



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:32 PM BST

PDB ID : 3JAQ
EMDB ID: : EMD-3049
Title : Structure of a partial yeast 48S preinitiation complex in open conformation
Authors : Llacer, J.L.; Hussain, T.; Ramakrishnan, V.
Deposited on : 2015-06-18
Resolution : 6.00 Å(reported)
Based on PDB ID : 1YFG, 2D74, 3CW2, 3J81, 4U1E

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

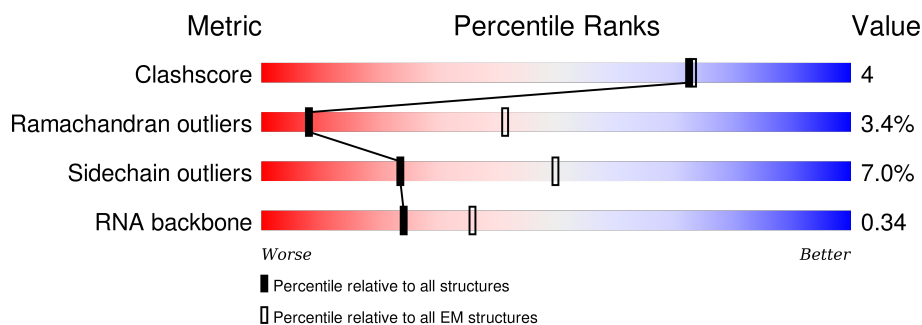
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.00 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.














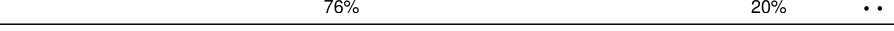







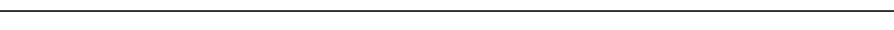

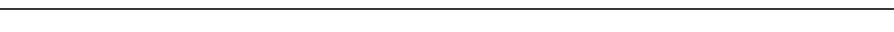
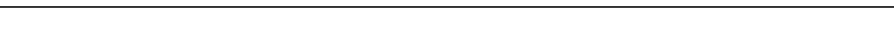


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1	75	35% 52% 13%
2	2	1781	43% 46% 11%
3	3	25	8% 92%
4	A	254	67% 15% 18%
5	B	255	72% 13% • 13%
6	C	259	71% 11% • 16%
7	D	237	78% 16% 6%
8	E	261	82% 17% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	F	227	
10	G	236	
11	H	190	
12	I	201	
13	J	188	
14	K	106	
15	L	156	
16	M	134	
17	N	151	
18	O	137	
19	P	142	
20	Q	143	
21	R	136	
22	S	146	
23	T	144	
24	U	117	
25	V	87	
26	W	130	
27	X	145	
28	Y	135	
29	Z	108	
30	a	119	
31	b	82	
32	c	67	
33	d	56	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	e	63	
35	f	150	
36	g	326	
37	h	25	
38	i	153	
39	j	304	
40	k	527	
41	l	285	
42	m	108	
43	o	92	
44	p	88	
45	q	347	
46	r	34	
47	s	52	

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 89768 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Met-tRNAi.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	75	Total	C	N	O	P	0	0
			1639	734	298	531	76		

- Molecule 2 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1780	Total	C	N	O	P	0	0
			37797	16892	6658	12467	1780		

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	2	Total	C	N	O	P	0	0
			42	19	7	14	2		

- Molecule 4 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	208	Total	C	N	O	S	0	0
			1626	1040	286	298	2		

- Molecule 5 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	222	Total	C	N	O	S	0	0
			1769	1117	324	325	3		

- Molecule 6 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	217	Total	C	N	O	S	0	0
			1629	1041	287	297	4		

- Molecule 7 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	223	Total	C	N	O	S	0	0
			1744	1108	313	318	5		

- Molecule 8 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	260	Total	C	N	O	S	0	0
			2078	1322	393	359	4		

- Molecule 9 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 10 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	226	Total	C	N	O	S	0	0
			1812	1134	348	326	4		

- Molecule 11 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	184	Total	C	N	O	S	0	0
			1483	950	270	263			

- Molecule 12 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	188	Total	C	N	O	S	0	0
			1489	923	300	265	1		

- Molecule 13 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	182	Total	C	N	O	S	0	0
			1471	929	287	254	1		

- Molecule 14 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	96	Total	C	N	O	S	0	0
			809	533	129	146	1		

- Molecule 15 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	155	Total	C	N	O	S	0	0
			1248	798	237	210	3		

- Molecule 16 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	117	Total	C	N	O	S	0	0
			885	553	161	171			

- Molecule 17 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	150	Total	C	N	O	S	0	0
			1187	756	223	206	2		

- Molecule 18 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	127	Total	C	N	O	S	0	0
			942	578	188	173	3		

- Molecule 19 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	119	Total	C	N	O	S	0	0
			943	604	171	163	5		

- Molecule 20 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	141	Total	C	N	O	S	0	0
			1105	709	204	192			

- Molecule 21 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	111	Total	C	N	O	S	0	0
			892	554	165	170	3		

- Molecule 22 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	145	Total	C	N	O	S	0	0
			1193	741	240	210	2		

- Molecule 23 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	143	Total	C	N	O	S	0	0
			1110	693	210	207			

- Molecule 24 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	106	Total	C	N	O	S	0	0
			845	540	152	152	1		

- Molecule 25 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	87	Total	C	N	O	S	0	0
			687	424	126	135	2		

- Molecule 26 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	129	Total	C	N	O	S	0	0
			1021	651	187	180	3		

- Molecule 27 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	144	Total	C	N	O	S	0	0
			1119	708	218	191	2		

- Molecule 28 is a protein called eS24.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	Y	134	Total	C	N	O		
			1061	665	207	189	0	0

- Molecule 29 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	70	Total	C	N	O	S		
			558	355	104	98	1	0	0

- Molecule 30 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	98	Total	C	N	O	S		
			779	480	165	129	5	0	0

- Molecule 31 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	81	Total	C	N	O	S		
			609	379	112	113	5	0	0

- Molecule 32 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	62	Total	C	N	O	S		
			487	301	97	88	1	0	0

- Molecule 33 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	53	Total	C	N	O	S		
			446	280	89	76	1	0	0

- Molecule 34 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	54	Total	C	N	O	S		
			433	271	88	73	1	0	0

- Molecule 35 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	69	Total	C	N	O	S	0	0
			549	352	102	91	4		

- Molecule 36 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	318	Total	C	N	O	S	0	0
			2466	1561	430	470	5		

- Molecule 37 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 38 is a protein called eIF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	95	Total	C	N	O	S	0	0
			765	475	142	143	5		

- Molecule 39 is a protein called eIF2 alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	249	Total	C	N	O	S	0	0
			2006	1283	333	382	8		

- Molecule 40 is a protein called eIF2 gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	396	Total	C	N	O	S	0	0
			3034	1932	542	544	16		

- Molecule 41 is a protein called eIF2 beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	128	Total	C	N	O	S	0	0
			1036	661	186	182	7		

- Molecule 42 is a protein called eIF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	86	Total	C	N	O	S	0	0
			695	439	128	124	4		

- Molecule 43 is a protein called eIF3a.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	o	92	Total	C	N	O	0	0
			460	276	92	92		

- Molecule 44 is a protein called eIF3c.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	p	88	Total	C	N	O	0	0
			440	264	88	88		

- Molecule 45 is a protein called eIF3i.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	342	Total	C	N	O	S	0	0
			2693	1711	443	530	9		

- Molecule 46 is a protein called eIF3b.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	r	34	Total	C	N	O	S	0	0
			300	192	52	54	2		

- Molecule 47 is a protein called eIF3g.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	s	52	Total	C	N	O	0	0
			418	257	82	79		

- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	2	79	Total	Mg	0
			79	79	
48	Q	1	Total	Mg	0
			1	1	
48	C	1	Total	Mg	0
			1	1	

Continued on next page...

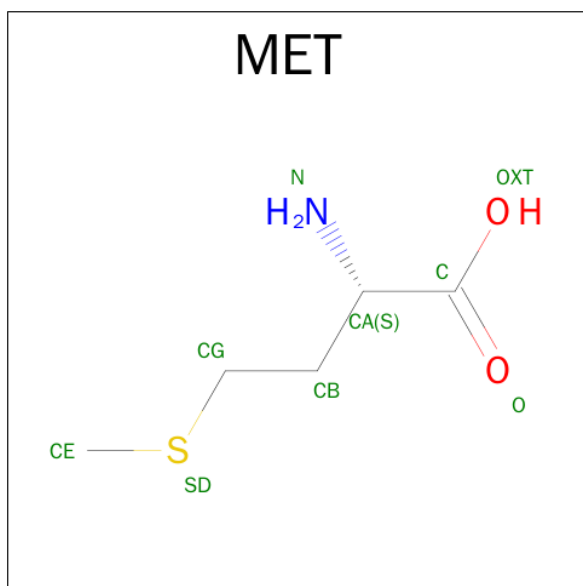
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
48	k	1	Total	Mg	0
			1	1	

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

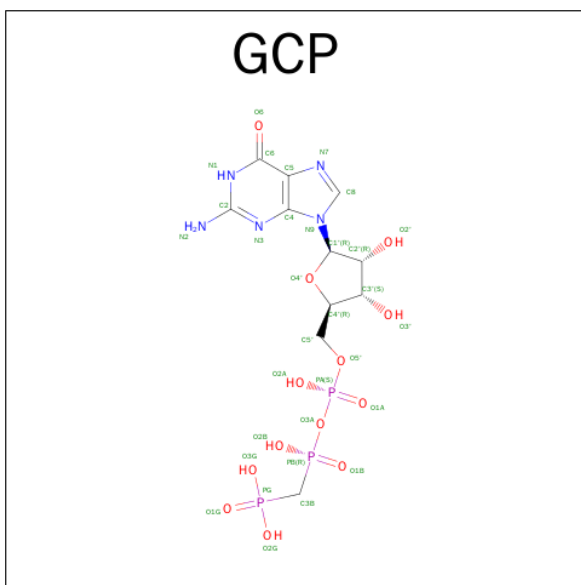
Mol	Chain	Residues	Atoms		AltConf
49	b	1	Total	Zn	0
			1	1	
49	a	1	Total	Zn	0
			1	1	
49	l	1	Total	Zn	0
			1	1	
49	f	1	Total	Zn	0
			1	1	

- Molecule 50 is METHIONINE (three-letter code: MET) (formula: C₅H₁₁NO₂S).



Mol	Chain	Residues	Atoms					AltConf
50	k	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 51 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).

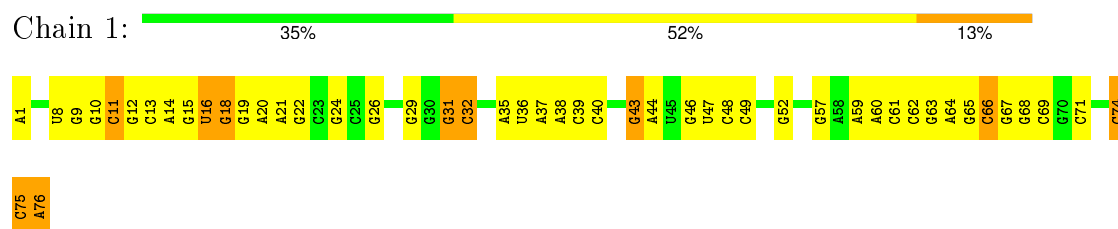


Mol	Chain	Residues	Atoms					AltConf
51	k	1	Total	C	N	O	P	0
			32	11	5	13	3	

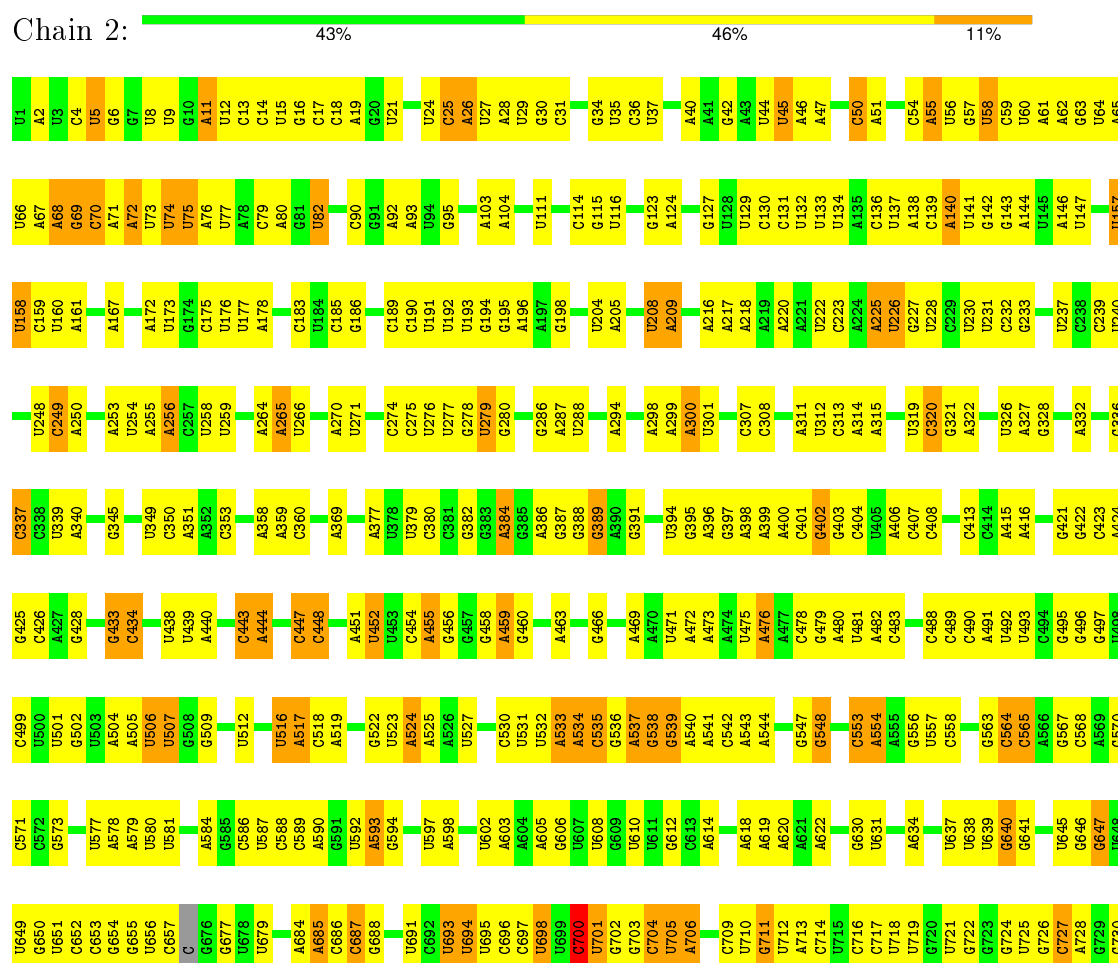
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Met-tRNAi



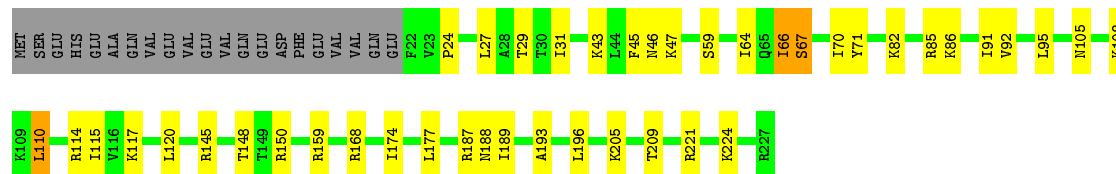
• Molecule 2: 18S rRNA




U1797	A1798	C1635	G1636	C1637	C1638	C1639	G1640	A1646	G1647	C1655	G1656	U1736	A1737	C1651	G1655	G1656	U1748	G1749	U1750	A1754	G1755	C1658	G1659	G1660	G1661	G1662	U1663	G1664	C1668	A1669	G1670	A1761	C1672	C1675	A1764	G1765	G1766	U1767	U1768	U1769	C1770	U1773	A1774	G1775	G1776	U1777	G1778	A1779	C1781	G1782	G1786	U1787	A1788	U1789	C1790	G1791	A1792	U1793	A1794	U1795	U1796	C1799	G1797	A1798	C1799	G1797	A1798	U1799	C1800	G1801	A1802	U1803	C1804	G1805	U1806	A1807	C1808	G1809	U1810	C1811	G1812	U1813	A1814	C1815	G1816	U1817	A1818	C1819	G1820	U1821	A1822	C1823	G1824	U1825	A1826	C1827	G1828	U1829	A1830	C1831	G1832	U1833	A1834	C1835	G1836	U1837	A1838	C1839	G1840	U1841	A1842	C1843	G1844	U1845	A1846	C1847	G1848	U1849	A1850	C1851	G1852	U1853	A1854	C1855	G1856	U1857	A1858	C1859	G1860	U1861	A1862	C1863	G1864	U1865	A1866	C1867	G1868	U1869	A1870	C1871	G1872	U1873	A1874	C1875	G1876	U1877	A1878	C1879	G1880	U1881	A1882	C1883	G1884	U1885	A1886	C1887	G1888	U1889	A1890	C1891	G1892	U1893	A1894	C1895	G1896	U1897	A1898	C1899	G1900	U1901	A1902	C1903	G1904	U1905	A1906	C1907	G1908	U1909	A1910	C1911	G1912	U1913	A1914	C1915	G1916	U1917	A1918	C1919	G1920	U1921	A1922	C1923	G1924	U1925	A1926	C1927	G1928	U1929	A1930	C1931	G1932	U1933	A1934	C1935	G1936	U1937	A1938	C1939	G1940	U1941	A1942	C1943	G1944	U1945	A1946	C1947	G1948	U1949	A1950	C1951	G1952	U1953	A1954	C1955	G1956	U1957	A1958	C1959	G1960	U1961	A1962	C1963	G1964	U1965	A1966	C1967	G1968	U1969	A1970	C1971	G1972	U1973	A1974	C1975	G1976	U1977	A1978	C1979	G1980	U1981	A1982	C1983	G1984	U1985	A1986	C1987	G1988	U1989	A1990	C1991	G1992	U1993	A1994	C1995	G1996	U1997	A1998	C1999	G2000	U2001	A2002	C2003	G2004	U2005	A2006	C2007	G2008	U2009	A2010	C2011	G2012	U2013	A2014	C2015	G2016	U2017	A2018	C2019	G2020	U2021	A2022	C2023	G2024	U2025	A2026	C2027	G2028	U2029	A2030	C2031	G2032	U2033	A2034	C2035	G2036	U2037	A2038	C2039	G2040	U2041	A2042	C2043	G2044	U2045	A2046	C2047	G2048	U2049	A2050	C2051	G2052	U2053	A2054	C2055	G2056	U2057	A2058	C2059	G2060	U2061	A2062	C2063	G2064	U2065	A2066	C2067	G2068	U2069	A2070	C2071	G2072	U2073	A2074	C2075	G2076	U2077	A2078	C2079	G2080	U2081	A2082	C2083	G2084	U2085	A2086	C2087	G2088	U2089	A2090	C2091	G2092	U2093	A2094	C2095	G2096	U2097	A2098	C2099	G2100	U2101	A2102	C2103	G2104	U2105	A2106	C2107	G2108	U2109	A2110	C2111	G2112	U2113	A2114	C2115	G2116	U2117	A2118	C2119	G2120	U2121	A2122	C2123	G2124	U2125	A2126	C2127	G2128	U2129	A2130	C2131	G2132	U2133	A2134	C2135	G2136	U2137	A2138	C2139	G2140	U2141	A2142	C2143	G2144	U2145	A2146	C2147	G2148	U2149	A2150	C2151	G2152	U2153	A2154	C2155	G2156	U2157	A2158	C2159	G2160	U2161	A2162	C2163	G2164	U2165	A2166	C2167	G2168	U2169	A2170	C2171	G2172	U2173	A2174	C2175	G2176	U2177	A2178	C2179	G2180	U2181	A2182	C2183	G2184	U2185	A2186	C2187	G2188	U2189	A2190	C2191	G2192	U2193	A2194	C2195	G2196	U2197	A2198	C2199	G2200	U2201	A2202	C2203	G2204	U2205	A2206	C2207	G2208	U2209	A2210	C2211	G2212	U2213	A2214	C2215	G2216	U2217	A2218	C2219	G2220	U2221	A2222	C2223	G2224	U2225	A2226	C2227	G2228	U2229	A2230	C2231	G2232	U2233	A2234	C2235	G2236	U2237	A2238	C2239	G2240	U2241	A2242	C2243	G2244	U2245	A2246	C2247	U2248	A2249	C2250	G2251	U2252	A2253	C2254	G2255	U2256	A2257	C2258	G2259	U2260	A2261	C2262	G2263	U2264	A2265	C2266	G2267	U2268	A2269	C2270	G2271	U2272	A2273	C2274	G2275	U2276	A2277	C2278	G2279	U2280	A2281	C2282	G2283	U2284	A2285	C2286	G2287	U2288	A2289	C2290	G2291	U2292	A2293	C2294	G2295	U2296	A2297	C2298	G2299	U2300	A2301	C2302	G2303	U2304	A2305	C2306	U2307	A2308	C2309	G2310	U2311	A2312	C2313	U2314	A2315	C2316	G2317	U2318	A2319	C2320	G2321	U2322	A2323	C2324	G2325	U2326	A2327	C2328	G2329	U2330	A2331	C2332	G2333	U2334	A2335	C2336	G2337	U2338	A2339	C2340	U2341	A2342	C2343	G2344	U2345	A2346	C2347	U2348	A2349	C2350	G2351	U2352	A2353	C2354	G2355	U2356	A2357	C2358	G2359	U2360	A2361	C2362	G2363	U2364	A2365	C2366	G2367	U2368	A2369	C2370	G2371	U2372	A2373	C2374	G2375	U2376	A2377	C2378	G2379	U2380	A2381	C2382	G2383	U2384	A2385	C2386	G2387	U2388	A2389	C2390	G2391	U2392	A2393	C2394	G2395	U2396	A2397	C2398	G2399	U2400	A2401	C2402	G2403	U2404	A2405	C2406	G2407	U2408	A2409	C2410	G2411	U2412	A2413	C2414	G2415	U2416	A2417	C2418	G2419	U2420	A2421	C2422	G2423	U2424	A2425	C2426	G2427	U2428	A2429	C2430	G2431	U2432	A2433	C2434	G2435	U2436	A2437	C2438	G2439	U2440	A2441	C2442	G2443	U2444	A2445	C2446	U2447	A2448	C2449	U2450	A2451	C2452	U2453	A2454	C2455	U2456	A2457	C2458	U2459	A2460	C2461	U2462	A2463	C2464	U2465	A2466	C2467	U2468	A2469	C2470	U2471	A2472	C2473	U2474	A2475	C2476	U2477	A2478	C2479	U2480	A2481	C2482	U2483	A2484	C2485	U2486	A2487	C2488	U2489	A2490	C2491	U2492	A2493	C2494	U2495	A2496	C2497	U2498	A2499	C2500	U2501	A2502	C2503	U2504	A2505	C2506	U2507	A2508	C2509	U2510	A2511	C2512	U2513	A2514	C2515	U2516	A2517	C2518	U2519	A2520	C2521	U2522	A2523	U2524	A2525	C2526	U2527	A2528	C2529	U2530	A2531	C2532	U2533	A2534	C2535	U2536	A2537	C2538	U2539	A2540	C2541	U2542	A2543	C2544	U2545	A2546	C2547	U2548	A2549	C2550	U2551	A2552	C2553	U2554	A2555	C2556	U2557	A2558	C2559	U2560	A2561	C2562	U2563	A2564	C2565	U2566	A2567	C2568	U2569	A2570	C2571	U2572	A2573	C2574	U2575	A2576	C2577	U2578	A2579	C2580	U2581	A2582	C2583	U2584	A2585	C2586	U2587	A2588	C2589	U2590	A2591	C2592	U2593	A2594	C2595	U2596	A2597	C2598	U2599	A2600	C2601	U2602	A2603	C2604	U2605	A2606	C2607	U2608	A2609	C2610	U2611	A2612	C2613	U2614	A2615	C2616	U2617	A2618	C2619	U2620	A2621	C2622	U2623	A2624	C2625	U2626	A2627	C2628	U2629	A2630	C2631	U2632	A2633	C2634	U2635	A2636	C2637	U2638	A2639	C2640	U2641	A2642	C2643	U2644	A2645	C2646	U2647	A2648	C2649	U2650	A2651	C2652	U2653	A2654	C2655	U2656	A2657	C2658	U2659	A2660	C2661	U2662	A2663	C2664	U2665	A2666	C2667	U2668	A2669	C2670	U2671	A2672	C2673	U2674	A2675	C2676	U2677	A2678	C2679	U2680	A2681	C2682	U2683	A2684	C2685	U2686	A2687	C2688	U2689	A2690	C2691	U2692	A2693	C2694	U2695	A2696	C2697	U2698	A2699	C2700	U2701	A2702	C2703	U2704	A2705	C2706	U2707	A2708	C2709	U2710	A2711	C2712	U2713	A2714	C2715	U2716	A2717	C2718	U2719	A2720	C2721	U2722	A2723	C2724	U2725	A2726	C2727	U2728	A2729	C2730	U2731	A2732	C2733	U2734	A2735	C2736	U2737	A2738	C2739	U2740	A2741	C2742	U2743	A2744	C2745	U2746	A2747	C2748	U2749	A2750	C2751	U2752	A2753	C2754	U2755	A2756	C2757	U2758	A2759	C2760	U2761	A2762	C2763	U2764	A2765	C2766	U2767	A2768	C2769	U2770	A2771	C2772	U2773	A2774	C2775	U2776	A2777	C2778	U2779	A2780	C2781	U2782	A2783	C2784	U2785	A2786	C2787	U2788	A2789	C2790	U2791	A2792	C2793	U2794	A2795	C2796	U2797	A2798	C2799	U2800	A2801	C2802	U2803	A2804	C2805	U2806	A2807	C2808	U2809	A2810	C2811	U2812	A2813	C2814	U2815	A2816	C2817	U2818	A2819	C2820	U2821	A2822	C2823	U2824	A2825	C2826	U2827	A2828	C2829	U2830	A2831	C2832	U2833	A2834	C2835	U2836	A2837	C2838	U2839	A2840	C2841	U2842	A2843	C2844	U2845	A2846	C2847	U2848	A2849	C2850	U2851	A2852	C2853	U2854	A2855	C2856	U2857	A2858	C2859	U2860	A2861	C2862	U2863	A2864	C2865	U2866	A2867	C2868	U2869	A2870	C2871	U2872	A2873	C2874	U2875	A2876	C2877	U2878	A2879	C2880	U2881	A2882	C2883	U2884	A2885	C2886	U2887	A2888	C2889	U2890	A2891	C2892	U2893	A2894	C2895	U2896	A2897	C2898	U2899	A2900	C2901	U2902	A2903	C2904	U2905	A2906	C2907	U2908	A2909	C2910	U2911	A2912	C2913	U2914	A2915	C2916	U2917	A2918	C2919	U2920	A2921	C2922	U2923	A2924	C2925	U2926	A2927	C2928	U2929	A2930	C2931	U2932	A2933	C2934	U2935	A2936	C2937	U2938	A2939	C2940	U2941	A2942	C2943	U2944	A2945	C2946	U2947	A2948	C2949	U2950	A2951	C2952	U2953	A2954	C2955	U2956	A2957	C2958	U2959	A2960	C2961	U2962	A2963	C2964	U2965	A2966	C2967	U2968	A2969	C2970	U2971	A2972	C2973	U2974	A2975	C2976	U2977	A2978	C2979	U2980	A2981	C2982	U2983	A2984	C2985	U2986	A2987	C2988	U2989	A2990	C2991	U2992	A2993	C2994	U2995	A2996	C2997	U2998	A2999	C3000	U3001	A3002	C3003	U3004	A3005	C3006	U3007	A3008	C3009	U3010	A3011	C3012	U3013	A3014	C3015	U3016	A3017	C3018	U3019	A3020	C3021	U3022	A3023	C3024	U3025	A3026	C3027	U3028	A3029	C3030	U3031	A3032	C3033	U3034	A3035	C3036	U3037	A3038	C3039	U3040	A3041	C3042	U3043	A3044	C3045	U3046	A3047	C3048	U304
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	------

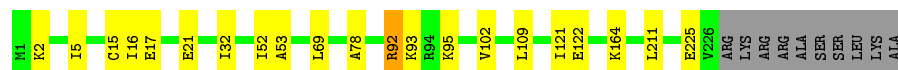
- Molecule 9: uS7

Chain F: 




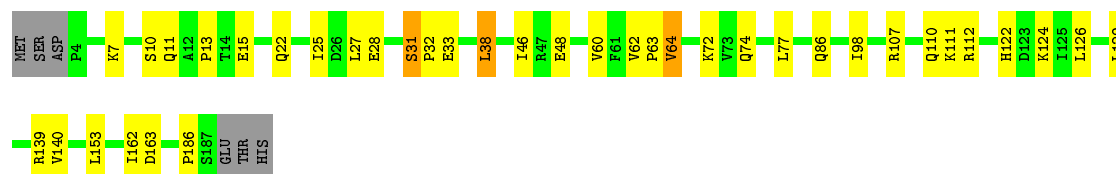
- Molecule 10: eS6

Chain G: 




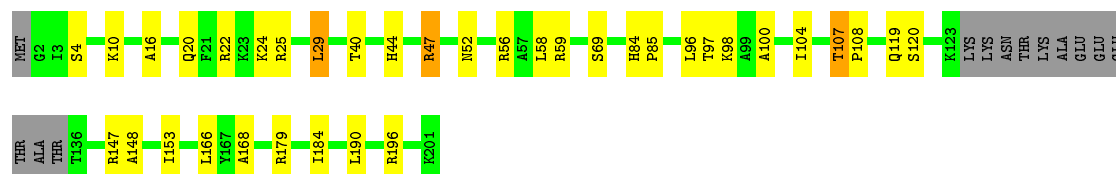
- Molecule 11: eS7

Chain H: 




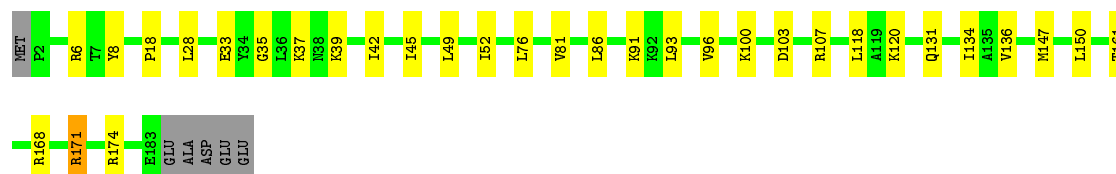
- Molecule 12: eS8

Chain I: 



- Molecule 13: uS4

Chain J: 

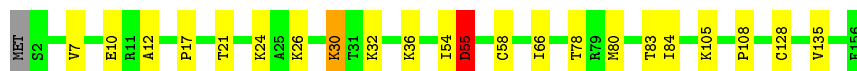
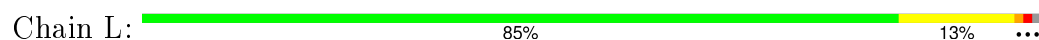


- Molecule 14: eS10

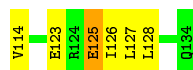
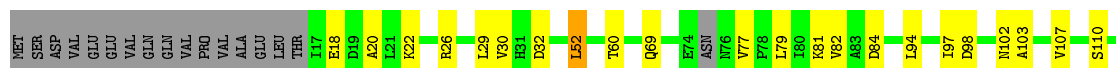
Chain K: 



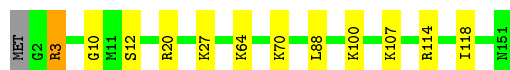
- Molecule 15: uS17



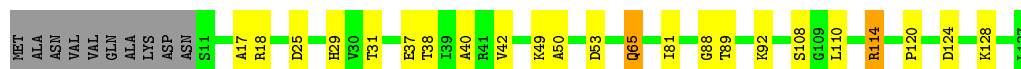
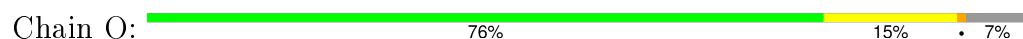
- Molecule 16: eS12



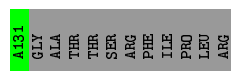
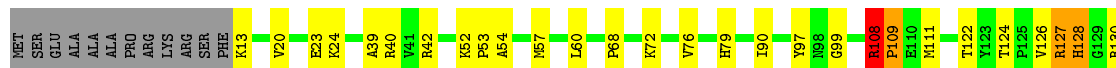
- Molecule 17: uS15



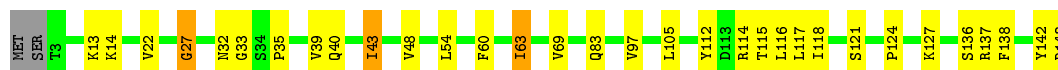
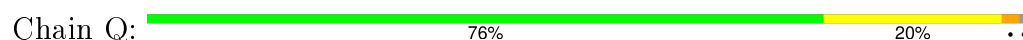
- Molecule 18: uS11



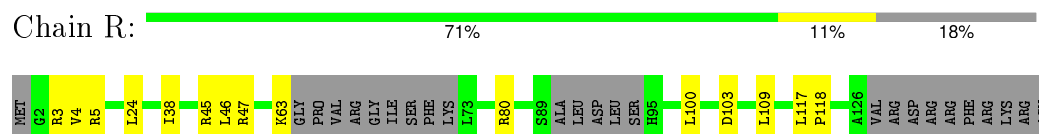
- Molecule 19: uS19



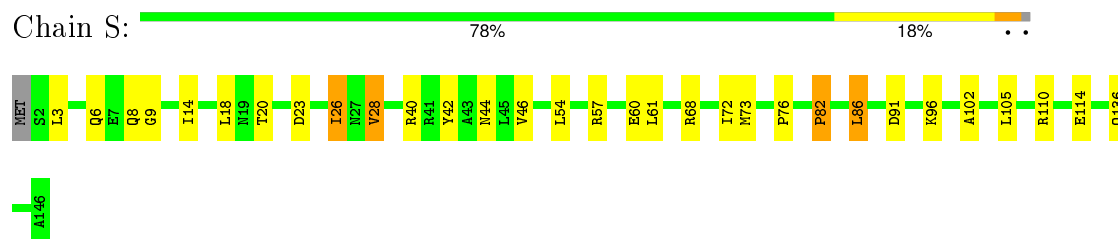
- Molecule 20: uS9



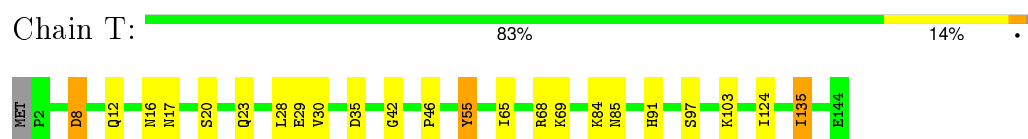
- Molecule 21: eS17



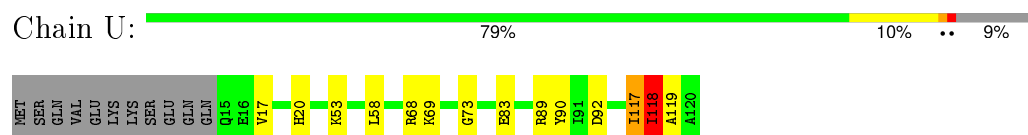
- Molecule 22: uS13



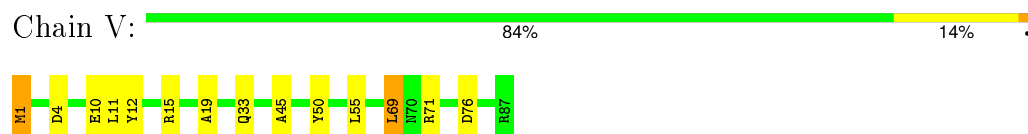
- Molecule 23: eS19



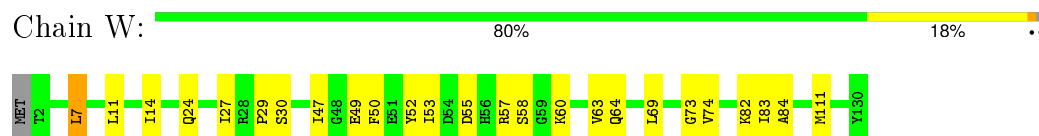
- Molecule 24: uS10



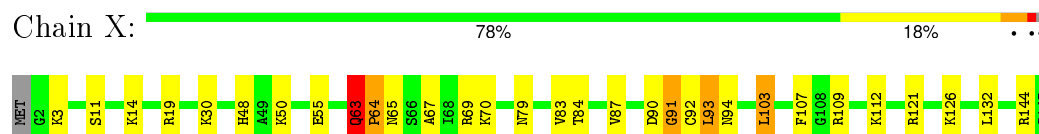
- Molecule 25: eS21




- Molecule 26: uS8



- Molecule 27: uS12



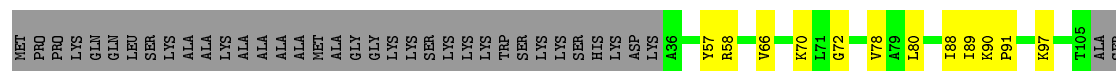
- Molecule 28: eS24

Chain Y:  84% 15% ..



- Molecule 29: eS25

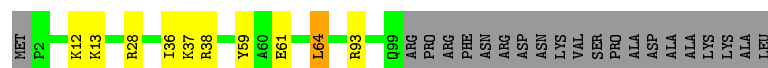
Chain Z:  54% 11% 35%



GLU

- Molecule 30: eS26

Chain a:  74% 8% 18%




- Molecule 31: eS27

Chain b:  93% 6% .




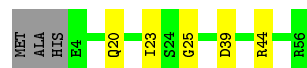
- Molecule 32: eS28

Chain c:  87% 6% 7%



- Molecule 33: uS14

Chain d:  86% 9% 5%




- Molecule 34: eS30

Chain e:  75% 11% 14%



- Molecule 35: eS31

Chain f:  37% 9% 54%

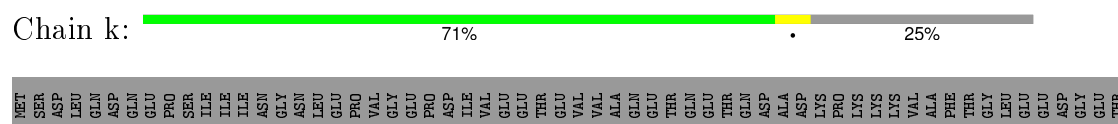
- Molecule 36: RACK1

- Molecule 37: eL41

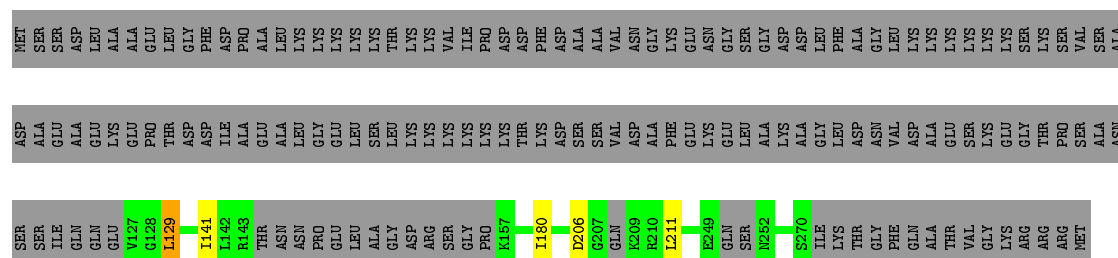
- Molecule 38: eIF1A

- Molecule 39: eIF2 alpha

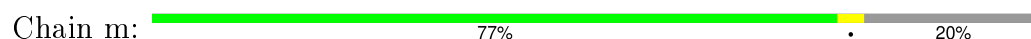
- Molecule 40: eIF2 gamma



- Molecule 41: eIF2 beta



- Molecule 42: eIF1



- Molecule 43: eIF3a



There are no outlier residues recorded for this chain.

- Molecule 44: eIF3c



There are no outlier residues recorded for this chain.

- Molecule 45: eIF3i



- Molecule 46: eIF3b



There are no outlier residues recorded for this chain.

- Molecule 47: eIF3g

Chain s:  98% .



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	4547	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	27	Depositor
Minimum defocus (nm)	4000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, H2U, 7MG, MG, GCP, 2MG, 5MC, 1MA, M2G, T6A, 1MG, RIA

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	1	0.45	2/1530 (0.1%)	0.76	4/2380 (0.2%)
10	G	0.38	0/1835	0.60	0/2451
11	H	0.41	0/1507	0.62	0/2028
12	I	0.41	0/1515	0.63	2/2029 (0.1%)
13	J	0.40	0/1495	0.67	2/2001 (0.1%)
14	K	0.46	0/831	0.61	0/1123
15	L	0.42	0/1276	0.58	0/1718
16	M	0.40	0/891	0.65	0/1201
17	N	0.39	0/1210	0.60	0/1628
18	O	0.39	0/953	0.61	0/1279
19	P	0.41	0/962	0.62	0/1294
2	2	0.24	0/42269	0.65	5/65862 (0.0%)
20	Q	0.41	0/1125	0.62	0/1510
21	R	0.39	0/899	0.60	0/1204
22	S	0.40	0/1212	0.66	0/1629
23	T	0.40	0/1129	0.58	0/1520
24	U	0.39	0/857	0.61	0/1158
25	V	0.38	0/696	0.61	0/938
26	W	0.40	0/1039	0.64	1/1399 (0.1%)
27	X	0.42	0/1137	0.66	2/1516 (0.1%)
28	Y	0.40	0/1075	0.59	0/1433
29	Z	0.41	0/567	0.60	0/762
3	3	0.22	0/46	0.64	0/69
30	a	0.38	0/791	0.64	0/1059
31	b	0.39	0/619	0.62	0/837
32	c	0.37	0/489	0.65	0/655
33	d	0.43	0/457	0.58	0/607
34	e	0.40	0/440	0.61	0/586
35	f	0.45	0/562	0.72	1/751 (0.1%)
36	g	0.41	0/2521	0.58	0/3431
37	h	0.35	0/234	0.61	0/300
38	i	0.38	0/775	0.60	0/1034

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	j	0.41	0/2034	0.63	0/2737
4	A	0.42	0/1666	0.63	1/2279 (0.0%)
40	k	0.39	0/3079	0.60	0/4157
41	l	0.41	0/1051	0.57	0/1402
42	m	0.39	0/703	0.58	0/938
45	q	0.42	0/2757	0.57	0/3733
46	r	0.42	0/306	0.52	0/407
47	s	0.39	0/426	0.54	0/571
5	B	0.40	0/1793	0.61	0/2414
6	C	0.40	0/1659	0.59	0/2252
7	D	0.41	0/1769	0.61	0/2378
8	E	0.40	0/2122	0.62	1/2861 (0.0%)
9	F	0.40	0/1628	0.63	1/2198 (0.0%)
All	All	0.34	2/93937 (0.0%)	0.64	20/135719 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
27	X	0	1
28	Y	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1	A	OP3-P	-9.98	1.49	1.61
1	1	65	G	P-O5'	-6.66	1.53	1.59

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	f	126	PRO	CA-N-CD	-8.85	99.11	111.50
1	1	65	G	OP1-P-OP2	-8.39	107.01	119.60
2	2	685	A	C2'-C3'-O3'	6.95	124.81	113.70
12	I	29	LEU	CA-CB-CG	6.73	130.78	115.30
1	1	65	G	O5'-P-OP2	6.33	118.29	110.70
1	1	65	G	O5'-P-OP1	6.14	118.06	110.70
2	2	1198	G	C2'-C3'-O3'	5.85	123.07	113.70
13	J	49	LEU	CA-CB-CG	5.83	128.70	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	700	C	C2'-C3'-O3'	5.61	122.68	113.70
1	1	65	G	O5'-C5'-C4'	-5.54	101.17	111.70
12	I	190	LEU	CA-CB-CG	5.47	127.89	115.30
2	2	822	G	C2'-C3'-O3'	5.34	122.25	113.70
9	F	110	LEU	CA-CB-CG	5.32	127.52	115.30
4	A	201	LEU	CA-CB-CG	5.29	127.47	115.30
27	X	103	LEU	CA-CB-CG	5.18	127.22	115.30
2	2	279	U	C2'-C3'-O3'	5.13	121.91	113.70
27	X	93	LEU	CA-CB-CG	5.11	127.05	115.30
26	W	69	LEU	CA-CB-CG	5.10	127.03	115.30
8	E	189	LEU	CA-CB-CG	5.08	127.00	115.30
13	J	93	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	X	63	GLN	Peptide
28	Y	29	HIS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1639	0	851	18	0
2	2	37797	0	19015	349	0
3	3	42	0	22	0	0
4	A	1626	0	1633	9	0
5	B	1769	0	1829	12	0
6	C	1629	0	1710	9	0
7	D	1744	0	1826	14	0
8	E	2078	0	2157	13	0
9	F	1609	0	1679	14	0
10	G	1812	0	1911	6	0
11	H	1483	0	1579	10	0
12	I	1489	0	1504	14	0
13	J	1471	0	1554	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	K	809	0	810	10	0
15	L	1248	0	1311	10	0
16	M	885	0	917	9	0
17	N	1187	0	1251	2	0
18	O	942	0	979	6	0
19	P	943	0	989	12	0
20	Q	1105	0	1170	8	0
21	R	892	0	932	3	0
22	S	1193	0	1217	12	0
23	T	1110	0	1124	9	0
24	U	845	0	913	5	0
25	V	687	0	682	4	0
26	W	1021	0	1056	9	0
27	X	1119	0	1198	11	0
28	Y	1061	0	1111	7	0
29	Z	558	0	585	4	0
30	a	779	0	830	0	0
31	b	609	0	629	0	0
32	c	487	0	528	0	0
33	d	446	0	436	0	0
34	e	433	0	470	0	0
35	f	549	0	562	0	0
36	g	2466	0	2406	0	0
37	h	233	0	284	0	0
38	i	765	0	769	0	0
39	j	2006	0	2066	0	0
40	k	3034	0	3195	0	0
41	l	1036	0	1080	0	0
42	m	695	0	729	0	0
43	o	460	0	106	0	0
44	p	440	0	102	0	0
45	q	2693	0	2609	0	0
46	r	300	0	297	0	0
47	s	418	0	411	0	0
48	2	79	0	0	0	0
48	C	1	0	0	0	0
48	Q	1	0	0	0	0
48	k	1	0	0	0	0
49	a	1	0	0	0	0
49	b	1	0	0	0	0
49	f	1	0	0	0	0
49	l	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	k	8	0	8	0	0
51	k	32	0	14	0	0
All	All	89768	0	71046	540	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 4.

All (540) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1330:A:H2'	2:2:1331:C:H5'	1.34	1.08
2:2:534:A:H3'	2:2:535:C:H5''	1.36	1.02
2:2:1330:A:C2'	2:2:1331:C:H5'	1.89	1.02
2:2:1328:A:C2'	2:2:1329:G:H5'	1.90	1.01
2:2:1328:A:H2'	2:2:1329:G:H5'	1.40	1.01
2:2:1327:G:C2'	2:2:1328:A:H5'	1.92	1.00
1:1:16:H2U:OP2	1:1:60:A:C2	2.19	0.95
2:2:1534:G:O2'	2:2:1535:C:OP1	1.88	0.90
2:2:1589:C:H2'	2:2:1590:A:C8	2.07	0.90
2:2:1323:G:H2'	2:2:1324:A:C4'	2.06	0.85
2:2:1323:G:H3'	2:2:1324:A:H5''	1.57	0.85
2:2:475:U:H6	2:2:475:U:H5''	1.43	0.84
2:2:534:A:C3'	2:2:535:C:H5''	2.07	0.84
2:2:1108:G:H1	2:2:1135:U:H3	1.27	0.83
2:2:447:C:H2'	2:2:448:C:C6	2.13	0.82
2:2:1534:G:N3	2:2:1534:G:H5''	1.95	0.82
2:2:1327:G:H2'	2:2:1328:A:H5'	1.61	0.81
2:2:1327:G:O2'	2:2:1328:A:H5'	1.80	0.81
2:2:459:A:H3'	2:2:460:G:H8	1.47	0.79
2:2:1563:C:H3'	2:2:1564:U:H6	1.46	0.79
2:2:1191:C:H3'	2:2:1192:A:H5''	1.63	0.79
2:2:813:A:H61	2:2:856:U:H3	1.30	0.79
2:2:1119:U:H3	2:2:1126:G:H1	1.30	0.79
2:2:455:A:H2'	2:2:456:G:O4'	1.83	0.78
2:2:538:G:H21	2:2:539:G:H1	1.30	0.77
2:2:1589:C:H2'	2:2:1590:A:H8	1.44	0.77
2:2:157:U:H4'	2:2:158:U:OP1	1.84	0.77
2:2:1563:C:H5''	2:2:1563:C:H6	1.48	0.76
1:1:66:C:H2'	1:1:67:G:H8	1.51	0.75
2:2:536:G:H5'	2:2:537:A:OP2	1.86	0.75
2:2:1176:C:H4'	2:2:1188:A:H61	1.51	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:12:U:H4'	2:2:1298:G:H1'	1.69	0.75
2:2:71:A:H3'	2:2:72:A:H5''	1.70	0.74
1:1:66:C:H2'	1:1:67:G:C8	2.22	0.74
2:2:1086:A:H2'	2:2:1087:A:C8	2.23	0.74
2:2:1563:C:H2'	2:2:1564:U:C6	2.23	0.74
2:2:1323:G:C3'	2:2:1324:A:H5''	2.16	0.74
1:1:16:H2U:OP2	1:1:60:A:H2	1.67	0.73
2:2:737:A:HO2'	2:2:738:G:H8	1.37	0.73
2:2:1563:C:H3'	2:2:1564:U:C6	2.23	0.72
2:2:516:U:H3	2:2:534:A:H61	1.37	0.72
2:2:1533:U:H4'	2:2:1534:G:C4	2.24	0.72
2:2:1329:G:H2'	2:2:1330:A:O4'	1.89	0.72
2:2:1563:C:C3'	2:2:1564:U:H6	2.03	0.71
2:2:1563:C:C5'	2:2:1563:C:H6	2.03	0.71
2:2:1563:C:H5''	2:2:1563:C:C6	2.26	0.70
2:2:1223:A:H3'	2:2:1224:U:H5''	1.72	0.70
2:2:538:G:H4'	2:2:539:G:O5'	1.92	0.70
2:2:1240:G:H5'	2:2:1241:A:OP2	1.90	0.70
2:2:11:A:H2	2:2:1298:G:H21	1.40	0.68
2:2:388:G:H3'	2:2:389:G:H5''	1.75	0.67
2:2:475:U:C6	2:2:475:U:H5''	2.28	0.67
2:2:813:A:N6	2:2:856:U:H3	1.91	0.67
2:2:1166:G:H3'	2:2:1167:U:H5''	1.76	0.66
2:2:534:A:H5'	2:2:535:C:OP2	1.96	0.66
4:A:53:THR:HG22	4:A:161:PRO:HB2	1.77	0.66
2:2:1330:A:C3'	2:2:1331:C:H5'	2.26	0.65
2:2:1589:C:O2'	2:2:1590:A:O4'	2.09	0.65
2:2:1534:G:HO2'	2:2:1535:C:P	2.20	0.65
2:2:1240:G:H1'	19:P:79:HIS:CG	2.32	0.65
5:B:157:GLN:HB2	5:B:160:HIS:HD2	1.61	0.65
2:2:1584:A:H5''	20:Q:136:SER:HB2	1.78	0.65
2:2:1488:A:H4'	2:2:1489:C:H4'	1.80	0.64
2:2:444:A:H8	2:2:524:A:H5''	1.63	0.64
2:2:867:G:H1	2:2:959:U:H3	1.45	0.63
2:2:693:U:H4'	2:2:694:U:OP2	1.97	0.63
2:2:1345:A:H2'	2:2:1345:A:N3	2.12	0.63
2:2:444:A:H61	2:2:460:G:H21	1.44	0.63
2:2:592:U:O3'	2:2:593:A:H4'	1.98	0.62
2:2:1314:U:H2'	2:2:1315:G:C8	2.34	0.62
2:2:1137:A:H2'	2:2:1138:A:C8	2.35	0.62
2:2:930:C:H3'	2:2:931:U:H5''	1.79	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1043:U:H2'	2:2:1043:U:O2	1.99	0.61
2:2:1534:G:H4'	2:2:1535:C:OP2	2.00	0.61
2:2:389:G:H5''	2:2:389:G:N3	2.15	0.61
2:2:1670:G:H2'	2:2:1671:G:C8	2.35	0.61
2:2:826:C:H2'	2:2:827:U:C6	2.35	0.61
2:2:396:A:H5''	12:I:47:ARG:HH12	1.64	0.61
27:X:103:LEU:HB3	27:X:126:LYS:HB2	1.83	0.61
2:2:536:G:H3'	13:J:171:ARG:NH1	2.16	0.60
2:2:388:G:H2'	2:2:389:G:O4'	2.01	0.60
1:1:16:H2U:OP2	1:1:60:A:N3	2.34	0.60
2:2:1323:G:H2'	2:2:1324:A:H4'	1.83	0.60
2:2:1710:A:H2'	2:2:1711:G:H4'	1.81	0.60
11:H:31:SER:HB2	11:H:32:PRO:HD3	1.82	0.60
2:2:1456:G:H21	19:P:128:HIS:HE1	1.50	0.60
24:U:53:LYS:HB2	24:U:92:ASP:HB3	1.83	0.60
11:H:46:ILE:HG12	11:H:60:VAL:HG12	1.81	0.60
1:1:16:H2U:C5'	1:1:16:H2U:H62	2.32	0.59
1:1:16:H2U:H5'	1:1:60:A:H2	1.67	0.59
1:1:62:C:O2'	1:1:63:G:H5'	2.02	0.59
2:2:1499:C:H42	2:2:1504:G:H1	1.50	0.59
23:T:42:GLY:HA2	23:T:84:LYS:HB2	1.85	0.59
2:2:1324:A:H2'	2:2:1325:A:C8	2.38	0.58
2:2:444:A:H61	2:2:460:G:N2	2.01	0.58
2:2:1330:A:H2'	2:2:1331:C:C5'	2.23	0.58
2:2:602:U:H2'	2:2:603:A:C8	2.38	0.58
2:2:711:G:H1	2:2:727:C:H42	1.51	0.58
2:2:1563:C:C2'	2:2:1564:U:C6	2.86	0.58
2:2:1323:G:H2'	2:2:1324:A:O4'	2.03	0.58
2:2:471:U:H2'	2:2:472:A:H8	1.69	0.58
2:2:946:U:HO2'	2:2:947:G:H8	1.52	0.58
2:2:1170:A:H2'	2:2:1171:G:C8	2.40	0.57
2:2:894:G:H1	2:2:916:U:H3	1.51	0.57
7:D:209:ILE:HG22	21:R:38:ILE:HG23	1.86	0.57
4:A:48:ILE:HG12	4:A:149:LEU:HD13	1.85	0.57
2:2:1456:G:H21	19:P:128:HIS:CE1	2.22	0.57
19:P:108:ARG:HB2	19:P:109:PRO:HD3	1.85	0.57
2:2:1558:U:H3	19:P:40:ARG:HH22	1.50	0.57
2:2:459:A:H3'	2:2:460:G:C8	2.35	0.57
25:V:15:ARG:HH11	25:V:33:GLN:HE21	1.52	0.57
7:D:23:GLU:HB3	14:K:61:TRP:HE1	1.70	0.57
2:2:1563:C:OP1	22:S:42:TYR:HE1	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:645:U:H2'	2:2:646:G:C8	2.40	0.57
1:1:16:H2U:H5'	1:1:60:A:C2	2.40	0.57
15:L:54:ILE:HG23	15:L:55:ASP:H	1.68	0.57
2:2:1333:U:H2'	2:2:1334:U:O4'	2.04	0.56
2:2:1557:A:H5'	2:2:1558:U:H5''	1.86	0.56
2:2:517:A:OP1	2:2:517:A:H4'	2.04	0.56
2:2:69:G:H1	2:2:82:U:H3	1.52	0.56
2:2:769:A:H2'	2:2:770:A:C8	2.41	0.56
2:2:384:A:H5'	12:I:25:ARG:HH22	1.70	0.56
2:2:1631:A:H5''	2:2:1631:A:H8	1.69	0.56
2:2:737:A:O2'	2:2:738:G:H8	1.87	0.56
2:2:705:U:H2'	2:2:706:A:C8	2.41	0.56
2:2:71:A:C3'	2:2:72:A:H5''	2.35	0.56
2:2:353:C:H5''	12:I:16:ALA:HB2	1.86	0.56
2:2:1166:G:C3'	2:2:1167:U:H5''	2.36	0.55
2:2:1419:A:H5'	7:D:160:SER:HB3	1.88	0.55
2:2:1290:G:H1	2:2:1323:G:H22	1.54	0.55
2:2:475:U:H6	2:2:475:U:C5'	2.18	0.55
2:2:1541:A:C2'	2:2:1542:U:H5'	2.36	0.55
2:2:1279:C:H4'	24:U:69:LYS:HB3	1.88	0.55
8:E:104:ASP:HB3	8:E:110:ALA:HB2	1.88	0.54
2:2:1586:G:H1	2:2:1606:U:H3	1.54	0.54
14:K:80:LEU:HB3	14:K:82:LEU:HD23	1.88	0.54
25:V:1:MET:HA	25:V:10:GLU:HB2	1.90	0.54
2:2:1116:U:H5'	2:2:1651:C:H5'	1.89	0.54
2:2:732:G:H1'	2:2:734:A:H61	1.73	0.54
12:I:44:HIS:HB2	12:I:56:ARG:HB2	1.89	0.54
2:2:778:G:H5'	2:2:780:A:H2	1.73	0.54
2:2:1051:U:H3'	2:2:1052:G:C5'	2.38	0.54
1:1:66:C:O2'	1:1:67:G:O4'	2.23	0.54
2:2:1323:G:H2'	2:2:1324:A:C5'	2.37	0.53
2:2:299:A:H2'	2:2:300:A:C8	2.43	0.53
27:X:109:ARG:HB3	27:X:112:LYS:HB2	1.90	0.53
2:2:1038:A:O2'	2:2:1039:G:H8	1.91	0.53
2:2:597:U:H2'	2:2:598:A:C8	2.44	0.53
2:2:14:C:O2'	2:2:1085:A:C8	2.61	0.53
2:2:937:G:H2'	2:2:938:A:H2'	1.89	0.53
2:2:1367:G:H5''	23:T:69:LYS:HB3	1.90	0.53
2:2:1087:A:H61	2:2:1092:A:H2	1.55	0.53
2:2:749:U:H3	2:2:799:U:H3	1.56	0.53
5:B:64:ARG:HH22	18:O:37:GLU:HB2	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:753:A:C2'	2:2:754:A:H5'	2.39	0.53
2:2:328:G:H5''	12:I:98:LYS:HB3	1.91	0.53
10:G:32:ILE:HG23	10:G:53:ALA:HA	1.91	0.53
2:2:979:G:H4'	2:2:1774:A:H4'	1.90	0.53
8:E:44:LEU:HD12	8:E:82:PHE:HB3	1.90	0.53
2:2:1602:U:C2	2:2:1603:G:C8	2.96	0.53
2:2:21:U:H4'	13:J:18:PRO:HG3	1.91	0.53
2:2:1533:U:O3'	2:2:1534:G:O4'	2.27	0.52
2:2:1563:C:H2'	2:2:1564:U:O4'	2.09	0.52
2:2:1043:U:O2	2:2:1043:U:C2'	2.56	0.52
7:D:74:GLU:HA	7:D:79:TYR:HB2	1.91	0.52
2:2:1329:G:C8	2:2:1330:A:C8	2.98	0.52
18:O:17:ALA:HB3	18:O:81:ILE:HA	1.91	0.52
2:2:730:G:N3	2:2:730:G:H2'	2.25	0.52
2:2:208:U:H2'	2:2:209:A:O4'	2.09	0.52
2:2:389:G:C5'	2:2:389:G:N3	2.73	0.52
5:B:117:TRP:HB3	5:B:153:THR:HA	1.92	0.52
2:2:248:U:H3	15:L:17:PRO:HG2	1.74	0.52
2:2:548:G:H1	2:2:588:C:H5	1.58	0.52
2:2:17:C:H2'	2:2:18:C:C6	2.45	0.52
2:2:925:A:H4'	2:2:1015:C:H4'	1.92	0.52
26:W:49:GLU:H	26:W:64:GLN:HB2	1.75	0.51
2:2:1639:C:H2'	2:2:1640:G:C8	2.45	0.51
2:2:1223:A:H3'	2:2:1224:U:C5'	2.40	0.51
23:T:17:ASN:HD22	23:T:135:ILE:HG23	1.76	0.51
6:C:50:VAL:HG21	6:C:73:ILE:HG23	1.92	0.51
14:K:58:GLN:HB2	14:K:65:TYR:HB2	1.93	0.51
2:2:452:U:H2'	2:2:452:U:O2	2.10	0.51
2:2:1144:U:H4'	2:2:1301:U:H5'	1.93	0.51
27:X:63:GLN:C	27:X:65:ASN:H	2.14	0.51
27:X:87:VAL:HG13	27:X:132:LEU:HD11	1.91	0.51
23:T:85:ASN:HA	23:T:91:HIS:HB3	1.93	0.51
5:B:121:ILE:HG12	5:B:161:ILE:HG23	1.93	0.51
12:I:85:PRO:HB3	15:L:12:ALA:HB2	1.93	0.51
2:2:842:U:H2'	2:2:843:A:C8	2.46	0.51
2:2:1290:G:H2'	2:2:1291:G:H8	1.76	0.51
2:2:1279:C:H2'	2:2:1280:G:H8	1.75	0.51
11:H:31:SER:CB	11:H:32:PRO:HD3	2.41	0.50
2:2:1660:G:H2'	2:2:1661:G:C8	2.46	0.50
2:2:50:C:H42	2:2:428:G:H1	1.59	0.50
2:2:1468:C:H4'	2:2:1538:G:H21	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1594:C:O2	2:2:1594:C:O4'	2.29	0.50
2:2:15:U:H2'	2:2:16:G:O4'	2.11	0.50
2:2:1080:A:H4'	2:2:1081:C:O5'	2.11	0.50
2:2:1563:C:C3'	2:2:1564:U:C6	2.88	0.50
2:2:1631:A:C8	2:2:1631:A:H5''	2.47	0.50
12:I:107:THR:H	12:I:108:PRO:HD2	1.77	0.50
7:D:69:LEU:HA	7:D:72:LEU:HD12	1.92	0.50
10:G:5:ILE:HD13	10:G:16:ILE:HD12	1.93	0.50
2:2:1191:C:H3'	2:2:1192:A:C5'	2.37	0.50
2:2:1534:G:N3	2:2:1534:G:C5'	2.73	0.50
15:L:66:ILE:HD13	15:L:128:CYS:HB3	1.94	0.50
2:2:158:U:H1'	28:Y:117:LYS:HA	1.92	0.49
2:2:1541:A:H2'	2:2:1542:U:H5'	1.93	0.49
2:2:868:A:H61	2:2:957:U:H5	1.60	0.49
2:2:1323:G:C3'	2:2:1324:A:C5'	2.90	0.49
2:2:1337:C:H2'	2:2:1338:C:O4'	2.12	0.49
2:2:5:U:H2'	2:2:6:G:C8	2.47	0.49
2:2:1257:U:O2	2:2:1257:U:O4'	2.29	0.49
2:2:404:C:H5'	10:G:93:LYS:HE2	1.93	0.49
2:2:1543:A:OP2	22:S:136:GLN:OE1	2.30	0.49
8:E:31:PRO:HG3	8:E:43:PRO:HG3	1.94	0.49
2:2:1137:A:H2'	2:2:1138:A:H8	1.74	0.49
2:2:1502:G:OP1	23:T:97:SER:HB2	2.12	0.49
16:M:26:ARG:HA	16:M:29:LEU:HD12	1.93	0.49
24:U:58:LEU:HD21	24:U:90:TYR:HD2	1.77	0.49
8:E:122:LYS:HB2	8:E:164:LEU:HD12	1.93	0.49
2:2:1602:U:H2'	2:2:1603:G:O4'	2.12	0.49
7:D:162:GLN:N	7:D:163:PRO:HD2	2.28	0.49
2:2:350:C:H5	2:2:630:G:H5'	1.78	0.49
6:C:58:ILE:HA	6:C:61:ILE:HD12	1.94	0.48
2:2:882:C:H42	2:2:944:U:H3	1.59	0.48
2:2:534:A:H3'	2:2:535:C:C5'	2.26	0.48
2:2:1239:U:H2'	2:2:1240:G:H5''	1.94	0.48
6:C:116:VAL:HG22	6:C:144:ILE:HD11	1.94	0.48
2:2:471:U:H2'	2:2:472:A:C8	2.49	0.48
2:2:320:C:H41	2:2:1664:U:H5''	1.79	0.48
2:2:1324:A:H2'	2:2:1325:A:H8	1.77	0.48
22:S:23:ASP:HB2	22:S:26:ILE:HD11	1.95	0.48
1:1:11:C:H42	1:1:24:G:H1	1.61	0.48
2:2:1328:A:H2'	2:2:1329:G:C5'	2.28	0.48
27:X:91:GLY:O	27:X:93:LEU:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1297:U:H2'	2:2:1298:G:C8	2.49	0.48
2:2:71:A:H3'	2:2:72:A:C5'	2.42	0.48
22:S:28:VAL:HG13	22:S:61:LEU:HD11	1.94	0.48
2:2:1087:A:C5	2:2:1088:U:H1'	2.49	0.48
2:2:1660:G:H2'	2:2:1661:G:H8	1.78	0.48
2:2:1343:A:H2'	2:2:1344:A:C8	2.48	0.48
2:2:1328:A:C3'	2:2:1329:G:H5'	2.43	0.48
2:2:564:C:H4'	2:2:565:C:OP2	2.14	0.48
12:I:168:ALA:HB2	12:I:184:ILE:HD12	1.95	0.48
2:2:40:A:H62	2:2:466:G:H21	1.60	0.48
2:2:1536:U:H2'	2:2:1537:G:H3'	1.95	0.48
2:2:1775:G:H1	2:2:1782:C:H42	1.62	0.48
26:W:14:ILE:HD11	26:W:27:ILE:HD11	1.96	0.48
11:H:63:PRO:O	11:H:64:VAL:HB	2.13	0.48
2:2:326:U:H2'	2:2:327:A:C8	2.49	0.48
2:2:602:U:H2'	2:2:603:A:H8	1.78	0.47
1:1:75:C:H5''	1:1:76:A:H5''	1.95	0.47
2:2:74:U:H4'	2:2:75:U:OP1	2.13	0.47
14:K:81:ASN:HB3	16:M:30:VAL:HG22	1.96	0.47
9:F:64:ILE:HG23	9:F:91:ILE:HG12	1.96	0.47
2:2:1563:C:C2'	2:2:1564:U:H6	2.24	0.47
2:2:1144:U:H3	2:2:1631:A:H2	1.60	0.47
15:L:21:THR:HG22	15:L:32:LYS:H	1.79	0.47
2:2:771:A:H3'	2:2:772:G:H8	1.79	0.47
2:2:533:A:OP1	13:J:168:ARG:NH2	2.47	0.47
2:2:1241:A:H8	2:2:1241:A:O5'	1.97	0.47
13:J:52:ILE:HG23	13:J:76:LEU:HD21	1.95	0.47
6:C:102:ARG:HE	6:C:122:THR:HG23	1.80	0.47
2:2:952:G:H2'	2:2:953:G:C8	2.50	0.47
2:2:1085:A:H5''	2:2:1086:A:OP2	2.14	0.47
22:S:57:ARG:HB2	22:S:60:GLU:HB2	1.96	0.47
2:2:1291:G:H2'	2:2:1292:U:O2	2.15	0.47
2:2:1512:U:O4'	2:2:1512:U:O2	2.31	0.47
2:2:1339:U:H6	2:2:1376:U:H4'	1.80	0.47
2:2:1087:A:N6	2:2:1092:A:H2	2.12	0.47
16:M:125:GLU:HA	16:M:128:LEU:HD12	1.97	0.47
13:J:39:LYS:HA	13:J:42:ILE:HD12	1.97	0.47
2:2:1001:G:H22	2:2:1758:G:H4'	1.80	0.47
18:O:65:GLN:HE21	18:O:108:SER:HB3	1.79	0.47
2:2:1326:C:C3'	2:2:1327:G:H5'	2.45	0.47
9:F:148:THR:HB	9:F:159:ARG:HD2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1239:U:H2'	2:2:1240:G:C5'	2.45	0.47
2:2:452:U:O2	2:2:452:U:C2'	2.62	0.47
2:2:506:U:H5'	2:2:507:U:H5''	1.97	0.47
2:2:249:C:H2'	2:2:250:A:H8	1.80	0.47
2:2:1328:A:O2'	2:2:1329:G:H5'	2.14	0.46
2:2:1563:C:C6	2:2:1563:C:C5'	2.89	0.46
27:X:50:LYS:HG3	27:X:103:LEU:HD23	1.97	0.46
2:2:646:G:H2'	2:2:647:G:O4'	2.16	0.46
2:2:45:U:H3	2:2:433:G:H1'	1.80	0.46
2:2:1155:C:H42	2:2:1620:G:H1	1.64	0.46
2:2:1326:C:C2'	2:2:1327:G:H5'	2.45	0.46
2:2:536:G:H3'	13:J:171:ARG:HH12	1.79	0.46
2:2:255:A:H2'	2:2:256:A:O4'	2.15	0.46
2:2:1571:A:H4'	2:2:1572:G:O5'	2.15	0.46
2:2:1279:C:H2'	2:2:1280:G:C8	2.50	0.46
8:E:94:ALA:HB1	28:Y:16:PRO:HB2	1.98	0.46
10:G:2:LYS:HG3	10:G:17:GLU:HG3	1.97	0.46
2:2:407:C:H2'	2:2:408:C:C6	2.50	0.46
19:P:39:ALA:HA	19:P:42:ARG:HD3	1.97	0.46
2:2:1198:G:H2'	2:2:1198:G:N3	2.31	0.46
10:G:78:ALA:HB2	10:G:92:ARG:HG3	1.96	0.46
2:2:1554:A:H3'	19:P:40:ARG:HD3	1.97	0.46
2:2:1408:A:H5''	20:Q:118:ILE:HG23	1.98	0.46
2:2:1179:C:H42	2:2:1456:G:H1	1.64	0.46
5:B:70:LEU:HD13	5:B:82:ARG:HG2	1.97	0.46
20:Q:54:LEU:HD21	20:Q:112:TYR:HE2	1.80	0.46
8:E:91:THR:HG22	8:E:98:ASN:HD22	1.80	0.46
4:A:60:ALA:HA	4:A:63:ILE:HD12	1.97	0.46
2:2:703:G:H3'	2:2:704:C:H3'	1.98	0.46
8:E:23:LEU:HD11	13:J:6:ARG:HD3	1.98	0.46
2:2:58:U:H5'	2:2:455:A:H1'	1.98	0.46
9:F:150:ARG:HA	9:F:159:ARG:HG2	1.97	0.46
14:K:18:GLU:HB3	14:K:20:VAL:HG12	1.96	0.46
2:2:1085:A:H3'	2:2:1086:A:C8	2.50	0.46
2:2:1095:C:H4'	2:2:1098:U:H4'	1.98	0.46
2:2:535:C:OP2	13:J:174:ARG:NH2	2.33	0.46
2:2:700:C:H42	2:2:738:G:H1	1.64	0.46
2:2:388:G:C3'	2:2:389:G:H5''	2.44	0.46
9:F:92:VAL:HA	9:F:95:LEU:HD12	1.97	0.46
2:2:1040:G:H1	2:2:1076:C:H42	1.64	0.46
9:F:117:LYS:HA	9:F:120:LEU:HD12	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:990:G:H21	2:2:1012:A:H62	1.63	0.45
16:M:52:LEU:HB3	16:M:114:VAL:HB	1.98	0.45
4:A:54:TRP:HA	4:A:57:ILE:HD12	1.98	0.45
2:2:1323:G:C2'	2:2:1324:A:H5''	2.45	0.45
2:2:1085:A:N3	2:2:1085:A:H2'	2.31	0.45
19:P:79:HIS:HA	19:P:97:TYR:HB3	1.99	0.45
2:2:1584:A:H2'	2:2:1585:A:O4'	2.16	0.45
13:J:81:VAL:HG11	13:J:91:LYS:HE2	1.98	0.45
11:H:153:LEU:HD22	11:H:186:PRO:HG3	1.98	0.45
15:L:108:PRO:HB2	15:L:135:VAL:HG22	1.97	0.45
8:E:47:PHE:HA	8:E:51:ARG:HB2	1.98	0.45
9:F:82:LYS:HB3	9:F:85:ARG:HB2	1.97	0.45
6:C:146:ARG:HD3	6:C:156:PRO:HG2	1.98	0.45
2:2:1331:C:OP1	21:R:45:ARG:HB3	2.16	0.45
2:2:1797:U:H5''	5:B:117:TRP:HE1	1.81	0.45
2:2:5:U:H2'	2:2:6:G:H8	1.81	0.45
19:P:52:LYS:HB2	19:P:53:PRO:HD3	1.97	0.45
2:2:1296:G:H21	2:2:1299:A:H62	1.64	0.45
2:2:1391:C:H42	2:2:1403:G:H1	1.65	0.45
22:S:68:ARG:O	22:S:72:ILE:HG12	2.16	0.45
2:2:444:A:N3	2:2:444:A:H3'	2.32	0.45
11:H:140:VAL:HB	26:W:52:TYR:HB3	1.98	0.45
2:2:394:U:H2'	2:2:395:G:O4'	2.16	0.45
2:2:391:G:O2'	2:2:1671:G:N3	2.49	0.45
2:2:1773:U:H2'	2:2:1774:A:H8	1.82	0.45
2:2:1072:G:H4'	17:N:10:GLY:HA2	1.99	0.45
9:F:114:ARG:HG3	20:Q:43:ILE:HG12	1.98	0.45
2:2:1236:G:H1	2:2:1247:C:H42	1.63	0.45
16:M:94:LEU:HB2	16:M:107:VAL:HG11	1.99	0.45
9:F:27:LEU:HB3	20:Q:27:GLY:HA3	1.97	0.45
16:M:20:ALA:HB3	16:M:127:LEU:HD12	1.99	0.45
2:2:1501:A:O2'	2:2:1502:G:C4	2.70	0.45
20:Q:35:PRO:HD3	23:T:8:ASP:HA	1.99	0.45
2:2:142:G:H2'	2:2:143:G:C8	2.52	0.45
2:2:1598:A:H2'	2:2:1598:A:N3	2.32	0.45
2:2:538:G:H1'	2:2:539:G:OP2	2.17	0.44
11:H:22:GLN:HA	11:H:25:ILE:HD12	1.98	0.44
2:2:225:A:H3'	2:2:226:U:H5'	1.99	0.44
2:2:895:U:H5'	5:B:23:PRO:HG2	1.99	0.44
8:E:197:HIS:CD2	8:E:199:GLU:HG3	2.52	0.44
2:2:1495:U:H2'	2:2:1496:G:C8	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:123:GLU:HA	16:M:126:ILE:HD12	2.00	0.44
15:L:78:THR:HG22	15:L:84:ILE:HD11	2.00	0.44
2:2:29:U:H2'	2:2:30:G:H8	1.82	0.44
2:2:1651:C:H42	2:2:1745:G:H1	1.65	0.44
4:A:11:SER:HB2	21:R:118:PRO:HD3	1.99	0.44
26:W:53:ILE:HB	26:W:60:LYS:HB3	2.00	0.44
28:Y:37:LYS:HA	28:Y:40:LEU:HD12	1.99	0.44
13:J:86:LEU:HD11	13:J:96:VAL:HG22	1.99	0.44
2:2:1558:U:O2	2:2:1558:U:O4'	2.35	0.44
11:H:28:GLU:HG3	11:H:38:LEU:HD22	1.99	0.44
2:2:512:U:O4'	2:2:512:U:O2	2.32	0.44
7:D:172:THR:HG22	7:D:185:LYS:HG2	1.99	0.44
2:2:406:A:H2'	2:2:407:C:C6	2.53	0.44
6:C:159:LEU:HB2	6:C:176:PRO:HG3	1.99	0.44
14:K:28:ASN:H	14:K:40:LEU:HD11	1.83	0.44
4:A:126:PRO:HG2	4:A:147:THR:HG22	2.00	0.44
2:2:1266:G:H1	2:2:1440:U:H3	1.65	0.44
2:2:1533:U:OP1	2:2:1534:G:C8	2.71	0.43
2:2:1533:U:H2'	2:2:1534:G:OP2	2.18	0.43
7:D:15:GLY:HA3	7:D:50:ILE:HG23	17.11	0.43
5:B:35:PRO:HB3	5:B:231:LEU:HD22	2.00	0.43
2:2:1668:G:O2'	2:2:1729:A:N6	2.52	0.43
9:F:66:ILE:HB	9:F:67:SER:H	1.71	0.43
2:2:947:G:H2'	2:2:948:C:O4'	2.18	0.43
27:X:63:GLN:HB3	27:X:64:PRO:CD	2.47	0.43
2:2:822:G:H2'	2:2:823:G:O4'	2.17	0.43
5:B:118:GLN:HE22	5:B:142:PHE:HB3	1.83	0.43
2:2:70:C:H2'	2:2:71:A:O4'	2.19	0.43
2:2:753:A:H2'	2:2:754:A:H5'	2.00	0.43
12:I:166:LEU:HB3	12:I:184:ILE:HD11	1.99	0.43
2:2:698:U:H1'	11:H:107:ARG:HG2	2.00	0.43
2:2:1171:G:H1	2:2:1465:C:H42	1.67	0.43
7:D:71:LEU:HB3	14:K:20:VAL:HG11	2.00	0.43
7:D:76:ARG:HH21	14:K:63:TYR:HB3	1.83	0.43
7:D:40:ARG:HH21	24:U:68:ARG:HB2	36.86	0.43
19:P:127:ARG:H	19:P:128:HIS:HD2	1.66	0.43
2:2:1773:U:H2'	2:2:1774:A:C8	2.53	0.43
4:A:162:CYS:SG	4:A:163:ASN:N	2.92	0.43
2:2:443:C:H5	28:Y:105:ARG:HH22	1.65	0.43
2:2:337:C:H5''	12:I:10:LYS:HG3	2.01	0.43
2:2:1471:U:C2	9:F:105:ASN:HB2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1209:C:H42	2:2:1451:G:H1	1.66	0.43
2:2:1437:C:H2'	2:2:1438:C:C6	2.53	0.43
2:2:1245:C:O2	2:2:1245:C:O4'	2.37	0.43
9:F:46:ASN:HD21	9:F:117:LYS:HD2	1.84	0.43
2:2:28:A:H2'	2:2:29:U:O4'	2.19	0.43
2:2:1168:G:H21	2:2:1574:A:H62	1.65	0.43
26:W:11:LEU:HD13	26:W:73:GLY:H	1.84	0.43
2:2:222:U:H2'	2:2:223:C:C6	2.54	0.43
2:2:1506:U:H2'	2:2:1507:C:C6	2.54	0.43
26:W:82:LYS:O	26:W:84:ALA:N	2.51	0.43
2:2:1602:U:H2'	2:2:1603:G:H8	1.83	0.42
7:D:68:GLU:HA	7:D:71:LEU:HD12	2.00	0.42
1:1:29:G:H4'	2:2:1460:G:H4'	2.01	0.42
2:2:14:C:O2'	2:2:1085:A:N9	2.53	0.42
2:2:1774:A:H2'	2:2:1775:G:C8	2.54	0.42
2:2:1736:U:H2'	2:2:1737:C:C6	2.55	0.42
2:2:687:C:H2'	2:2:688:G:C8	2.54	0.42
2:2:1335:A:H2'	2:2:1336:A:O4'	2.18	0.42
2:2:1602:U:H2'	2:2:1603:G:C8	2.54	0.42
2:2:1501:A:O2'	2:2:1502:G:C5	2.71	0.42
6:C:136:ILE:HA	6:C:139:LEU:HD12	2.01	0.42
23:T:20:SER:HA	23:T:23:GLN:HE21	1.84	0.42
22:S:44:ASN:HD22	23:T:46:PRO:HG2	1.84	0.42
2:2:1061:A:H2'	2:2:1062:U:O4'	2.19	0.42
18:O:50:ALA:HB3	18:O:53:ASP:HB2	2.02	0.42
4:A:69:ASN:HA	4:A:70:PRO:HD3	1.89	0.42
2:2:1292:U:O4	2:2:1321:A:N1	2.53	0.42
15:L:55:ASP:HB3	15:L:58:CYS:HB2	2.01	0.42
2:2:249:C:H2'	2:2:250:A:C8	2.54	0.42
2:2:606:G:H1	2:2:1098:U:H3	1.67	0.42
9:F:95:LEU:HG	9:F:174:ILE:HD11	2.01	0.42
24:U:117:ILE:HG22	24:U:118:ILE:H	1.84	0.42
12:I:84:HIS:HD2	12:I:100:ALA:HB2	1.85	0.42
8:E:54:TYR:HA	28:Y:22:GLN:HE22	1.84	0.42
29:Z:88:ILE:HG22	29:Z:89:ILE:HG13	2.02	0.42
2:2:1711:G:H2'	2:2:1711:G:N3	2.35	0.42
2:2:533:A:N3	2:2:533:A:H2'	2.34	0.42
9:F:43:LYS:HE2	20:Q:54:LEU:HA	2.01	0.42
2:2:186:G:H22	2:2:196:A:H2'	1.84	0.42
1:1:31:G:H3'	1:1:32:C:C6	2.55	0.42
18:O:31:THR:HG22	18:O:38:THR:HG22	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1261:U:H2'	2:2:1262:G:C8	2.55	0.42
2:2:1326:C:H2'	2:2:1327:G:H5'	2.01	0.42
2:2:1290:G:H2'	2:2:1291:G:C8	2.55	0.42
2:2:1240:G:H1'	19:P:79:HIS:ND1	2.35	0.42
2:2:1174:U:H2'	2:2:1175:G:H8	1.85	0.42
25:V:19:ALA:HA	25:V:71:ARG:HH22	1.84	0.42
26:W:7:LEU:HD22	26:W:74:VAL:HG21	2.02	0.42
8:E:155:LYS:HB3	8:E:156:VAL:H	1.76	0.42
2:2:389:G:H8	2:2:1729:A:HO2'	1.67	0.41
2:2:1143:U:H2'	2:2:1144:U:C6	2.55	0.41
18:O:89:THR:HB	18:O:128:LYS:HG3	2.01	0.41
22:S:3:LEU:H	29:Z:78:VAL:HG13	1.84	0.41
28:Y:122:GLY:HA2	28:Y:125:ILE:HD12	2.02	0.41
2:2:253:A:H2'	2:2:254:U:C6	2.55	0.41
8:E:179:LYS:HA	8:E:231:PRO:HD3	2.01	0.41
2:2:475:U:C6	2:2:475:U:C3'	3.03	0.41
2:2:1223:A:H5'	2:2:1224:U:OP2	2.19	0.41
29:Z:90:LYS:HA	29:Z:91:PRO:HD3	1.88	0.41
5:B:186:SER:HA	5:B:189:ILE:HD12	2.00	0.41
2:2:339:U:H2'	2:2:340:A:C8	2.55	0.41
4:A:123:VAL:HG11	4:A:133:ILE:HD11	2.02	0.41
2:2:1292:U:O4'	2:2:1292:U:O2	2.37	0.41
2:2:1339:U:H4'	2:2:1340:A:H5''	2.02	0.41
8:E:94:ALA:C	8:E:96:ASN:H	2.24	0.41
2:2:512:U:H1'	13:J:131:GLN:HG3	2.03	0.41
2:2:1262:G:H2'	2:2:1263:G:O4'	2.20	0.41
25:V:55:LEU:HD11	25:V:69:LEU:HD23	2.02	0.41
2:2:1206:C:H4'	2:2:1207:A:OP1	2.20	0.41
2:2:140:A:H2	2:2:265:A:H4'	1.85	0.41
22:S:26:ILE:H	22:S:26:ILE:HG13	1.55	0.41
26:W:50:PHE:HB3	26:W:63:VAL:HG13	2.02	0.41
15:L:26:LYS:HB3	15:L:30:LYS:HE3	2.01	0.41
12:I:104:ILE:HD13	12:I:168:ALA:HB3	2.02	0.41
28:Y:53:ASP:HB3	28:Y:96:LEU:HD21	2.02	0.41
1:1:18:G:N2	1:1:57:G:H2'	2.35	0.41
19:P:20:VAL:HG11	19:P:24:LYS:HD2	2.02	0.41
2:2:1229:A:H62	2:2:1254:G:H21	1.68	0.41
2:2:25:C:H4'	2:2:26:A:OP2	2.20	0.41
2:2:26:A:H61	2:2:598:A:H61	1.69	0.41
7:D:162:GLN:HA	7:D:165:ASN:HD22	1.86	0.41
22:S:46:VAL:HG21	22:S:73:MET:HG2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1227:G:H22	16:M:60:THR:HB	1.84	0.41
29:Z:66:VAL:HG22	29:Z:72:GLY:HA2	2.02	0.41
2:2:645:U:H2'	2:2:646:G:H8	1.83	0.41
6:C:155:GLN:HA	6:C:156:PRO:HD2	1.87	0.41
2:2:819:U:H2'	2:2:820:U:H4'	2.02	0.41
2:2:1219:C:H2'	2:2:1220:A:C8	2.55	0.41
2:2:1626:U:H2'	2:2:1627:G:C8	2.55	0.41
10:G:102:VAL:HG11	10:G:109:LEU:HD11	2.03	0.41
2:2:1637:C:H42	2:2:1761:A:H61	1.68	0.41
2:2:1327:G:H2'	2:2:1328:A:C5'	2.42	0.41
27:X:63:GLN:C	27:X:65:ASN:N	2.74	0.41
1:1:74:C:H4'	1:1:75:C:O5'	2.21	0.41
2:2:553:C:H1'	2:2:554:A:N7	2.35	0.41
12:I:69:SER:HB3	15:L:24:LYS:HD2	2.02	0.41
2:2:631:U:H4'	27:X:11:SER:HB3	2.02	0.41
2:2:843:A:H2'	2:2:844:G:C8	2.56	0.41
2:2:639:U:H2'	2:2:640:G:O4'	2.19	0.41
26:W:55:ASP:C	26:W:57:ARG:H	2.24	0.41
2:2:434:C:H1'	27:X:48:HIS:HB2	2.03	0.41
2:2:204:U:H2'	2:2:205:A:C8	2.55	0.41
22:S:86:LEU:CD2	22:S:86:LEU:H	2.34	0.41
7:D:34:TYR:HE1	7:D:37:VAL:HG23	1.86	0.41
2:2:1563:C:C4'	2:2:1563:C:C6	3.04	0.41
2:2:68:A:H4'	2:2:69:G:OP2	2.20	0.41
2:2:1659:U:H2'	2:2:1660:G:C8	2.55	0.41
5:B:176:VAL:HA	5:B:184:LEU:HD21	2.04	0.41
9:F:115:ILE:HG23	9:F:193:ALA:HB2	2.03	0.41
16:M:69:GLN:HG2	16:M:79:LEU:HD22	2.02	0.41
1:1:43:G:H2'	1:1:44:A:C8	2.55	0.41
2:2:476:A:H62	2:2:538:G:H22	1.68	0.40
2:2:1501:A:H61	22:S:82:PRO:HB2	1.85	0.40
14:K:38:LYS:HB2	14:K:41:PHE:HD2	1.86	0.40
14:K:25:LYS:HB2	14:K:62:GLN:HB2	2.03	0.40
2:2:589:C:H2'	2:2:590:A:C8	2.56	0.40
17:N:114:ARG:O	17:N:118:ILE:HG12	2.21	0.40
2:2:1086:A:OP2	2:2:1086:A:C8	2.74	0.40
2:2:687:C:H2'	2:2:688:G:H8	1.87	0.40
5:B:176:VAL:O	5:B:177:GLN:HB2	2.21	0.40
2:2:980:U:H3	2:2:1019:A:H61	1.69	0.40
20:Q:60:PHE:HD1	20:Q:63:ILE:HG21	1.86	0.40
2:2:1675:C:H2'	2:2:1676:A:O4'	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:67:ALA:HB3	27:X:69:ARG:HH21	1.87	0.40
2:2:885:U:H2'	2:2:886:A:C8	2.56	0.40
2:2:1323:G:H2'	2:2:1324:A:H5''	2.03	0.40
1:1:67:G:H2'	1:1:68:G:H8	1.87	0.40
2:2:1499:C:N4	2:2:1504:G:H1	2.19	0.40
2:2:55:A:H3'	2:2:402:G:H1	1.85	0.40
2:2:1161:C:H3'	2:2:1162:A:C8	2.57	0.40
2:2:700:C:H2'	2:2:701:U:C6	2.56	0.40
2:2:842:U:H2'	2:2:843:A:H8	1.87	0.40
11:H:62:VAL:HG12	11:H:64:VAL:H	1.85	0.40
2:2:1439:C:H2'	2:2:1440:U:C6	2.57	0.40
6:C:175:ILE:HB	6:C:202:TYR:HB2	2.03	0.40
2:2:1044:C:H2'	2:2:1045:G:C8	2.57	0.40
12:I:4:SER:HB3	12:I:24:LYS:HD3	2.03	0.40
23:T:55:TYR:HD1	23:T:55:TYR:H	1.69	0.40
2:2:1272:G:N7	2:2:1428:U:H3'	2.37	0.40
2:2:92:A:H5'	2:2:93:A:H5''	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	206/254 (81%)	177 (86%)	23 (11%)	6 (3%)	6	43
5	B	218/255 (86%)	191 (88%)	18 (8%)	9 (4%)	3	35
6	C	215/259 (83%)	193 (90%)	17 (8%)	5 (2%)	8	48
7	D	221/237 (93%)	198 (90%)	17 (8%)	6 (3%)	6	44
8	E	258/261 (99%)	230 (89%)	23 (9%)	5 (2%)	10	52
9	F	204/227 (90%)	170 (83%)	28 (14%)	6 (3%)	6	43
10	G	224/236 (95%)	204 (91%)	17 (8%)	3 (1%)	15	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	H	182/190 (96%)	166 (91%)	8 (4%)	8 (4%)	3	33
12	I	184/201 (92%)	163 (89%)	12 (6%)	9 (5%)	3	31
13	J	180/188 (96%)	153 (85%)	19 (11%)	8 (4%)	3	33
14	K	94/106 (89%)	80 (85%)	9 (10%)	5 (5%)	2	29
15	L	153/156 (98%)	133 (87%)	16 (10%)	4 (3%)	7	45
16	M	113/134 (84%)	86 (76%)	16 (14%)	11 (10%)	1	14
17	N	148/151 (98%)	141 (95%)	5 (3%)	2 (1%)	14	58
18	O	125/137 (91%)	101 (81%)	16 (13%)	8 (6%)	2	25
19	P	117/142 (82%)	91 (78%)	18 (15%)	8 (7%)	1	23
20	Q	139/143 (97%)	114 (82%)	13 (9%)	12 (9%)	1	17
21	R	105/136 (77%)	92 (88%)	10 (10%)	3 (3%)	6	43
22	S	143/146 (98%)	115 (80%)	20 (14%)	8 (6%)	2	28
23	T	141/144 (98%)	128 (91%)	13 (9%)	0	100	100
24	U	104/117 (89%)	88 (85%)	11 (11%)	5 (5%)	3	31
25	V	85/87 (98%)	79 (93%)	4 (5%)	2 (2%)	7	47
26	W	127/130 (98%)	114 (90%)	9 (7%)	4 (3%)	5	41
27	X	142/145 (98%)	121 (85%)	13 (9%)	8 (6%)	2	28
28	Y	132/135 (98%)	120 (91%)	8 (6%)	4 (3%)	5	42
29	Z	68/108 (63%)	55 (81%)	12 (18%)	1 (2%)	13	57
30	a	96/119 (81%)	83 (86%)	8 (8%)	5 (5%)	2	29
31	b	79/82 (96%)	69 (87%)	8 (10%)	2 (2%)	7	46
32	c	60/67 (90%)	56 (93%)	3 (5%)	1 (2%)	11	55
33	d	51/56 (91%)	37 (72%)	12 (24%)	2 (4%)	4	36
34	e	52/63 (82%)	41 (79%)	9 (17%)	2 (4%)	4	37
35	f	67/150 (45%)	50 (75%)	12 (18%)	5 (8%)	1	20
36	g	312/326 (96%)	267 (86%)	39 (12%)	6 (2%)	10	52
37	h	23/25 (92%)	23 (100%)	0	0	100	100
38	i	93/153 (61%)	82 (88%)	8 (9%)	3 (3%)	5	40
39	j	243/304 (80%)	212 (87%)	24 (10%)	7 (3%)	6	43
40	k	388/527 (74%)	335 (86%)	39 (10%)	14 (4%)	4	38
41	l	120/285 (42%)	106 (88%)	13 (11%)	1 (1%)	24	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	m	84/108 (78%)	74 (88%)	8 (10%)	2 (2%)	7	47
45	q	340/347 (98%)	307 (90%)	29 (8%)	4 (1%)	16	61
46	r	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
47	s	50/52 (96%)	44 (88%)	5 (10%)	1 (2%)	9	51
All	All	6118/7123 (86%)	5319 (87%)	594 (10%)	205 (3%)	8	40

All (205) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	H	31	SER
11	H	64	VAL
11	H	74	GLN
14	K	88	PRO
19	P	126	VAL
20	Q	138	PHE
22	S	40	ARG
24	U	118	ILE
26	W	83	ILE
27	X	64	PRO
27	X	92	CYS
28	Y	30	PRO
30	a	59	TYR
31	b	21	LEU
34	e	47	VAL
42	m	72	PRO
4	A	202	TYR
5	B	221	PRO
7	D	4	ILE
7	D	216	PRO
7	D	220	PRO
9	F	66	ILE
10	G	122	GLU
10	G	225	GLU
11	H	110	GLN
11	H	163	ASP
12	I	40	THR
12	I	148	ALA
12	I	153	ILE
13	J	150	LEU
15	L	55	ASP
16	M	98	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	N	3	ARG
18	O	40	ALA
18	O	124	ASP
20	Q	27	GLY
20	Q	39	VAL
20	Q	115	THR
20	Q	116	LEU
20	Q	121	SER
21	R	103	ASP
24	U	119	ALA
25	V	12	TYR
27	X	90	ASP
33	d	23	ILE
33	d	25	GLY
35	f	102	VAL
38	i	64	LYS
39	j	49	SER
39	j	196	GLU
41	l	129	LEU
5	B	8	ARG
5	B	131	ASP
5	B	207	LEU
6	C	111	ASP
6	C	253	THR
8	E	95	THR
8	E	195	ILE
8	E	205	PHE
9	F	67	SER
9	F	205	LYS
11	H	10	SER
12	I	22	ARG
12	I	52	ASN
12	I	120	SER
13	J	171	ARG
14	K	23	ALA
15	L	30	LYS
15	L	105	LYS
16	M	82	VAL
16	M	102	ASN
18	O	25	ASP
19	P	54	ALA
20	Q	14	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	Q	40	GLN
20	Q	124	PRO
20	Q	142	TYR
22	S	102	ALA
25	V	45	ALA
26	W	58	SER
27	X	3	LYS
28	Y	36	SER
30	a	13	LYS
32	c	35	ASP
36	g	4	SER
36	g	146	LEU
39	j	57	ARG
39	j	64	ARG
40	k	127	ARG
40	k	255	ARG
40	k	383	GLU
45	q	164	LYS
47	s	63	GLY
4	A	39	LYS
4	A	103	THR
4	A	109	ASN
4	A	207	PRO
5	B	54	LEU
5	B	224	ASP
6	C	151	THR
6	C	155	GLN
7	D	219	GLU
8	E	77	ARG
9	F	71	TYR
13	J	118	LEU
13	J	136	VAL
14	K	89	ALA
16	M	18	GLU
16	M	84	ASP
17	N	12	SER
18	O	18	ARG
18	O	42	VAL
18	O	114	ARG
19	P	90	ILE
19	P	108	ARG
19	P	128	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	Q	32	ASN
21	R	24	LEU
24	U	17	VAL
24	U	89	ARG
26	W	29	PRO
27	X	144	ARG
28	Y	64	TYR
29	Z	97	LYS
35	f	85	TYR
36	g	129	ASP
38	i	44	ASN
39	j	6	CYS
40	k	126	VAL
40	k	273	THR
45	q	116	MET
45	q	261	LYS
4	A	158	VAL
5	B	22	ASP
5	B	177	GLN
6	C	96	ARG
7	D	196	THR
8	E	245	LYS
9	F	24	PRO
9	F	59	SER
11	H	13	PRO
11	H	98	ILE
12	I	59	ARG
12	I	107	THR
13	J	120	LYS
13	J	134	ILE
13	J	147	MET
14	K	54	PHE
16	M	32	ASP
16	M	77	VAL
16	M	81	LYS
16	M	110	SER
21	R	5	ARG
22	S	14	ILE
22	S	28	VAL
22	S	76	PRO
22	S	91	ASP
26	W	30	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	X	63	GLN
28	Y	4	ALA
30	a	36	ILE
30	a	61	GLU
31	b	62	VAL
35	f	90	LYS
36	g	201	GLY
39	j	120	GLN
40	k	321	PHE
40	k	408	ARG
40	k	497	GLU
45	q	165	GLY
5	B	148	ASN
12	I	147	ARG
13	J	35	GLY
14	K	64	TYR
15	L	7	VAL
16	M	103	ALA
19	P	109	PRO
27	X	70	LYS
30	a	64	LEU
35	f	98	VAL
36	g	64	GLY
39	j	5	HIS
40	k	225	PRO
40	k	324	ASN
7	D	63	GLY
16	M	97	ILE
27	X	91	GLY
34	e	12	GLY
38	i	45	GLY
18	O	120	PRO
20	Q	33	GLY
22	S	82	PRO
24	U	73	GLY
40	k	270	ILE
18	O	88	GLY
19	P	68	PRO
19	P	99	GLY
22	S	9	GLY
42	m	97	GLY
10	G	69	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	f	122	PRO
40	k	176	ARG
40	k	392	PRO
36	g	106	GLY
40	k	335	GLY

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	174/211 (82%)	159 (91%)	15 (9%)	13	47
5	B	198/228 (87%)	182 (92%)	16 (8%)	15	50
6	C	176/203 (87%)	161 (92%)	15 (8%)	13	48
7	D	185/196 (94%)	171 (92%)	14 (8%)	16	53
8	E	223/224 (100%)	201 (90%)	22 (10%)	10	39
9	F	174/194 (90%)	156 (90%)	18 (10%)	9	37
10	G	192/200 (96%)	184 (96%)	8 (4%)	36	70
11	H	164/170 (96%)	146 (89%)	18 (11%)	8	34
12	I	147/159 (92%)	138 (94%)	9 (6%)	23	60
13	J	153/158 (97%)	144 (94%)	9 (6%)	24	61
14	K	88/96 (92%)	82 (93%)	6 (7%)	20	57
15	L	136/137 (99%)	131 (96%)	5 (4%)	41	73
16	M	93/109 (85%)	90 (97%)	3 (3%)	46	76
17	N	127/128 (99%)	119 (94%)	8 (6%)	22	59
18	O	96/104 (92%)	90 (94%)	6 (6%)	22	59
19	P	101/119 (85%)	89 (88%)	12 (12%)	6	31
20	Q	117/119 (98%)	103 (88%)	14 (12%)	6	31
21	R	102/124 (82%)	93 (91%)	9 (9%)	12	45
22	S	128/129 (99%)	117 (91%)	11 (9%)	13	47
23	T	117/118 (99%)	104 (89%)	13 (11%)	8	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	U	96/107 (90%)	92 (96%)	4 (4%)	36	70
25	V	73/73 (100%)	67 (92%)	6 (8%)	14	49
26	W	110/111 (99%)	106 (96%)	4 (4%)	42	74
27	X	119/120 (99%)	109 (92%)	10 (8%)	14	49
28	Y	108/109 (99%)	101 (94%)	7 (6%)	21	58
29	Z	60/88 (68%)	56 (93%)	4 (7%)	20	57
30	a	83/100 (83%)	77 (93%)	6 (7%)	18	55
31	b	71/72 (99%)	68 (96%)	3 (4%)	36	70
32	c	54/59 (92%)	51 (94%)	3 (6%)	26	62
33	d	46/48 (96%)	43 (94%)	3 (6%)	21	58
34	e	47/55 (86%)	42 (89%)	5 (11%)	8	36
35	f	58/133 (44%)	51 (88%)	7 (12%)	6	31
36	g	265/272 (97%)	244 (92%)	21 (8%)	15	51
37	h	23/23 (100%)	22 (96%)	1 (4%)	35	70
38	i	81/130 (62%)	75 (93%)	6 (7%)	17	54
39	j	224/274 (82%)	193 (86%)	31 (14%)	4	27
40	k	332/449 (74%)	324 (98%)	8 (2%)	57	82
41	l	119/246 (48%)	114 (96%)	5 (4%)	36	70
42	m	77/96 (80%)	76 (99%)	1 (1%)	76	89
45	q	297/301 (99%)	290 (98%)	7 (2%)	57	82
46	r	33/33 (100%)	33 (100%)	0	100	100
47	s	43/43 (100%)	43 (100%)	0	100	100
All	All	5310/6068 (88%)	4937 (93%)	373 (7%)	23	56

All (373) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	LEU
4	A	37	VAL
4	A	59	LEU
4	A	72	ASP
4	A	88	LYS
4	A	93	THR
4	A	101	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	112	THR
4	A	134	LYS
4	A	165	ARG
4	A	167	LYS
4	A	170	ILE
4	A	177	LEU
4	A	193	GLN
4	A	198	MET
5	B	29	TRP
5	B	54	LEU
5	B	70	LEU
5	B	82	ARG
5	B	104	ASP
5	B	118	GLN
5	B	124	ASN
5	B	127	VAL
5	B	140	ILE
5	B	155	TYR
5	B	171	ILE
5	B	181	LEU
5	B	184	LEU
5	B	196	GLU
5	B	208	GLN
5	B	228	LEU
6	C	83	ASP
6	C	84	GLU
6	C	91	VAL
6	C	96	ARG
6	C	101	THR
6	C	116	VAL
6	C	145	ARG
6	C	146	ARG
6	C	166	LYS
6	C	212	LEU
6	C	230	LEU
6	C	233	ASN
6	C	234	LEU
6	C	235	TRP
6	C	236	GLU
7	D	5	ILE
7	D	20	GLU
7	D	68	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	D	75	LYS
7	D	94	ARG
7	D	113	LEU
7	D	115	ILE
7	D	116	ARG
7	D	120	TYR
7	D	146	ARG
7	D	168	ILE
7	D	200	LYS
7	D	212	LYS
7	D	214	GLU
8	E	7	LYS
8	E	22	LYS
8	E	38	LEU
8	E	51	ARG
8	E	60	GLU
8	E	69	HIS
8	E	75	LYS
8	E	77	ARG
8	E	79	ASP
8	E	88	ASP
8	E	108	ARG
8	E	113	ARG
8	E	123	LEU
8	E	168	THR
8	E	180	LEU
8	E	181	VAL
8	E	189	LEU
8	E	212	ASP
8	E	225	VAL
8	E	230	GLU
8	E	233	ARG
8	E	248	ILE
9	F	29	THR
9	F	31	ILE
9	F	45	PHE
9	F	47	LYS
9	F	70	ILE
9	F	86	LYS
9	F	108	LYS
9	F	110	LEU
9	F	145	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	F	168	ARG
9	F	177	LEU
9	F	187	ARG
9	F	188	ASN
9	F	189	ILE
9	F	196	LEU
9	F	209	THR
9	F	221	ARG
9	F	224	LYS
10	G	15	CYS
10	G	21	GLU
10	G	52	ILE
10	G	92	ARG
10	G	95	LYS
10	G	121	ILE
10	G	164	LYS
10	G	211	LEU
11	H	7	LYS
11	H	11	GLN
11	H	15	GLU
11	H	27	LEU
11	H	33	GLU
11	H	38	LEU
11	H	48	GLU
11	H	72	LYS
11	H	77	LEU
11	H	86	GLN
11	H	111	LYS
11	H	112	ARG
11	H	122	HIS
11	H	124	LYS
11	H	126	LEU
11	H	129	LEU
11	H	139	ARG
11	H	162	ILE
12	I	20	GLN
12	I	29	LEU
12	I	47	ARG
12	I	58	LEU
12	I	96	LEU
12	I	97	THR
12	I	119	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	I	179	ARG
12	I	196	ARG
13	J	8	TYR
13	J	28	LEU
13	J	33	GLU
13	J	37	LYS
13	J	45	ILE
13	J	100	LYS
13	J	103	ASP
13	J	107	ARG
13	J	161	THR
14	K	6	GLU
14	K	21	LEU
14	K	44	LYS
14	K	47	GLN
14	K	64	TYR
14	K	76	LEU
15	L	10	GLU
15	L	36	LYS
15	L	55	ASP
15	L	80	MET
15	L	83	THR
16	M	22	LYS
16	M	52	LEU
16	M	125	GLU
17	N	3	ARG
17	N	20	ARG
17	N	27	LYS
17	N	64	LYS
17	N	70	LYS
17	N	88	LEU
17	N	100	LYS
17	N	107	LYS
18	O	29	HIS
18	O	49	LYS
18	O	65	GLN
18	O	92	LYS
18	O	110	LEU
18	O	114	ARG
19	P	13	LYS
19	P	23	GLU
19	P	57	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	P	60	LEU
19	P	72	LYS
19	P	76	VAL
19	P	108	ARG
19	P	111	MET
19	P	122	THR
19	P	124	THR
19	P	127	ARG
19	P	130	ARG
20	Q	13	LYS
20	Q	22	VAL
20	Q	43	ILE
20	Q	48	VAL
20	Q	63	ILE
20	Q	69	VAL
20	Q	83	GLN
20	Q	97	VAL
20	Q	105	LEU
20	Q	114	ARG
20	Q	117	LEU
20	Q	127	LYS
20	Q	137	ARG
20	Q	143	ARG
21	R	3	ARG
21	R	4	VAL
21	R	46	LEU
21	R	47	ARG
21	R	63	LYS
21	R	80	ARG
21	R	100	LEU
21	R	109	LEU
21	R	117	LEU
22	S	6	GLN
22	S	8	GLN
22	S	18	LEU
22	S	20	THR
22	S	26	ILE
22	S	54	LEU
22	S	86	LEU
22	S	96	LYS
22	S	105	LEU
22	S	110	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	S	114	GLU
23	T	8	ASP
23	T	12	GLN
23	T	16	ASN
23	T	28	LEU
23	T	29	GLU
23	T	30	VAL
23	T	35	ASP
23	T	55	TYR
23	T	65	ILE
23	T	68	ARG
23	T	103	LYS
23	T	124	ILE
23	T	135	ILE
24	U	20	HIS
24	U	83	GLU
24	U	117	ILE
24	U	118	ILE
25	V	1	MET
25	V	4	ASP
25	V	11	LEU
25	V	50	TYR
25	V	69	LEU
25	V	76	ASP
26	W	7	LEU
26	W	24	GLN
26	W	47	ILE
26	W	111	MET
27	X	14	LYS
27	X	19	ARG
27	X	30	LYS
27	X	55	GLU
27	X	79	ASN
27	X	83	VAL
27	X	84	THR
27	X	94	ASN
27	X	107	PHE
27	X	121	ARG
28	Y	5	ILE
28	Y	8	ARG
28	Y	35	VAL
28	Y	72	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	Y	84	LYS
28	Y	99	LYS
28	Y	105	ARG
29	Z	57	TYR
29	Z	58	ARG
29	Z	70	LYS
29	Z	80	LEU
30	a	12	LYS
30	a	28	ARG
30	a	37	LYS
30	a	38	ARG
30	a	64	LEU
30	a	93	ARG
31	b	3	LEU
31	b	57	GLU
31	b	67	THR
32	c	9	LEU
32	c	33	LEU
32	c	50	GLU
33	d	20	GLN
33	d	39	ASP
33	d	44	ARG
34	e	15	LYS
34	e	20	LYS
34	e	39	LEU
34	e	49	LEU
34	e	54	ARG
35	f	97	LYS
35	f	103	LEU
35	f	111	GLU
35	f	119	LYS
35	f	120	GLU
35	f	138	TYR
35	f	143	HIS
36	g	6	ILE
36	g	8	LEU
36	g	10	LEU
36	g	50	GLU
36	g	70	GLN
36	g	77	ASP
36	g	103	ARG
36	g	124	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	g	146	LEU
36	g	151	TRP
36	g	172	ILE
36	g	175	VAL
36	g	188	LEU
36	g	198	ASP
36	g	206	ILE
36	g	210	GLN
36	g	238	PHE
36	g	281	LEU
36	g	297	VAL
36	g	314	ASP
36	g	321	GLN
37	h	21	ARG
38	i	23	LYS
38	i	24	ARG
38	i	62	ARG
38	i	70	TRP
38	i	89	CYS
38	i	114	LYS
39	j	7	ARG
39	j	11	ASN
39	j	13	TYR
39	j	19	ILE
39	j	38	GLU
39	j	39	TYR
39	j	43	GLU
39	j	45	MET
39	j	46	ILE
39	j	47	LEU
39	j	57	ARG
39	j	59	ILE
39	j	64	ARG
39	j	87	LYS
39	j	103	GLN
39	j	113	ARG
39	j	121	ILE
39	j	123	LEU
39	j	126	LEU
39	j	127	TYR
39	j	137	LYS
39	j	152	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	j	154	VAL
39	j	159	GLU
39	j	166	LEU
39	j	172	TYR
39	j	185	ARG
39	j	230	LEU
39	j	235	LEU
39	j	244	LEU
39	j	251	ILE
40	k	228	GLN
40	k	291	ILE
40	k	337	VAL
40	k	395	LEU
40	k	402	VAL
40	k	403	ASP
40	k	410	ASP
40	k	432	ILE
41	l	129	LEU
41	l	141	ILE
41	l	180	ILE
41	l	206	ASP
41	l	211	LEU
42	m	49	TYR
45	q	94	VAL
45	q	244	VAL
45	q	253	ILE
45	q	272	LYS
45	q	276	ARG
45	q	317	ILE
45	q	328	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	69	ASN
4	A	109	ASN
5	B	49	ASN
5	B	118	GLN
5	B	124	ASN
5	B	160	HIS
5	B	220	GLN
6	C	76	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	C	233	ASN
7	D	165	ASN
8	E	69	HIS
8	E	98	ASN
8	E	112	HIS
9	F	188	ASN
10	G	10	ASN
11	H	155	ASN
12	I	84	HIS
15	L	8	GLN
15	L	22	ASN
18	O	65	GLN
19	P	98	ASN
19	P	103	ASN
19	P	128	HIS
20	Q	77	GLN
20	Q	83	GLN
20	Q	94	GLN
20	Q	100	GLN
20	Q	139	GLN
21	R	29	GLN
22	S	89	GLN
22	S	136	GLN
23	T	16	ASN
23	T	17	ASN
23	T	23	GLN
24	U	105	GLN
25	V	33	GLN
26	W	80	ASN
27	X	22	ASN
27	X	79	ASN
28	Y	22	GLN
32	c	27	GLN
34	e	17	GLN
35	f	133	HIS
36	g	18	ASN
36	g	292	GLN
39	j	26	GLN
39	j	238	GLN
40	k	102	ASN
40	k	221	ASN
40	k	248	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	k	286	GLN
40	k	376	ASN
40	k	465	ASN
42	m	43	GLN
42	m	67	ASN
42	m	79	GLN
42	m	99	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	73/75 (97%)	38 (52%)	12 (16%)
2	2	1778/1781 (99%)	814 (45%)	118 (6%)
3	3	1/25 (4%)	0	0
All	All	1852/1881 (98%)	852 (46%)	130 (7%)

All (852) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	8	U
1	1	9	1MG
1	1	10	2MG
1	1	11	C
1	1	12	G
1	1	13	C
1	1	14	A
1	1	15	G
1	1	16	H2U
1	1	18	G
1	1	19	G
1	1	20	A
1	1	21	A
1	1	22	G
1	1	26	M2G
1	1	31	G
1	1	32	C
1	1	35	A
1	1	36	U
1	1	37	T6A
1	1	38	A
1	1	39	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	40	C
1	1	43	G
1	1	46	7MG
1	1	47	H2U
1	1	48	5MC
1	1	49	5MC
1	1	52	G
1	1	59	A
1	1	61	C
1	1	64	RIA
1	1	66	C
1	1	69	C
1	1	71	C
1	1	74	C
1	1	75	C
1	1	76	A
2	2	2	A
2	2	4	C
2	2	5	U
2	2	8	U
2	2	9	U
2	2	11	A
2	2	13	C
2	2	19	A
2	2	24	U
2	2	25	C
2	2	26	A
2	2	27	U
2	2	31	C
2	2	34	G
2	2	35	U
2	2	36	C
2	2	37	U
2	2	42	G
2	2	45	U
2	2	46	A
2	2	47	A
2	2	50	C
2	2	51	A
2	2	54	C
2	2	55	A
2	2	56	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	57	G
2	2	59	C
2	2	60	U
2	2	61	A
2	2	62	A
2	2	63	G
2	2	64	U
2	2	65	A
2	2	67	A
2	2	68	A
2	2	69	G
2	2	70	C
2	2	72	A
2	2	73	U
2	2	74	U
2	2	75	U
2	2	76	A
2	2	77	U
2	2	79	C
2	2	80	A
2	2	82	U
2	2	90	C
2	2	95	G
2	2	104	A
2	2	111	U
2	2	114	C
2	2	116	U
2	2	123	G
2	2	124	A
2	2	127	G
2	2	129	U
2	2	130	C
2	2	131	C
2	2	132	U
2	2	133	U
2	2	134	U
2	2	136	C
2	2	137	U
2	2	138	A
2	2	139	C
2	2	140	A
2	2	141	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	144	A
2	2	146	A
2	2	147	U
2	2	157	U
2	2	158	U
2	2	159	C
2	2	160	U
2	2	161	A
2	2	167	A
2	2	172	A
2	2	173	U
2	2	175	C
2	2	176	U
2	2	177	U
2	2	178	A
2	2	183	C
2	2	185	C
2	2	190	C
2	2	191	U
2	2	192	U
2	2	194	G
2	2	195	G
2	2	198	G
2	2	208	U
2	2	209	A
2	2	217	A
2	2	218	A
2	2	220	A
2	2	225	A
2	2	226	U
2	2	227	G
2	2	228	U
2	2	230	U
2	2	231	U
2	2	232	C
2	2	233	G
2	2	237	U
2	2	239	C
2	2	240	U
2	2	249	C
2	2	256	A
2	2	259	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	264	A
2	2	265	A
2	2	266	U
2	2	270	A
2	2	271	U
2	2	274	C
2	2	275	C
2	2	276	U
2	2	277	U
2	2	278	G
2	2	279	U
2	2	280	G
2	2	286	G
2	2	287	A
2	2	288	U
2	2	294	A
2	2	298	A
2	2	300	A
2	2	301	U
2	2	307	C
2	2	308	C
2	2	311	A
2	2	312	U
2	2	313	C
2	2	314	A
2	2	315	A
2	2	319	U
2	2	320	C
2	2	321	G
2	2	322	A
2	2	332	A
2	2	336	G
2	2	337	C
2	2	345	G
2	2	349	U
2	2	351	A
2	2	358	A
2	2	359	A
2	2	360	C
2	2	369	A
2	2	377	A
2	2	379	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	380	C
2	2	382	G
2	2	384	A
2	2	386	A
2	2	387	G
2	2	389	G
2	2	397	G
2	2	398	A
2	2	399	A
2	2	400	A
2	2	401	C
2	2	402	G
2	2	403	G
2	2	413	C
2	2	415	A
2	2	416	A
2	2	421	G
2	2	422	G
2	2	423	C
2	2	424	A
2	2	425	G
2	2	426	C
2	2	433	G
2	2	434	C
2	2	438	U
2	2	439	U
2	2	440	A
2	2	443	C
2	2	444	A
2	2	447	C
2	2	448	C
2	2	452	U
2	2	455	A
2	2	458	G
2	2	459	A
2	2	463	A
2	2	469	A
2	2	473	A
2	2	476	A
2	2	478	C
2	2	479	G
2	2	480	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	481	U
2	2	482	A
2	2	483	C
2	2	488	C
2	2	489	C
2	2	490	C
2	2	491	A
2	2	492	U
2	2	493	U
2	2	495	G
2	2	496	G
2	2	497	G
2	2	499	C
2	2	501	U
2	2	502	G
2	2	504	A
2	2	505	A
2	2	506	U
2	2	507	U
2	2	509	G
2	2	516	U
2	2	517	A
2	2	518	C
2	2	519	A
2	2	522	G
2	2	523	U
2	2	524	A
2	2	525	A
2	2	527	U
2	2	530	C
2	2	531	U
2	2	532	U
2	2	533	A
2	2	534	A
2	2	535	C
2	2	537	A
2	2	538	G
2	2	539	G
2	2	540	A
2	2	541	A
2	2	542	C
2	2	543	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	544	A
2	2	547	G
2	2	548	G
2	2	553	C
2	2	554	A
2	2	556	G
2	2	557	U
2	2	558	C
2	2	563	G
2	2	564	C
2	2	565	C
2	2	567	G
2	2	568	C
2	2	570	G
2	2	571	C
2	2	573	G
2	2	577	U
2	2	578	A
2	2	579	A
2	2	580	U
2	2	581	U
2	2	584	A
2	2	586	C
2	2	587	U
2	2	593	A
2	2	594	G
2	2	605	A
2	2	610	U
2	2	612	G
2	2	614	A
2	2	618	A
2	2	619	A
2	2	620	A
2	2	622	A
2	2	634	A
2	2	637	U
2	2	638	U
2	2	640	G
2	2	641	G
2	2	647	G
2	2	649	U
2	2	650	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	651	U
2	2	652	C
2	2	653	C
2	2	654	G
2	2	655	G
2	2	656	U
2	2	657	C
2	2	677	G
2	2	679	U
2	2	684	A
2	2	686	C
2	2	687	C
2	2	691	U
2	2	693	U
2	2	694	U
2	2	696	C
2	2	697	C
2	2	698	U
2	2	700	C
2	2	701	U
2	2	702	G
2	2	704	C
2	2	705	U
2	2	706	A
2	2	709	C
2	2	710	U
2	2	711	G
2	2	712	U
2	2	713	A
2	2	714	C
2	2	716	C
2	2	717	C
2	2	718	U
2	2	719	U
2	2	721	U
2	2	722	G
2	2	725	U
2	2	726	G
2	2	727	C
2	2	728	A
2	2	731	C
2	2	732	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	733	A
2	2	734	A
2	2	735	C
2	2	736	C
2	2	738	G
2	2	741	C
2	2	742	U
2	2	744	U
2	2	745	U
2	2	747	C
2	2	753	A
2	2	754	A
2	2	755	A
2	2	762	A
2	2	764	U
2	2	765	G
2	2	766	U
2	2	767	U
2	2	768	C
2	2	771	A
2	2	774	A
2	2	775	G
2	2	778	G
2	2	780	A
2	2	781	A
2	2	782	G
2	2	783	C
2	2	784	U
2	2	785	C
2	2	786	G
2	2	788	A
2	2	791	U
2	2	793	U
2	2	794	U
2	2	796	G
2	2	803	A
2	2	806	A
2	2	809	G
2	2	810	A
2	2	811	A
2	2	813	A
2	2	814	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	817	C
2	2	818	G
2	2	819	U
2	2	820	U
2	2	822	G
2	2	823	G
2	2	825	U
2	2	826	C
2	2	827	U
2	2	828	A
2	2	829	U
2	2	840	U
2	2	845	G
2	2	847	C
2	2	851	C
2	2	854	A
2	2	855	A
2	2	856	U
2	2	859	U
2	2	861	A
2	2	862	A
2	2	863	U
2	2	864	A
2	2	872	U
2	2	875	G
2	2	876	G
2	2	881	U
2	2	895	U
2	2	897	A
2	2	898	G
2	2	904	A
2	2	905	A
2	2	907	U
2	2	908	U
2	2	910	U
2	2	912	G
2	2	913	G
2	2	915	U
2	2	918	A
2	2	919	U
2	2	920	U
2	2	924	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	925	A
2	2	927	U
2	2	930	C
2	2	931	U
2	2	932	A
2	2	933	C
2	2	934	U
2	2	938	A
2	2	939	A
2	2	941	G
2	2	944	U
2	2	946	U
2	2	947	G
2	2	950	A
2	2	956	G
2	2	957	U
2	2	958	U
2	2	965	A
2	2	970	A
2	2	972	A
2	2	981	U
2	2	982	A
2	2	983	G
2	2	984	G
2	2	991	A
2	2	995	U
2	2	997	A
2	2	1000	A
2	2	1001	G
2	2	1002	A
2	2	1003	U
2	2	1004	A
2	2	1009	C
2	2	1011	U
2	2	1012	A
2	2	1015	C
2	2	1018	A
2	2	1020	C
2	2	1022	A
2	2	1024	A
2	2	1025	A
2	2	1026	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1027	C
2	2	1030	U
2	2	1031	G
2	2	1034	G
2	2	1038	A
2	2	1039	G
2	2	1041	G
2	2	1043	U
2	2	1044	C
2	2	1047	G
2	2	1048	U
2	2	1049	G
2	2	1050	G
2	2	1051	U
2	2	1052	G
2	2	1054	U
2	2	1055	U
2	2	1056	U
2	2	1057	U
2	2	1058	C
2	2	1059	U
2	2	1060	U
2	2	1062	U
2	2	1068	A
2	2	1069	C
2	2	1070	U
2	2	1075	A
2	2	1080	A
2	2	1081	C
2	2	1082	G
2	2	1084	G
2	2	1085	A
2	2	1086	A
2	2	1089	C
2	2	1090	A
2	2	1091	A
2	2	1093	G
2	2	1095	C
2	2	1096	U
2	2	1097	U
2	2	1098	U
2	2	1099	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1100	G
2	2	1102	U
2	2	1103	U
2	2	1105	U
2	2	1108	G
2	2	1112	A
2	2	1113	G
2	2	1114	U
2	2	1117	G
2	2	1118	G
2	2	1119	U
2	2	1121	G
2	2	1123	A
2	2	1124	A
2	2	1129	G
2	2	1137	A
2	2	1144	U
2	2	1145	G
2	2	1146	A
2	2	1149	G
2	2	1150	A
2	2	1151	A
2	2	1153	G
2	2	1155	C
2	2	1157	C
2	2	1158	C
2	2	1161	C
2	2	1162	A
2	2	1163	G
2	2	1165	A
2	2	1166	G
2	2	1167	U
2	2	1169	G
2	2	1172	C
2	2	1174	U
2	2	1176	C
2	2	1182	A
2	2	1184	U
2	2	1188	A
2	2	1190	U
2	2	1192	A
2	2	1193	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1197	G
2	2	1198	G
2	2	1199	G
2	2	1200	G
2	2	1201	A
2	2	1202	A
2	2	1203	A
2	2	1207	A
2	2	1211	G
2	2	1216	A
2	2	1217	G
2	2	1223	A
2	2	1224	U
2	2	1226	A
2	2	1227	G
2	2	1228	G
2	2	1229	A
2	2	1230	U
2	2	1231	U
2	2	1234	C
2	2	1236	G
2	2	1240	G
2	2	1241	A
2	2	1243	A
2	2	1244	G
2	2	1246	U
2	2	1253	U
2	2	1254	G
2	2	1255	A
2	2	1256	U
2	2	1258	U
2	2	1259	U
2	2	1260	G
2	2	1266	G
2	2	1268	U
2	2	1269	G
2	2	1272	G
2	2	1273	C
2	2	1275	U
2	2	1279	C
2	2	1282	U
2	2	1283	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1284	U
2	2	1285	U
2	2	1286	A
2	2	1287	G
2	2	1292	U
2	2	1295	A
2	2	1296	G
2	2	1297	U
2	2	1298	G
2	2	1300	U
2	2	1303	G
2	2	1305	C
2	2	1306	U
2	2	1309	U
2	2	1310	U
2	2	1312	A
2	2	1313	U
2	2	1314	U
2	2	1315	G
2	2	1316	C
2	2	1317	G
2	2	1320	A
2	2	1321	A
2	2	1323	G
2	2	1324	A
2	2	1327	G
2	2	1328	A
2	2	1329	G
2	2	1331	C
2	2	1332	C
2	2	1333	U
2	2	1336	A
2	2	1337	C
2	2	1338	C
2	2	1339	U
2	2	1343	A
2	2	1344	A
2	2	1345	A
2	2	1346	U
2	2	1347	A
2	2	1352	U
2	2	1353	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1355	U
2	2	1361	U
2	2	1362	U
2	2	1364	C
2	2	1366	G
2	2	1369	U
2	2	1370	G
2	2	1371	A
2	2	1374	C
2	2	1375	U
2	2	1376	U
2	2	1378	U
2	2	1380	A
2	2	1381	G
2	2	1383	G
2	2	1386	A
2	2	1388	U
2	2	1389	A
2	2	1391	C
2	2	1393	G
2	2	1396	U
2	2	1397	C
2	2	1398	A
2	2	1400	G
2	2	1410	G
2	2	1411	U
2	2	1412	U
2	2	1413	U
2	2	1418	C
2	2	1419	A
2	2	1420	A
2	2	1425	A
2	2	1426	G
2	2	1428	U
2	2	1429	C
2	2	1430	U
2	2	1431	G
2	2	1433	G
2	2	1434	A
2	2	1435	U
2	2	1442	A
2	2	1444	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1445	C
2	2	1448	U
2	2	1449	C
2	2	1455	C
2	2	1456	G
2	2	1457	C
2	2	1461	C
2	2	1463	C
2	2	1467	A
2	2	1469	A
2	2	1470	C
2	2	1471	U
2	2	1476	G
2	2	1479	C
2	2	1482	G
2	2	1483	C
2	2	1484	G
2	2	1488	A
2	2	1489	C
2	2	1490	A
2	2	1491	A
2	2	1492	C
2	2	1494	U
2	2	1499	C
2	2	1502	G
2	2	1504	G
2	2	1508	U
2	2	1509	G
2	2	1512	U
2	2	1513	A
2	2	1514	A
2	2	1515	U
2	2	1516	C
2	2	1519	G
2	2	1521	G
2	2	1522	A
2	2	1523	A
2	2	1529	G
2	2	1532	G
2	2	1533	U
2	2	1534	G
2	2	1535	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1536	U
2	2	1538	G
2	2	1540	G
2	2	1541	A
2	2	1542	U
2	2	1543	A
2	2	1544	G
2	2	1548	A
2	2	1551	G
2	2	1554	A
2	2	1555	U
2	2	1557	A
2	2	1563	C
2	2	1564	U
2	2	1566	C
2	2	1570	G
2	2	1571	A
2	2	1572	G
2	2	1573	G
2	2	1575	A
2	2	1581	A
2	2	1582	G
2	2	1583	U
2	2	1589	C
2	2	1590	A
2	2	1595	A
2	2	1597	C
2	2	1598	A
2	2	1599	G
2	2	1604	C
2	2	1608	G
2	2	1613	C
2	2	1614	G
2	2	1616	C
2	2	1617	C
2	2	1620	G
2	2	1621	C
2	2	1625	U
2	2	1626	U
2	2	1629	A
2	2	1630	C
2	2	1631	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1632	C
2	2	1633	A
2	2	1635	C
2	2	1636	G
2	2	1637	C
2	2	1638	C
2	2	1640	G
2	2	1646	A
2	2	1647	G
2	2	1649	A
2	2	1655	U
2	2	1656	G
2	2	1662	C
2	2	1676	A
2	2	1678	G
2	2	1679	A
2	2	1682	U
2	2	1685	U
2	2	1686	U
2	2	1687	A
2	2	1688	G
2	2	1692	A
2	2	1693	G
2	2	1694	G
2	2	1695	G
2	2	1696	G
2	2	1697	G
2	2	1698	C
2	2	1699	A
2	2	1700	A
2	2	1701	C
2	2	1702	U
2	2	1703	C
2	2	1705	A
2	2	1706	U
2	2	1707	C
2	2	1709	C
2	2	1710	A
2	2	1711	G
2	2	1712	A
2	2	1725	G
2	2	1730	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1742	A
2	2	1743	G
2	2	1744	A
2	2	1745	G
2	2	1748	A
2	2	1750	U
2	2	1754	A
2	2	1755	G
2	2	1758	G
2	2	1760	A
2	2	1763	A
2	2	1764	A
2	2	1766	G
2	2	1767	U
2	2	1768	U
2	2	1769	U
2	2	1770	C
2	2	1777	U
2	2	1778	G
2	2	1780	A
2	2	1781	C
2	2	1786	G
2	2	1787	G
2	2	1789	A
2	2	1790	G
2	2	1791	G
2	2	1792	A
2	2	1793	U
2	2	1794	C
2	2	1795	A
2	2	1796	U
2	2	1797	U

All (130) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	9	1MG
1	1	10	2MG
1	1	16	H2U
1	1	19	G
1	1	20	A
1	1	36	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	37	T6A
1	1	38	A
1	1	46	7MG
1	1	47	H2U
1	1	48	5MC
1	1	74	C
2	2	25	C
2	2	44	U
2	2	45	U
2	2	46	A
2	2	55	A
2	2	58	U
2	2	61	A
2	2	66	U
2	2	68	A
2	2	74	U
2	2	103	A
2	2	115	G
2	2	130	C
2	2	131	C
2	2	133	U
2	2	134	U
2	2	157	U
2	2	177	U
2	2	189	C
2	2	190	C
2	2	193	U
2	2	216	A
2	2	217	A
2	2	239	C
2	2	258	U
2	2	265	A
2	2	270	A
2	2	271	U
2	2	275	C
2	2	277	U
2	2	279	U
2	2	321	G
2	2	349	U
2	2	379	U
2	2	399	A
2	2	451	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	454	C
2	2	497	G
2	2	524	A
2	2	538	G
2	2	542	C
2	2	543	A
2	2	564	C
2	2	580	U
2	2	593	A
2	2	608	U
2	2	619	A
2	2	637	U
2	2	654	G
2	2	685	A
2	2	693	U
2	2	695	U
2	2	700	C
2	2	721	U
2	2	724	G
2	2	784	U
2	2	793	U
2	2	810	A
2	2	812	U
2	2	813	A
2	2	822	G
2	2	826	C
2	2	827	U
2	2	828	A
2	2	854	A
2	2	855	A
2	2	896	C
2	2	907	U
2	2	911	U
2	2	912	G
2	2	918	A
2	2	945	U
2	2	946	U
2	2	956	G
2	2	1000	A
2	2	1001	G
2	2	1002	A
2	2	1015	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1022	A
2	2	1030	U
2	2	1051	U
2	2	1056	U
2	2	1080	A
2	2	1096	U
2	2	1097	U
2	2	1099	G
2	2	1107	G
2	2	1123	A
2	2	1195	A
2	2	1198	G
2	2	1206	C
2	2	1226	A
2	2	1284	U
2	2	1314	U
2	2	1343	A
2	2	1363	G
2	2	1380	A
2	2	1411	U
2	2	1412	U
2	2	1424	C
2	2	1430	U
2	2	1455	C
2	2	1487	U
2	2	1488	A
2	2	1491	A
2	2	1514	A
2	2	1534	G
2	2	1537	G
2	2	1571	A
2	2	1613	C
2	2	1631	A
2	2	1655	U
2	2	1678	G
2	2	1706	U
2	2	1765	G
2	2	1789	A
2	2	1790	G
2	2	1792	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	2MG	1	10	1	18,26,27	1.43	2 (11%)	21,38,41	2.44	7 (33%)
1	H2U	1	16	1	17,21,22	0.85	1 (5%)	23,30,33	1.41	5 (21%)
1	M2G	1	26	1	18,27,28	1.70	3 (16%)	22,40,43	2.19	6 (27%)
1	T6A	1	37	1	23,34,35	1.17	1 (4%)	26,49,52	2.93	8 (30%)
1	7MG	1	46	1	20,26,27	1.77	3 (15%)	23,39,42	3.16	6 (26%)
1	H2U	1	47	1	17,21,22	0.83	0	23,30,33	1.94	5 (21%)
1	5MC	1	48	1	14,22,23	1.62	2 (14%)	17,32,35	1.18	2 (11%)
1	5MC	1	49	1	14,22,23	1.61	1 (7%)	17,32,35	1.14	1 (5%)
1	1MA	1	58	1	15,25,26	2.05	4 (26%)	15,37,40	1.18	1 (6%)
1	RIA	1	64	1	31,38,39	1.23	2 (6%)	38,57,60	2.08	8 (21%)
1	1MG	1	9	1	17,26,27	1.71	3 (17%)	19,39,42	1.08	2 (10%)

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
1	2MG	1	10	1	-	0/5/27/28	0/3/3/3
1	H2U	1	16	1	-	0/7/38/39	0/2/2/2
1	M2G	1	26	1	-	0/7/29/30	0/3/3/3
1	T6A	1	37	1	-	1/15/41/42	0/3/3/3
1	7MG	1	46	1	-	0/7/37/38	0/3/3/3
1	H2U	1	47	1	-	0/7/38/39	0/2/2/2
1	5MC	1	48	1	-	0/3/25/26	0/2/2/2
1	5MC	1	49	1	-	0/3/25/26	0/2/2/2
1	1MA	1	58	1	-	0/3/25/26	0/3/3/3
1	RIA	1	64	1	-	0/13/51/52	0/4/4/4
1	1MG	1	9	1	-	0/3/25/26	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	64	RIA	P'-O3X	-4.10	1.40	1.54
1	1	16	H2U	C2-N3	-2.04	1.34	1.38
1	1	64	RIA	C2-N1	2.04	1.37	1.33
1	1	48	5MC	O4'-C1'	2.17	1.44	1.41
1	1	46	7MG	C1'-N9	2.60	1.50	1.44
1	1	58	1MA	C2-N3	2.86	1.35	1.30
1	1	9	1MG	C6-N1	3.06	1.42	1.38
1	1	26	M2G	C5-C4	3.21	1.47	1.40
1	1	10	2MG	C5-C4	3.38	1.48	1.40
1	1	58	1MA	C5-C4	3.45	1.48	1.40
1	1	9	1MG	C5-C4	3.57	1.48	1.40
1	1	46	7MG	C5-C4	3.58	1.48	1.39
1	1	37	T6A	C5-C4	3.59	1.48	1.40
1	1	26	M2G	C6-C5	3.79	1.49	1.41
1	1	10	2MG	C6-C5	3.80	1.49	1.41
1	1	58	1MA	C6-N6	3.96	1.36	1.29
1	1	26	M2G	C2-N2	4.32	1.42	1.34
1	1	9	1MG	C6-C5	4.36	1.49	1.40
1	1	58	1MA	C6-C5	4.63	1.49	1.40
1	1	48	5MC	C5-C4	5.41	1.49	1.41
1	1	49	5MC	C5-C4	5.41	1.49	1.41
1	1	46	7MG	C6-C5	5.48	1.49	1.41

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	46	7MG	C5-C4-N3	-8.53	118.05	126.74
1	1	37	T6A	N3-C2-N1	-7.54	122.95	128.87
1	1	64	RIA	O2A-C1'-C2'	-6.69	94.14	107.91
1	1	47	H2U	C5-C6-N1	-5.11	105.17	110.76
1	1	46	7MG	C5-C6-N1	-4.94	116.03	123.39
1	1	37	T6A	O10-C10-N6	-4.22	117.14	123.59
1	1	10	2MG	C5-C6-N1	-4.06	118.22	123.52
1	1	26	M2G	C5-C6-N1	-3.87	118.47	123.52
1	1	26	M2G	C6-C5-C4	-3.42	116.95	120.86
1	1	26	M2G	N3-C2-N1	-3.15	121.00	126.35
1	1	10	2MG	C6-C5-C4	-2.99	117.44	120.86
1	1	10	2MG	N3-C2-N1	-2.88	121.87	126.19
1	1	64	RIA	O2X-P'-O5'	-2.78	98.61	106.72
1	1	16	H2U	C4-N3-C2	-2.61	123.40	125.77
1	1	37	T6A	N6-C6-N1	-2.55	116.58	118.82
1	1	47	H2U	C4-N3-C2	-2.44	123.56	125.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	16	H2U	C5-C6-N1	-2.42	108.11	110.76
1	1	64	RIA	N3-C2-N1	-2.26	127.09	128.87
1	1	46	7MG	C8-N9-C1'	-2.24	115.70	122.43
1	1	64	RIA	O3X-P'-O1X	-2.20	103.44	110.63
1	1	37	T6A	C13-C12-N11	-2.16	109.25	113.40
1	1	9	1MG	C6-C5-C4	-2.11	118.42	119.93
1	1	46	7MG	C2-N3-C4	2.03	120.28	114.50
1	1	10	2MG	C4'-O4'-C1'	2.04	111.80	109.64
1	1	16	H2U	C6-N1-C2	2.05	125.32	122.16
1	1	26	M2G	C4'-O4'-C1'	2.11	111.88	109.64
1	1	48	5MC	O4'-C1'-N1	2.11	112.12	108.10
1	1	47	H2U	C3'-C2'-C1'	2.23	105.91	101.44
1	1	9	1MG	N2-C2-N1	2.29	120.96	118.26
1	1	49	5MC	O4'-C1'-N1	2.36	112.58	108.10
1	1	37	T6A	O3'-C3'-C4'	2.36	118.06	111.01
1	1	48	5MC	C4'-O4'-C1'	2.40	112.19	109.64
1	1	16	H2U	C3'-C2'-C1'	2.43	106.31	101.44
1	1	37	T6A	O4'-C1'-N9	2.51	112.84	108.11
1	1	64	RIA	O3X-P'-O5'	2.53	114.09	106.72
1	1	16	H2U	C1'-N1-C2	2.60	121.83	118.19
1	1	64	RIA	O1'-C1'-C2'	2.69	108.54	104.83
1	1	47	H2U	C5-C4-N3	2.87	119.65	116.62
1	1	26	M2G	N1-C2-N2	2.96	120.36	117.14
1	1	10	2MG	N2-C2-N3	3.59	121.11	116.94
1	1	58	1MA	C2-N3-C4	3.70	122.05	116.44
1	1	64	RIA	C1'-O2A-C2A	4.54	130.07	118.00
1	1	37	T6A	N6-C10-N11	5.14	122.12	113.75
1	1	47	H2U	C1'-N1-C2	5.15	125.41	118.19
1	1	10	2MG	C6-N1-C2	5.19	122.68	115.24
1	1	46	7MG	C6-N1-C2	6.00	122.91	115.88
1	1	64	RIA	O5'-P'-O1X	6.10	122.43	107.08
1	1	10	2MG	C2-N3-C4	6.12	121.70	114.99
1	1	26	M2G	C2-N3-C4	6.75	122.39	114.99
1	1	46	7MG	N3-C4-N9	8.58	138.07	126.98
1	1	37	T6A	C2-N1-C6	8.99	122.94	116.47

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	37	T6A	C5-C6-N6-C10

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	16	H2U	6	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 88 ligands modelled in this entry, 86 are monoatomic - leaving 2 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	$\# Z > 2$
50	MET	k	601	-	5,7,8	0.41	0	4,7,9	0.94	0
51	GCP	k	603	48	29,34,34	1.79	7 (24%)	32,54,54	1.77	5 (15%)

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
50	MET	k	601	-	-	0/4/6/8	0/0/0/0
51	GCP	k	603	48	-	0/15/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	k	603	GCP	PG-O3G	-2.63	1.48	1.54
51	k	603	GCP	PB-O2B	2.14	1.61	1.56
51	k	603	GCP	PG-O2G	2.58	1.61	1.54
51	k	603	GCP	PB-O3A	2.69	1.61	1.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	k	603	GCP	C5-C4	3.35	1.48	1.40
51	k	603	GCP	C6-C5	4.09	1.49	1.41
51	k	603	GCP	PG-O1G	5.02	1.61	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	k	603	GCP	C5-C6-N1	-3.99	118.31	123.52
51	k	603	GCP	N3-C2-N1	-3.71	122.51	127.56
51	k	603	GCP	C6-C5-C4	-3.38	116.99	120.86
51	k	603	GCP	O4'-C1'-N9	2.92	113.61	108.11
51	k	603	GCP	C6-N1-C2	5.48	122.31	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.