	X	1793	A
1	X	1799	A
1	X	1800	A
1	X	1801	C
1	X	1807	A
1	X	1808	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1810	U
1	X	1811	A
1	X	1812	U
1	X	1813	A
1	X	1821	A
1	X	1825	C
1	X	1830	C
1	X	1831	G
1	X	1839	A
1	X	1840	A
1	X	1852	G
1	X	1861	G
1	X	1867	A
1	X	1874	G
1	X	1883	A
1	X	1886	G
1	X	1910	A
1	X	1912	G
1	X	1913	G
1	X	1919	A
1	X	1920	A
1	X	1921	A
1	X	1923	U
1	X	1924	C
1	X	1927	U
1	X	1937	G
1	X	1938	U
1	X	1939	U
1	X	1943	A
1	X	1946	U
1	X	1947	G
1	X	1950	C
1	X	1953	A
1	X	1954	A
1	X	1955	G
1	X	1964	A
1	X	1965	U
1	X	1975	G
1	X	1976	U
1	X	1980	A
1	X	2003	A
1	X	2006	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	2014	A
1	X	2015	G
1	X	2018	G
1	X	2019	C
1	X	2026	C
1	X	2033	C
1	X	2035	G
1	X	2038	C
1	X	2039	G
1	X	2043	A
1	X	2044	G
1	X	2045	A
1	X	2046	C
1	X	2052	G
1	X	2063	A
1	X	2075	U
1	X	2076	G
1	X	2078	G
1	X	2079	A
1	X	2089	C
1	X	2090	U
1	X	2166	G
1	X	2171	U
1	X	2181	A
1	X	2189	A
1	X	2190	A
1	X	2191	A
1	X	2193	C
1	X	2195	C
1	X	2196	U
1	X	2197	U
1	X	2199	C
1	X	2204	A
1	X	2205	C
1	X	2214	G
1	X	2217	G
1	X	2218	G
1	X	2228	U
1	X	2229	G
1	X	2246	A
1	X	2247	A
1	X	2257	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	2262	C
1	X	2265	A
1	X	2266	A
1	X	2268	G
1	X	2283	G
1	X	2284	U
1	X	2285	U
1	X	2286	G
1	X	2287	G
1	X	2288	A
1	X	2289	A
1	X	2291	U
1	X	2295	C
1	X	2298	U
1	X	2299	A
1	X	2300	G
1	X	2301	A
1	X	2305	C
1	X	2306	A
1	X	2313	G
1	X	2315	A
1	X	2323	U
1	X	2324	G
1	X	2326	C
1	X	2329	C
1	X	2330	G
1	X	2333	A
1	X	2340	C
1	X	2351	G
1	X	2358	C
1	X	2362	G
1	X	2363	G
1	X	2364	C
1	X	2370	G
1	X	2371	A
1	X	2374	C
1	X	2381	A
1	X	2382	C
1	X	2385	U
1	X	2389	G
1	X	2396	C
1	X	2397	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	2401	A
1	X	2402	U
1	X	2404	A
1	X	2405	A
1	X	2406	C
1	X	2407	G
1	X	2408	G
1	X	2409	A
1	X	2410	U
1	X	2415	G
1	X	2420	C
1	X	2426	G
1	X	2427	A
1	X	2438	A
1	X	2447	G
1	X	2448	A
1	X	2453	C
1	X	2455	A
1	X	2457	A
1	X	2459	C
1	X	2461	G
1	X	2463	G
1	X	2466	G
1	X	2470	U
1	X	2477	C
1	X	2480	C
1	X	2481	G
1	X	2483	U
1	X	2484	G
1	X	2485	U
1	X	2498	U
1	X	2499	C
1	X	2508	G
1	X	2509	A
1	X	2514	G
1	X	2528	G
1	X	2529	G
1	X	2545	A
1	X	2546	G
1	X	2548	G
1	X	2552	C
1	X	2557	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	2560	G
1	X	2561	G
1	X	2562	G
1	X	2564	U
1	X	2565	C
1	X	2580	C
1	X	2581	A
1	X	2582	G
1	X	2588	U
1	X	2590	U
1	X	2591	C
1	X	2593	A
1	X	2594	U
1	X	2608	A
1	X	2609	G
1	X	2611	A
1	X	2613	A
1	X	2615	U
1	X	2616	U
1	X	2618	A
1	X	2621	G
1	X	2633	A
1	X	2634	G
1	X	2640	G
1	X	2642	G
1	X	2650	G
1	X	2668	U
1	X	2691	C
1	X	2692	A
1	X	2693	U
1	X	2694	G
1	X	2706	U
1	X	2713	A
1	X	2718	A
1	X	2719	U
1	X	2728	A
1	X	2731	G
1	X	2732	C
1	X	2735	C
1	X	2737	A
1	X	2745	A
1	X	2758	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	2759	U
1	X	2760	G
1	X	2769	C
1	X	2770	A
1	X	2771	C
1	X	2774	U
1	X	2776	U
1	X	2778	U
1	X	2779	C
1	X	2780	A
1	X	2793	G
1	X	2795	A
1	X	2796	A
1	X	2798	A
1	X	2800	C
1	X	2807	U
1	X	2808	U
1	X	2809	A
1	X	2824	C
1	X	2825	A
1	X	2841	U
1	X	2843	A
1	X	2846	G
1	X	2847	G
1	X	2848	A
1	X	2849	C
1	X	2854	G
1	X	2855	C
1	X	2861	A
1	X	2864	C
1	X	2866	A
1	X	2868	G
1	X	2877	A
2	Y	11	G
2	Y	14	C
2	Y	15	A
2	Y	17	A
2	Y	18	G
2	Y	26	G
2	Y	27	A
2	Y	28	A
2	Y	37	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Y	38	C
2	Y	39	C
2	Y	42	U
2	Y	43	G
2	Y	44	C
2	Y	46	G
2	Y	47	A
2	Y	48	A
2	Y	49	C
2	Y	52	G
2	Y	53	G
2	Y	54	U
2	Y	58	G
2	Y	59	A
2	Y	69	G
2	Y	75	A
2	Y	76	U
2	Y	77	G
2	Y	86	A
2	Y	87	C
2	Y	88	C
2	Y	89	G
2	Y	90	C
2	Y	91	A
2	Y	92	G
2	Y	99	G
2	Y	102	A
2	Y	106	U
2	Y	110	U
2	Y	111	C
2	Y	112	A
2	Y	115	G
2	Y	116	C
2	Y	123	U

All (262) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	13	A
1	X	33	C
1	X	34	U
1	X	48	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	61	U
1	X	62	U
1	X	70	A
1	X	71	A
1	X	73	A
1	X	74	G
1	X	82	G
1	X	83	A
1	X	89	A
1	X	98	U
1	X	99	U
1	X	100	G
1	X	117	A
1	X	173	A
1	X	176	A
1	X	181	A
1	X	190	A
1	X	198	A
1	X	204	A
1	X	242	A
1	X	247	A
1	X	312	G
1	X	321	A
1	X	322	A
1	X	332	C
1	X	333	A
1	X	334	G
1	X	339	U
1	X	341	A
1	X	342	G
1	X	343	A
1	X	387	A
1	X	396	U
1	X	399	G
1	X	400	U
1	X	408	U
1	X	416	U
1	X	417	C
1	X	425	A
1	X	447	U
1	X	454	G
1	X	458	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	466	A
1	X	467	U
1	X	469	G
1	X	513	A
1	X	522	G
1	X	539	A
1	X	540	G
1	X	557	U
1	X	558	G
1	X	559	C
1	X	580	A
1	X	582	G
1	X	583	C
1	X	596	C
1	X	631	G
1	X	648	A
1	X	657	A
1	X	664	C
1	X	672	C
1	X	682	G
1	X	683	A
1	X	687	G
1	X	698	A
1	X	717	G
1	X	731	A
1	X	765	C
1	X	775	U
1	X	777	A
1	X	788	G
1	X	802	A
1	X	803	C
1	X	806	A
1	X	813	A
1	X	824	U
1	X	840	U
1	X	841	G
1	X	842	A
1	X	858	G
1	X	859	U
1	X	878	C
1	X	883	A
1	X	886	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	925	U
1	X	938	G
1	X	939	C
1	X	943	U
1	X	956	A
1	X	969	U
1	X	970	A
1	X	972	C
1	X	995	A
1	X	1000	G
1	X	1019	U
1	X	1036	G
1	X	1037	U
1	X	1053	G
1	X	1055	A
1	X	1056	U
1	X	1057	A
1	X	1072	U
1	X	1080	A
1	X	1081	A
1	X	1086	C
1	X	1096	A
1	X	1099	A
1	X	1122	A
1	X	1129	A
1	X	1139	A
1	X	1142	G
1	X	1143	A
1	X	1152	C
1	X	1185	C
1	X	1186	G
1	X	1191	G
1	X	1223	G
1	X	1249	G
1	X	1250	A
1	X	1266	G
1	X	1278	A
1	X	1288	A
1	X	1313	U
1	X	1314	A
1	X	1325	U
1	X	1333	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1337	G
1	X	1345	G
1	X	1353	A
1	X	1357	U
1	X	1404	C
1	X	1409	U
1	X	1412	C
1	X	1433	A
1	X	1434	U
1	X	1439	G
1	X	1441	A
1	X	1442	C
1	X	1459	U
1	X	1467	U
1	X	1473	U
1	X	1474	A
1	X	1475	U
1	X	1489	C
1	X	1496	G
1	X	1508	G
1	X	1513	U
1	X	1562	G
1	X	1570	C
1	X	1574	A
1	X	1575	C
1	X	1583	A
1	X	1600	U
1	X	1601	U
1	X	1602	G
1	X	1607	A
1	X	1613	G
1	X	1618	U
1	X	1624	A
1	X	1631	C
1	X	1632	A
1	X	1634	A
1	X	1685	A
1	X	1686	A
1	X	1710	U
1	X	1711	C
1	X	1732	U
1	X	1749	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1775	A
1	X	1777	A
1	X	1790	G
1	X	1791	C
1	X	1795	C
1	X	1799	A
1	X	1800	A
1	X	1810	U
1	X	1811	A
1	X	1820	G
1	X	1830	C
1	X	1839	A
1	X	1883	A
1	X	1909	U
1	X	1920	A
1	X	1921	A
1	X	1923	U
1	X	1937	G
1	X	1938	U
1	X	1953	A
1	X	1975	G
1	X	2018	G
1	X	2032	G
1	X	2075	U
1	X	2165	A
1	X	2189	A
1	X	2204	A
1	X	2217	G
1	X	2228	U
1	X	2254	C
1	X	2258	G
1	X	2261	G
1	X	2295	C
1	X	2298	U
1	X	2299	A
1	X	2305	C
1	X	2312	A
1	X	2314	A
1	X	2323	U
1	X	2343	C
1	X	2363	G
1	X	2370	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	2381	A
1	X	2396	C
1	X	2401	A
1	X	2409	A
1	X	2447	G
1	X	2482	A
1	X	2497	A
1	X	2508	G
1	X	2528	G
1	X	2545	A
1	X	2560	G
1	X	2561	G
1	X	2564	U
1	X	2580	C
1	X	2593	A
1	X	2608	A
1	X	2615	U
1	X	2660	C
1	X	2669	C
1	X	2691	C
1	X	2693	U
1	X	2731	G
1	X	2736	U
1	X	2758	A
1	X	2759	U
1	X	2770	A
1	X	2778	U
1	X	2795	A
1	X	2807	U
1	X	2808	U
1	X	2824	C
1	X	2832	G
1	X	2846	G
1	X	2848	A
1	X	2854	G
1	X	2867	G
2	Y	14	C
2	Y	46	G
2	Y	47	A
2	Y	49	C
2	Y	58	G
2	Y	86	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Y	90	C
2	Y	92	G
2	Y	94	G
2	Y	111	C
2	Y	116	C
2	Y	117	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 36 ligands modelled in this entry, 35 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	1F4	X	2929	-	61,62,62	1.27	6 (9%)	81,95,95	2.75	37 (45%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	1F4	X	2929	-	-	33/74/119/119	1/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2929	1F4	C41-N40	4.52	1.39	1.33
32	X	2929	1F4	C52-C51	3.41	1.44	1.39
32	X	2929	1F4	C22-C9	2.87	1.58	1.52
32	X	2929	1F4	O46-C44	2.19	1.24	1.21
32	X	2929	1F4	C4-N40	2.09	1.49	1.45
32	X	2929	1F4	C12-C13	-2.01	1.50	1.54

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2929	1F4	C51-C47-N45	-8.29	98.37	113.03
32	X	2929	1F4	C6-O10-C11	6.74	129.97	118.20
32	X	2929	1F4	C22-C9-C7	-5.34	103.00	111.17
32	X	2929	1F4	C21-C14-C13	5.10	120.37	111.40
32	X	2929	1F4	O43-C13-C14	5.05	119.16	107.52
32	X	2929	1F4	C4-N40-C41	-4.82	106.10	112.39
32	X	2929	1F4	C58-C49-C50	-4.68	104.57	110.77
32	X	2929	1F4	C9-C7-C2	-4.54	108.70	116.10
32	X	2929	1F4	C9-C8-C14	4.36	120.20	113.54
32	X	2929	1F4	O42-C41-N40	-4.18	124.25	129.19
32	X	2929	1F4	O17-C41-N40	4.07	112.94	109.80
32	X	2929	1F4	C58-C49-C57	4.07	115.94	109.52
32	X	2929	1F4	O18-C9-C8	3.95	115.63	107.82
32	X	2929	1F4	C22-C9-C8	-3.73	104.32	109.79
32	X	2929	1F4	C54-N55-C56	3.69	123.32	116.85
32	X	2929	1F4	C2-C3-C1	3.61	125.24	119.13
32	X	2929	1F4	C51-C56-N55	-3.59	118.45	124.05
32	X	2929	1F4	O46-C44-N45	-3.51	120.22	124.21
32	X	2929	1F4	C21-C14-C8	3.48	120.06	112.42
32	X	2929	1F4	O10-C6-C23	3.23	113.37	107.36
32	X	2929	1F4	C19-C2-C7	-3.16	104.01	109.88
32	X	2929	1F4	O20-C28-O29	-3.14	102.43	110.69
32	X	2929	1F4	C57-C49-C48	-3.04	105.87	111.22
32	X	2929	1F4	C28-O20-C8	-2.96	111.22	116.26
32	X	2929	1F4	C48-C47-C51	-2.80	108.23	113.64
32	X	2929	1F4	C28-O29-C30	-2.73	108.70	112.91
32	X	2929	1F4	C7-C9-C8	2.67	113.41	110.18
32	X	2929	1F4	O15-C3-C2	-2.61	116.59	121.30
32	X	2929	1F4	C24-C5-C6	2.50	116.81	112.36
32	X	2929	1F4	C31-C32-C33	2.50	113.61	110.02
32	X	2929	1F4	C16-C1-C3	2.47	112.41	108.09
32	X	2929	1F4	C13-O43-C44	2.36	120.33	117.01
32	X	2929	1F4	C7-C2-C3	-2.26	109.54	113.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2929	1F4	C23-C6-C5	-2.16	112.26	115.23
32	X	2929	1F4	O10-C11-O26	2.10	127.74	123.95
32	X	2929	1F4	C50-N45-C47	-2.05	108.31	112.52
32	X	2929	1F4	C31-C32-N34	-2.04	109.85	115.59

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	X	2929	1F4	C4-C5-C6-O10
32	X	2929	1F4	C4-C5-C6-C23
32	X	2929	1F4	O17-C5-C6-O10
32	X	2929	1F4	O17-C5-C6-C23
32	X	2929	1F4	C24-C5-C6-O10
32	X	2929	1F4	C24-C5-C6-C23
32	X	2929	1F4	O20-C8-C9-C22
32	X	2929	1F4	C7-C9-O18-C39
32	X	2929	1F4	C14-C13-O43-C44
32	X	2929	1F4	C31-C32-N34-C35
32	X	2929	1F4	C31-C32-N34-C36
32	X	2929	1F4	C33-C32-N34-C35
32	X	2929	1F4	C33-C32-N34-C36
32	X	2929	1F4	C12-C13-O43-C44
32	X	2929	1F4	C25-C23-C6-O10
32	X	2929	1F4	O43-C13-C14-C8
32	X	2929	1F4	C12-C13-C14-C8
32	X	2929	1F4	C19-C2-C7-C9
32	X	2929	1F4	C13-C14-C8-C9
32	X	2929	1F4	C25-C23-C6-C5
32	X	2929	1F4	C14-C8-C9-C7
32	X	2929	1F4	C14-C8-C9-O18
32	X	2929	1F4	C14-C8-C9-C22
32	X	2929	1F4	O20-C8-C9-C7
32	X	2929	1F4	O20-C8-C9-O18
32	X	2929	1F4	O46-C44-O43-C13
32	X	2929	1F4	N45-C44-O43-C13
32	X	2929	1F4	C22-C9-O18-C39
32	X	2929	1F4	C13-C14-C8-O20
32	X	2929	1F4	C4-C1-C3-C2
32	X	2929	1F4	C3-C2-C7-C9
32	X	2929	1F4	C4-C1-C3-O15
32	X	2929	1F4	C8-C9-O18-C39

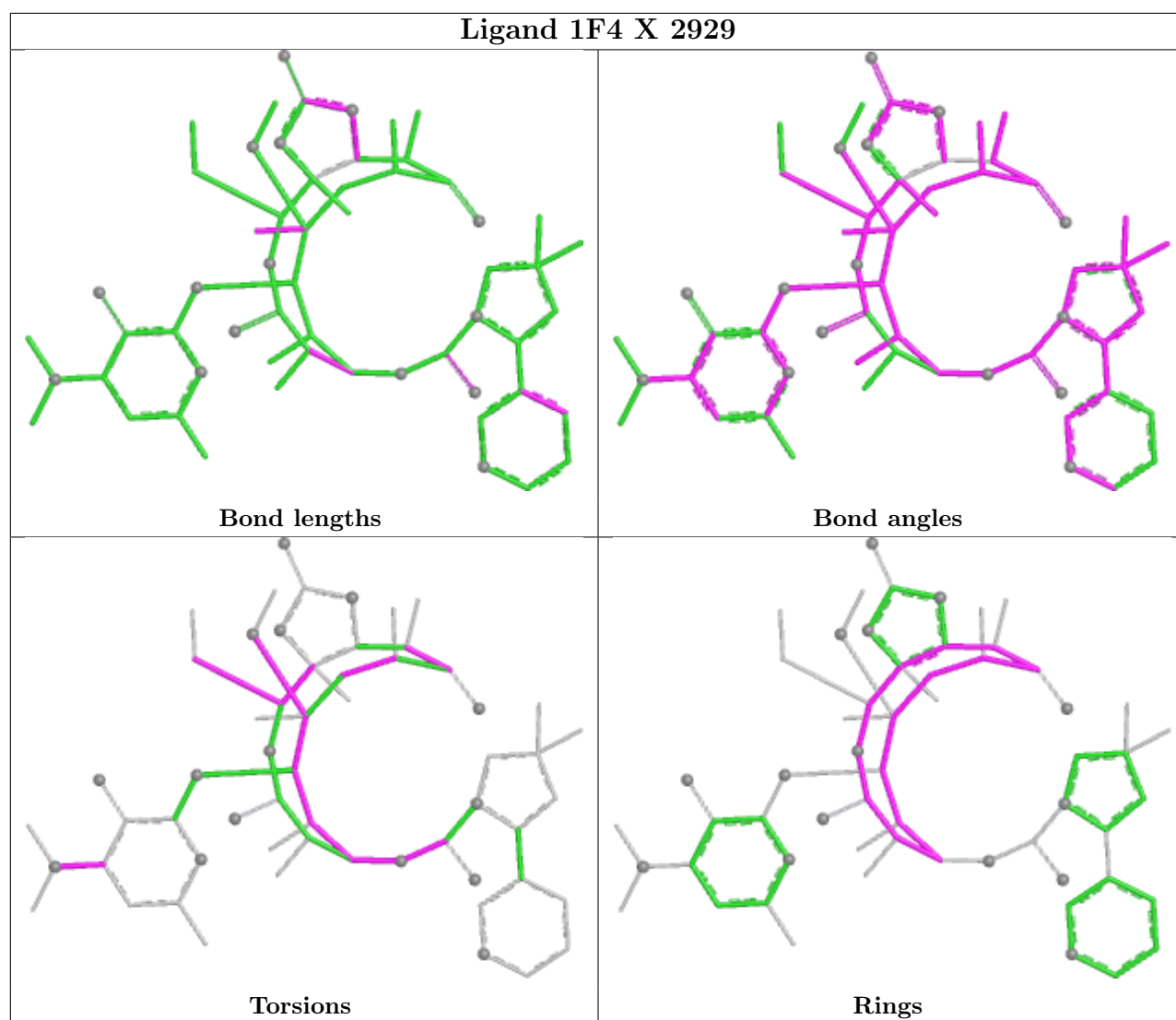
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	X	2929	1F4	C1-C11-C12-C13-C14-C2-C3-C4-C5-C6-C7-C8-C9-O10

1 monomer is involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	2929	1F4	19	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	X	2686/2880 (93%)	0.11	116 (4%) 40 22	43, 92, 197, 276	0
2	Y	122/123 (99%)	0.32	5 (4%) 41 23	83, 135, 170, 191	0
3	A	240/274 (87%)	0.49	24 (10%) 12 10	68, 115, 146, 172	0
4	B	205/211 (97%)	0.08	3 (1%) 72 44	45, 73, 105, 154	0
5	C	197/205 (96%)	0.57	17 (8%) 16 12	57, 114, 154, 187	0
6	D	177/180 (98%)	0.33	7 (3%) 42 24	146, 183, 216, 227	0
7	E	171/185 (92%)	0.10	7 (4%) 41 23	92, 143, 192, 206	0
8	F	71/144 (49%)	0.76	6 (8%) 16 12	211, 236, 252, 257	0
9	G	142/174 (81%)	0.38	9 (6%) 26 16	72, 97, 144, 161	0
10	H	134/134 (100%)	0.02	1 (0%) 84 61	50, 70, 97, 121	0
11	I	141/156 (90%)	1.26	35 (24%) 2 2	67, 129, 174, 204	0
12	J	136/141 (96%)	0.43	11 (8%) 18 12	74, 103, 149, 184	0
13	K	113/116 (97%)	0.22	6 (5%) 32 19	35, 60, 79, 91	0
14	L	104/114 (91%)	0.63	15 (14%) 6 6	98, 134, 156, 168	0
15	M	108/166 (65%)	-0.04	1 (0%) 81 56	50, 73, 111, 145	0
16	N	117/118 (99%)	0.36	9 (7%) 19 13	59, 90, 128, 159	0
17	O	94/100 (94%)	0.38	8 (8%) 16 12	66, 115, 157, 173	0
18	P	127/134 (94%)	-0.15	0 100 100	50, 68, 107, 158	0
19	Q	93/95 (97%)	0.27	5 (5%) 31 18	73, 106, 162, 195	0
20	R	110/115 (95%)	0.67	13 (11%) 9 8	88, 117, 170, 178	0
21	S	175/237 (73%)	0.42	11 (6%) 26 16	121, 155, 175, 190	0
22	T	84/91 (92%)	0.43	7 (8%) 17 12	79, 107, 186, 200	0
23	U	72/81 (88%)	0.97	10 (13%) 6 6	92, 128, 153, 161	0
24	V	66/67 (98%)	-0.24	0 100 100	100, 132, 211, 216	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	55/55 (100%)	0.08	3 (5%) 30 18	80, 98, 126, 152	0
26	Z	58/60 (96%)	0.39	3 (5%) 33 19	49, 70, 105, 114	0
27	1	53/55 (96%)	6.95	40 (75%) 0 0	8, 32, 62, 93	0
28	2	46/47 (97%)	10.41	46 (100%) 0 0	3, 15, 38, 59	0
29	3	63/66 (95%)	8.83	50 (79%) 0 0	3, 25, 40, 61	0
30	4	37/37 (100%)	2.84	23 (62%) 0 0	228, 254, 266, 269	0
All	All	5997/6561 (91%)	0.49	491 (8%) 17 12	3, 100, 196, 276	0

All (491) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	1	7	ARG	58.7
28	2	31	LEU	54.2
29	3	28	GLY	43.9
29	3	41	ILE	37.1
27	1	34	LYS	31.9
29	3	22	VAL	27.7
27	1	31	THR	26.0
29	3	30	ARG	25.8
28	2	39	ARG	24.6
29	3	43	GLY	23.3
29	3	38	GLY	23.1
29	3	60	LEU	23.1
28	2	46	ASP	22.6
28	2	38	GLY	21.2
29	3	31	HIS	20.4
29	3	33	ASN	19.4
29	3	63	PRO	19.2
29	3	58	MET	19.2
29	3	3	LYS	18.2
29	3	2	PRO	17.8
28	2	35	ARG	17.3
27	1	43	VAL	17.1
28	2	14	LYS	16.7
29	3	9	MET	16.4
28	2	27	GLY	15.3
27	1	44	ALA	14.9
27	1	21	TYR	13.4
28	2	7	PRO	13.1
28	2	8	ASN	13.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
29	3	45	GLY	12.9
28	2	40	HIS	12.9
29	3	29	LYS	12.6
27	1	40	TYR	12.5
28	2	10	ARG	11.7
28	2	34	ARG	11.5
29	3	40	GLU	11.2
28	2	30	ILE	11.1
28	2	4	THR	11.0
27	1	2	ALA	10.9
27	1	19	GLY	10.9
27	1	52	GLU	10.9
29	3	42	ARG	10.8
26	Z	2	ALA	10.7
28	2	42	LEU	10.6
28	2	6	GLN	10.6
28	2	43	THR	10.5
27	1	26	LYS	10.5
28	2	1	MET	10.5
29	3	19	THR	10.5
28	2	9	ASN	10.4
28	2	36	ALA	10.2
28	2	21	ARG	10.1
30	4	19	ARG	9.8
27	1	41	ASP	9.1
28	2	26	SER	9.1
1	X	731	A	9.0
28	2	11	LYS	8.7
28	2	32	ALA	8.5
28	2	5	TYR	8.4
29	3	37	SER	8.2
27	1	54	LYS	8.1
28	2	45	SER	8.0
11	I	9	THR	8.0
5	C	44	SER	7.8
11	I	48	PHE	7.7
28	2	41	GLN	7.7
29	3	17	THR	7.7
29	3	34	THR	7.5
29	3	18	GLY	7.5
28	2	18	PHE	7.3
27	1	3	LYS	7.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
28	2	15	THR	7.3
27	1	25	THR	7.2
28	2	2	LYS	7.2
27	1	18	THR	7.2
27	1	46	LYS	7.2
29	3	20	GLY	7.1
11	I	8	PRO	7.1
1	X	248	A	7.1
30	4	31	LYS	7.0
28	2	16	HIS	6.8
29	3	52	LYS	6.8
27	1	47	HIS	6.8
11	I	53	ARG	6.8
29	3	4	MET	6.7
3	A	237	GLU	6.6
23	U	47	HIS	6.6
11	I	29	THR	6.6
27	1	42	PRO	6.4
28	2	20	ALA	6.4
28	2	24	THR	6.4
29	3	51	ALA	6.3
28	2	13	ALA	6.3
29	3	8	LYS	6.2
28	2	3	ARG	6.1
29	3	54	GLU	6.1
4	B	135	HIS	6.1
30	4	3	VAL	6.1
28	2	12	ARG	6.0
30	4	21	GLY	5.9
1	X	1083	C	5.9
28	2	37	LYS	5.9
27	1	4	ASP	5.7
11	I	52	GLY	5.7
27	1	27	ASN	5.7
22	T	9	SER	5.7
23	U	16	ASN	5.7
6	D	42	SER	5.7
11	I	63	ARG	5.6
30	4	17	VAL	5.6
3	A	224	SER	5.5
29	3	46	LYS	5.5
11	I	31	GLY	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	223	GLY	5.5
17	O	36	LYS	5.4
30	4	18	ARG	5.4
3	A	203	ASN	5.4
28	2	28	ARG	5.3
29	3	47	GLY	5.2
29	3	32	GLN	5.2
12	J	84	MET	5.1
30	4	37	GLY	5.1
29	3	24	ALA	5.1
30	4	23	VAL	5.0
3	A	220	HIS	5.0
30	4	1	MET	5.0
1	X	2323	U	4.9
20	R	100	ASP	4.9
28	2	29	ASN	4.9
3	A	91	ARG	4.9
29	3	12	ARG	4.9
13	K	17	ARG	4.8
7	E	5	GLY	4.8
28	2	22	MET	4.8
1	X	2329	C	4.8
5	C	49	ALA	4.7
8	F	123	ALA	4.7
1	X	2330	G	4.7
11	I	17	LYS	4.7
29	3	62	LEU	4.6
9	G	97	ASP	4.6
1	X	774	A	4.6
20	R	82	ALA	4.6
29	3	13	ARG	4.6
27	1	35	LEU	4.6
29	3	39	ASP	4.6
27	1	37	LEU	4.5
11	I	74	VAL	4.5
23	U	65	ASN	4.5
1	X	1091	C	4.5
16	N	48	ARG	4.5
1	X	1068	A	4.5
21	S	67	LYS	4.5
27	1	20	PHE	4.5
27	1	45	LYS	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	N	4	ALA	4.4
29	3	35	GLY	4.4
30	4	24	LEU	4.4
1	X	346	C	4.4
1	X	74	G	4.3
23	U	39	LYS	4.3
1	X	2776	U	4.3
30	4	33	LYS	4.2
14	L	57	ALA	4.1
29	3	56	ALA	4.1
19	Q	62	ARG	4.1
20	R	78	ALA	4.1
2	Y	123	U	4.1
8	F	126	THR	4.0
1	X	1951	G	4.0
11	I	32	ARG	4.0
20	R	57	ASN	4.0
20	R	7	GLY	4.0
27	1	30	ASN	3.9
30	4	35	ARG	3.9
29	3	21	LYS	3.9
9	G	163	PRO	3.9
11	I	57	ILE	3.9
27	1	50	PHE	3.9
30	4	20	HIS	3.9
5	C	48	ARG	3.9
1	X	358	C	3.8
1	X	170	U	3.8
1	X	225	G	3.8
30	4	4	ARG	3.8
29	3	7	HIS	3.8
1	X	2265	A	3.7
27	1	24	THR	3.7
28	2	44	VAL	3.7
29	3	14	ILE	3.7
6	D	85	VAL	3.7
3	A	219	PRO	3.7
26	Z	8	LYS	3.7
1	X	1067	G	3.7
13	K	104	ARG	3.7
30	4	30	VAL	3.6
30	4	5	SER	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	C	189	ASP	3.6
16	N	94	VAL	3.6
25	W	6	VAL	3.6
22	T	10	SER	3.6
28	2	23	LYS	3.6
7	E	68	THR	3.6
27	1	32	GLN	3.6
23	U	62	LEU	3.6
17	O	78	VAL	3.5
20	R	81	VAL	3.5
27	1	36	GLU	3.5
19	Q	69	ILE	3.5
29	3	44	LYS	3.5
1	X	730	C	3.5
1	X	483	A	3.5
1	X	1092	U	3.5
11	I	15	ASP	3.5
16	N	56	ASP	3.5
17	O	5	ILE	3.5
30	4	2	LYS	3.4
1	X	356	A	3.4
28	2	19	ARG	3.4
14	L	36	LYS	3.4
27	1	33	ALA	3.4
1	X	1082	G	3.4
5	C	47	THR	3.4
12	J	86	LYS	3.4
8	F	115	LEU	3.3
21	S	1	MET	3.3
17	O	39	PHE	3.3
11	I	36	GLY	3.3
1	X	123	A	3.3
16	N	91	ASN	3.3
11	I	30	ALA	3.3
1	X	2270	U	3.3
9	G	103	TYR	3.3
29	3	11	LYS	3.3
25	W	50	LEU	3.3
27	1	29	ARG	3.3
11	I	102	LYS	3.2
22	T	15	ASP	3.2
19	Q	56	MET	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
23	U	52	ARG	3.2
14	L	53	ALA	3.2
19	Q	64	ARG	3.2
20	R	58	VAL	3.2
9	G	129	HIS	3.2
30	4	22	ARG	3.2
7	E	37	TYR	3.2
27	1	9	ILE	3.1
11	I	60	LEU	3.1
12	J	67	ILE	3.1
16	N	3	ARG	3.1
22	T	14	ARG	3.1
29	3	6	THR	3.1
6	D	153	ASP	3.1
30	4	8	LYS	3.1
14	L	20	THR	3.1
11	I	54	SER	3.0
1	X	435	A	3.0
11	I	64	GLY	3.0
1	X	1912	G	3.0
1	X	2557	G	3.0
11	I	62	LYS	3.0
7	E	71	LEU	3.0
14	L	21	THR	3.0
25	W	7	ARG	3.0
28	2	25	LYS	2.9
1	X	1069	G	2.9
1	X	1913	G	2.9
1	X	2283	G	2.9
1	X	2327	U	2.9
3	A	250	TRP	2.9
17	O	34	GLU	2.9
27	1	6	PRO	2.9
5	C	55	GLY	2.9
1	X	2328	G	2.9
27	1	13	GLU	2.9
4	B	205	SER	2.9
14	L	111	GLY	2.9
8	F	130	THR	2.9
1	X	1089	C	2.9
1	X	887	G	2.9
1	X	1954	A	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	L	34	SER	2.8
1	X	1090	C	2.8
3	A	261	ARG	2.8
5	C	82	VAL	2.8
30	4	36	GLN	2.8
12	J	17	ARG	2.8
11	I	33	GLY	2.8
21	S	38	ALA	2.8
5	C	39	ARG	2.8
5	C	57	LYS	2.8
5	C	161	ALA	2.8
1	X	2456	U	2.8
1	X	398	C	2.8
1	X	434	C	2.8
1	X	653	G	2.8
11	I	56	LEU	2.8
1	X	2777	A	2.8
28	2	17	GLY	2.8
14	L	40	ALA	2.8
30	4	29	ASN	2.8
3	A	52	ARG	2.7
5	C	193	LEU	2.7
22	T	7	VAL	2.7
12	J	27	TYR	2.7
1	X	1104	G	2.7
13	K	12	ARG	2.7
1	X	1299	A	2.7
8	F	86	LYS	2.7
1	X	2326	C	2.7
3	A	46	ARG	2.7
27	1	28	ARG	2.7
6	D	154	ILE	2.7
30	4	6	SER	2.7
1	X	1060	C	2.7
3	A	236	GLY	2.7
11	I	42	GLY	2.7
12	J	141	ALA	2.7
29	3	59	LYS	2.7
1	X	1066	G	2.6
29	3	57	ARG	2.6
20	R	91	ALA	2.6
11	I	41	SER	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	X	842	A	2.6
1	X	1365	U	2.6
1	X	558	G	2.6
1	X	2408	G	2.6
1	X	1087	C	2.6
29	3	10	ALA	2.6
1	X	193	A	2.6
1	X	416	U	2.6
1	X	230	C	2.6
1	X	520	C	2.6
1	X	2409	A	2.6
3	A	225	ALA	2.6
3	A	243	GLY	2.6
3	A	33	LEU	2.5
1	X	2400	G	2.5
12	J	22	ALA	2.5
5	C	66	ASN	2.5
11	I	27	ASP	2.5
23	U	29	GLY	2.5
23	U	63	SER	2.5
1	X	940	G	2.5
1	X	1079	G	2.5
9	G	40	ASN	2.5
1	X	1753	A	2.5
21	S	94	VAL	2.5
4	B	204	ALA	2.5
17	O	21	ARG	2.5
23	U	21	ARG	2.5
1	X	1585	A	2.5
17	O	11	GLN	2.5
11	I	100	ARG	2.5
27	1	51	ARG	2.5
1	X	559	C	2.4
1	X	1086	C	2.4
2	Y	29	C	2.4
6	D	43	SER	2.4
12	J	18	MET	2.4
1	X	2174	G	2.4
3	A	208	LYS	2.4
20	R	102	LYS	2.4
9	G	110	LEU	2.4
5	C	75	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	L	19	THR	2.4
1	X	75	C	2.4
1	X	180	C	2.4
1	X	652	C	2.4
20	R	4	PRO	2.4
1	X	192	G	2.4
1	X	361	G	2.4
23	U	8	THR	2.4
27	1	23	THR	2.4
29	3	55	TRP	2.4
20	R	79	SER	2.4
1	X	387	A	2.4
1	X	1428	G	2.4
21	S	108	VAL	2.4
14	L	99	ARG	2.4
9	G	162	LYS	2.4
1	X	169	C	2.3
1	X	1468	A	2.3
1	X	1516	A	2.3
1	X	2267	A	2.3
1	X	2344	G	2.3
5	C	53	LYS	2.3
17	O	23	GLU	2.3
9	G	90	LEU	2.3
19	Q	88	ILE	2.3
1	X	2290	A	2.3
11	I	12	SER	2.3
7	E	43	VAL	2.3
1	X	1847	G	2.3
11	I	109	LEU	2.3
12	J	82	THR	2.3
1	X	1078	A	2.3
16	N	83	LEU	2.3
9	G	98	LYS	2.3
11	I	28	LYS	2.3
11	I	55	ARG	2.3
1	X	413	G	2.3
1	X	1656	U	2.3
1	X	2774	U	2.3
13	K	52	ILE	2.3
5	C	190	ALA	2.3
21	S	24	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	X	665	A	2.3
1	X	583	C	2.3
11	I	45	LYS	2.3
3	A	222	ARG	2.3
11	I	82	ASP	2.3
14	L	18	ARG	2.3
20	R	43	ASP	2.3
3	A	272	THR	2.2
6	D	38	GLU	2.2
3	A	242	ALA	2.2
7	E	17	VAL	2.2
15	M	34	ARG	2.2
16	N	2	PRO	2.2
1	X	1071	U	2.2
1	X	843	G	2.2
1	X	655	A	2.2
2	Y	27	A	2.2
20	R	89	GLY	2.2
22	T	8	GLY	2.2
1	X	1077	U	2.2
1	X	406	G	2.2
1	X	1543	G	2.2
21	S	22	VAL	2.2
21	S	30	VAL	2.2
21	S	92	VAL	2.2
11	I	11	GLY	2.2
21	S	143	ILE	2.2
26	Z	40	LYS	2.2
7	E	69	ARG	2.1
14	L	33	ARG	2.1
1	X	1059	A	2.1
1	X	1355	A	2.1
3	A	36	ALA	2.1
13	K	33	ARG	2.1
16	N	12	ARG	2.1
1	X	45	C	2.1
1	X	1472	C	2.1
2	Y	111	C	2.1
8	F	127	VAL	2.1
11	I	118	VAL	2.1
5	C	174	GLY	2.1
1	X	2778	U	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	L	104	ALA	2.1
21	S	23	ALA	2.1
14	L	41	GLN	2.1
1	X	247	A	2.1
1	X	1888	C	2.1
28	2	33	ARG	2.1
10	H	64	VAL	2.1
12	J	124	HIS	2.1
27	1	17	GLY	2.1
1	X	984	A	2.1
1	X	1429	A	2.1
2	Y	68	A	2.1
5	C	188	ILE	2.1
3	A	252	LYS	2.1
27	1	16	ALA	2.1
29	3	50	LEU	2.1
1	X	2271	C	2.1
1	X	2628	C	2.1
13	K	82	GLU	2.1
1	X	1106	A	2.0
1	X	1588	A	2.0
1	X	1867	A	2.0
14	L	97	HIS	2.0
22	T	6	GLY	2.0
12	J	83	ARG	2.0
11	I	108	LEU	2.0
1	X	641	G	2.0
1	X	1062	G	2.0
1	X	1085	G	2.0
1	X	2567	G	2.0
1	X	1112	U	2.0
3	A	149	PRO	2.0
3	A	248	THR	2.0
1	X	2289	A	2.0
30	4	26	ILE	2.0
3	A	201	HIS	2.0
1	X	1779	C	2.0
1	X	2237	C	2.0
1	X	2446	C	2.0
1	X	871	U	2.0
1	X	1909	U	2.0
6	D	146	VAL	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.

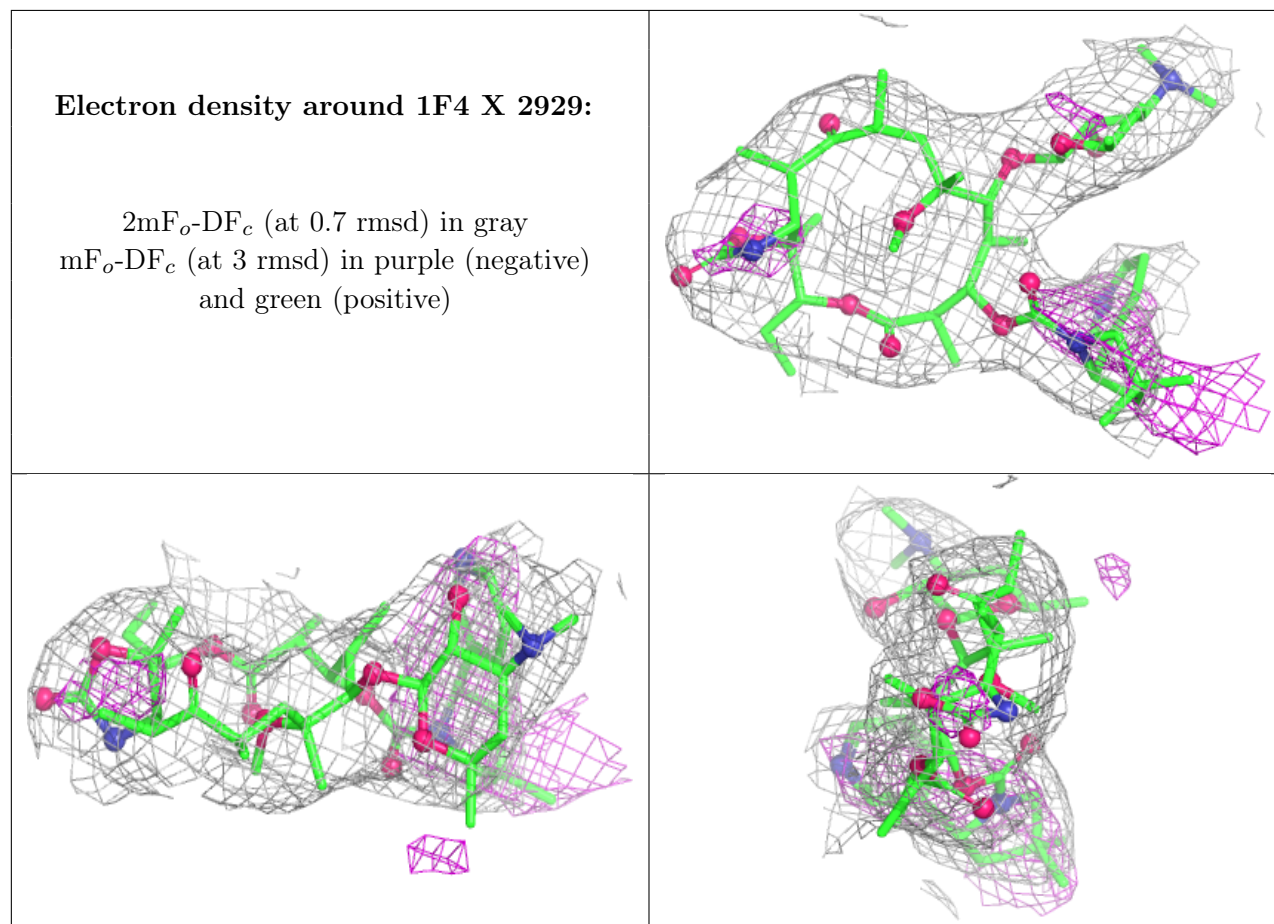
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	Y	204	1/1	0.20	0.51	86,86,86,86	0
31	MG	X	2909	1/1	0.25	0.45	97,97,97,97	0
31	MG	Y	202	1/1	0.49	0.92	88,88,88,88	0
31	MG	X	2924	1/1	0.53	0.79	70,70,70,70	0
31	MG	X	2903	1/1	0.65	1.03	89,89,89,89	0
31	MG	Y	206	1/1	0.67	0.11	78,78,78,78	0
31	MG	X	2913	1/1	0.68	2.56	60,60,60,60	0
31	MG	X	2920	1/1	0.68	0.81	113,113,113,113	0
31	MG	X	2917	1/1	0.70	0.62	55,55,55,55	0
31	MG	X	2928	1/1	0.73	1.28	61,61,61,61	0
31	MG	X	2906	1/1	0.75	0.75	58,58,58,58	0
31	MG	M	201	1/1	0.75	0.47	23,23,23,23	0
31	MG	X	2910	1/1	0.77	0.41	41,41,41,41	0
31	MG	X	2905	1/1	0.78	0.46	65,65,65,65	0
31	MG	X	2907	1/1	0.79	0.77	51,51,51,51	0
31	MG	X	2902	1/1	0.80	0.17	94,94,94,94	0
31	MG	Y	201	1/1	0.80	0.17	98,98,98,98	0
31	MG	X	2914	1/1	0.83	0.40	27,27,27,27	0
31	MG	X	2922	1/1	0.85	0.89	44,44,44,44	0
31	MG	X	2912	1/1	0.86	0.54	71,71,71,71	0
31	MG	X	2925	1/1	0.86	0.20	122,122,122,122	0
31	MG	X	2919	1/1	0.87	0.60	30,30,30,30	0
31	MG	X	2918	1/1	0.88	0.84	42,42,42,42	0
31	MG	X	2915	1/1	0.88	1.64	57,57,57,57	0
31	MG	X	2927	1/1	0.88	0.64	64,64,64,64	0
31	MG	X	2911	1/1	0.89	0.35	68,68,68,68	0
31	MG	X	2921	1/1	0.89	0.82	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	2923	1/1	0.90	0.47	34,34,34,34	0
31	MG	X	2926	1/1	0.90	0.88	45,45,45,45	0
31	MG	X	2908	1/1	0.90	0.73	37,37,37,37	0
31	MG	X	2916	1/1	0.93	0.96	37,37,37,37	0
31	MG	Y	203	1/1	0.94	0.41	59,59,59,59	0
32	1F4	X	2929	58/58	0.94	0.09	20,20,20,20	0
31	MG	Y	205	1/1	0.96	0.19	82,82,82,82	0
31	MG	X	2901	1/1	0.97	1.85	50,50,50,50	0
31	MG	X	2904	1/1	0.97	0.11	110,110,110,110	0

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



6.5 Other polymers ⓘ

There are no such residues in this entry.