



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:08 PM GMT

PDB ID : 1N8R
Title : Structure of large ribosomal subunit in complex with virginiamycin M
Authors : Hansen, J.L.; Moore, P.B.; Steitz, T.A.
Deposited on : 2002-11-21
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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) : trunk26865

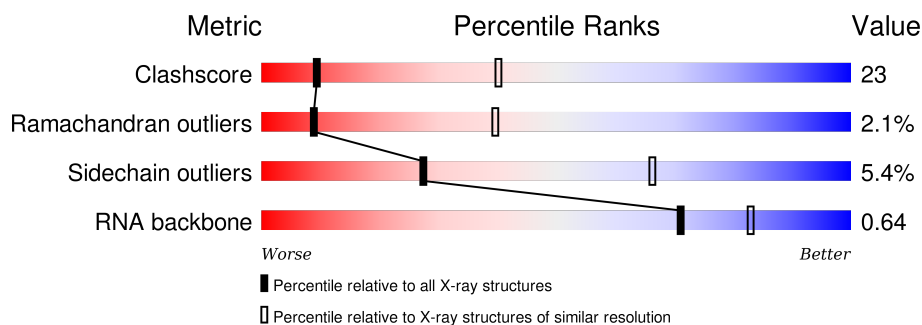
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)







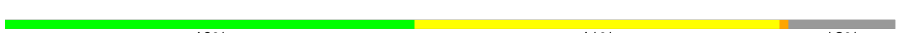



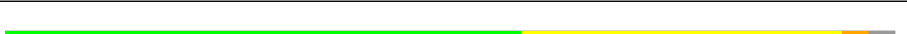



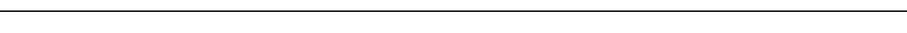
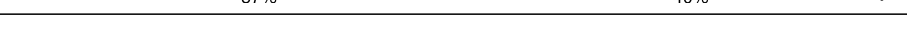
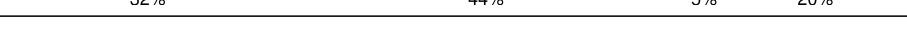



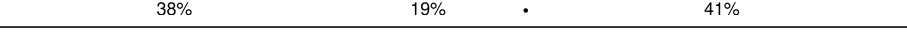
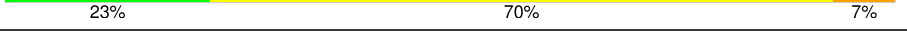


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	2922	
2	B	122	
3	C	239	
4	D	337	
5	E	246	
6	F	176	

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Mol	Chain	Length	Quality of chain
7	G	177	
8	H	119	
9	I	348	
10	J	167	
11	K	145	
12	L	132	
13	M	164	
14	N	194	
15	O	186	
16	P	115	
17	Q	148	
18	R	95	
19	S	154	
20	T	84	
21	U	119	
22	V	66	
23	W	70	
24	X	154	
25	Y	91	
26	Z	240	
27	1	73	
28	2	56	
29	3	48	
30	4	92	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	CL	M	8510	-	-	X	-
35	CL	N	8518	-	-	X	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 98569 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	0	0
			1754	1072	352	325	5			

- Molecule 4 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	337	Total	C	N	O	S	0	0	0
			2624	1616	493	510	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	DELETION	UNP P20279
D	310	ARG	PHE	CONFLICT	UNP P20279

- Molecule 5 is a protein called 50S ribosomal protein L4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	246	Total	C	N	O	S	0	0	0
			1858	1131	344	382	1			

- Molecule 6 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 7 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 8 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	119	Total	C	N	O	S	0	0	0
			885	552	141	191	1			

- Molecule 9 is a protein called Acidic ribosomal protein P0 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 10 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	156	Total	C	N	O	S	0	0	0
			1215	766	233	212	4			

- Molecule 11 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	142	Total	C	N	O	S	0	0	0
			1119	696	199	221	3			

- Molecule 12 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

- Molecule 13 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	145	Total	C	N	O	0	0	0
			1114	668	222	224			

- Molecule 14 is a protein called 50S ribosomal protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	194	Total	C	N	O	S	0	0	0
			1605	988	346	266	5			

- Molecule 15 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

- Molecule 16 is a protein called 50S ribosomal protein L18E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	P	115	Total	C	N	O	0	0	0
			864	529	161	174			

- Molecule 17 is a protein called 50S ribosomal protein L19E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	Q	143	Total	C	N	O	0	0	0
			1133	680	230	223			

- Molecule 18 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	95	Total	C	N	O	0	0	0
			734	450	141	143			

- Molecule 19 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	150	Total	C	N	O	S	0	0	0
			1149	713	209	223	4			

- Molecule 20 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	81	Total	C	N	O	S	0	0	0
			641	389	111	138	3			

- Molecule 21 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	119	Total	C	N	O		0	0	0
			949	568	180	201				

- Molecule 22 is a protein called 50S ribosomal protein L24E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	53	Total	C	N	O	S	0	0	0
			410	244	75	86	5			

- Molecule 23 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 24 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	154	Total	C	N	O	S	0	0	0
			1195	737	209	243	6			

- Molecule 25 is a protein called 50S ribosomal protein L31E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 26 is a protein called 50S ribosomal protein L32E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	142	Total	C	N	O		0	0	0
			1130	686	228	216				

- Molecule 27 is a protein called 50S ribosomal protein L37AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 28 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

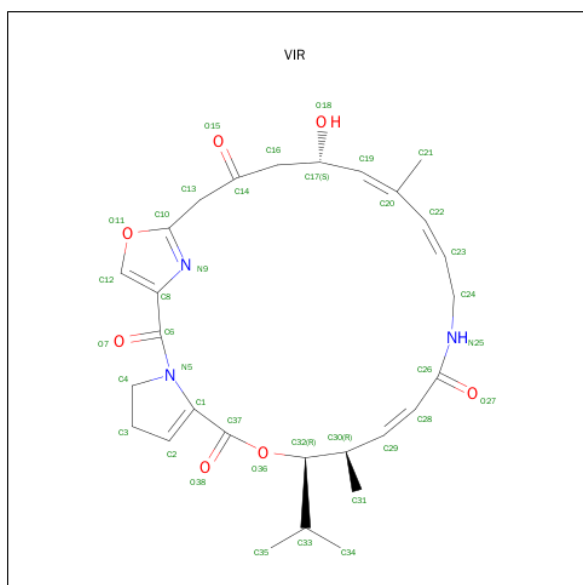
- Molecule 29 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

- Molecule 30 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is VIRGINIAMYCIN M1 (three-letter code: VIR) (formula: $C_{28}H_{35}N_3O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	N	O	0	0
			38	28	3	7		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	D	1	Total Mg 1 1	0	0
32	B	1	Total Mg 1 1	0	0
32	C	2	Total Mg 2 2	0	0
32	Z	1	Total Mg 1 1	0	0
32	A	109	Total Mg 109 109	0	0
32	4	1	Total Mg 1 1	0	0
32	U	1	Total Mg 1 1	0	0
32	L	1	Total Mg 1 1	0	0

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total K 1 1	0	0

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	J	2	Total Na 2 2	0	0
34	K	1	Total Na 1 1	0	0
34	E	1	Total Na 1 1	0	0
34	B	2	Total Na 2 2	0	0
34	C	1	Total Na 1 1	0	0
34	A	71	Total Na 71 71	0	0
34	T	1	Total Na 1 1	0	0
34	N	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	U	1	Total 1	Na 1	0	0
34	4	1	Total 1	Na 1	0	0
34	R	1	Total 1	Na 1	0	0
34	S	2	Total 2	Na 2	0	0
34	M	1	Total 1	Na 1	0	0

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	P	1	Total 1	Cl 1	0	0
35	D	1	Total 1	Cl 1	0	0
35	K	3	Total 3	Cl 3	0	0
35	C	1	Total 1	Cl 1	0	0
35	Z	2	Total 2	Cl 2	0	0
35	A	8	Total 8	Cl 8	0	0
35	4	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	O	1	Total 1	Cl 1	0	0
35	L	1	Total 1	Cl 1	0	0
35	S	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	P	1	Total Cd 1 1	0	0
36	2	1	Total Cd 1 1	0	0
36	1	1	Total Cd 1 1	0	0
36	4	1	Total Cd 1 1	0	0
36	V	1	Total Cd 1 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	A	5881	Total O 5881 5881	0	0
37	B	146	Total O 146 146	0	0
37	C	135	Total O 135 135	0	0
37	D	141	Total O 141 141	0	0
37	E	178	Total O 178 178	0	0
37	F	49	Total O 49 49	0	0
37	G	43	Total O 43 43	0	0
37	H	30	Total O 30 30	0	0
37	I	21	Total O 21 21	0	0
37	J	76	Total O 76 76	0	0
37	K	55	Total O 55 55	0	0
37	L	64	Total O 64 64	0	0
37	M	85	Total O 85 85	0	0
37	N	141	Total O 141 141	0	0
37	O	67	Total O 67 67	0	0

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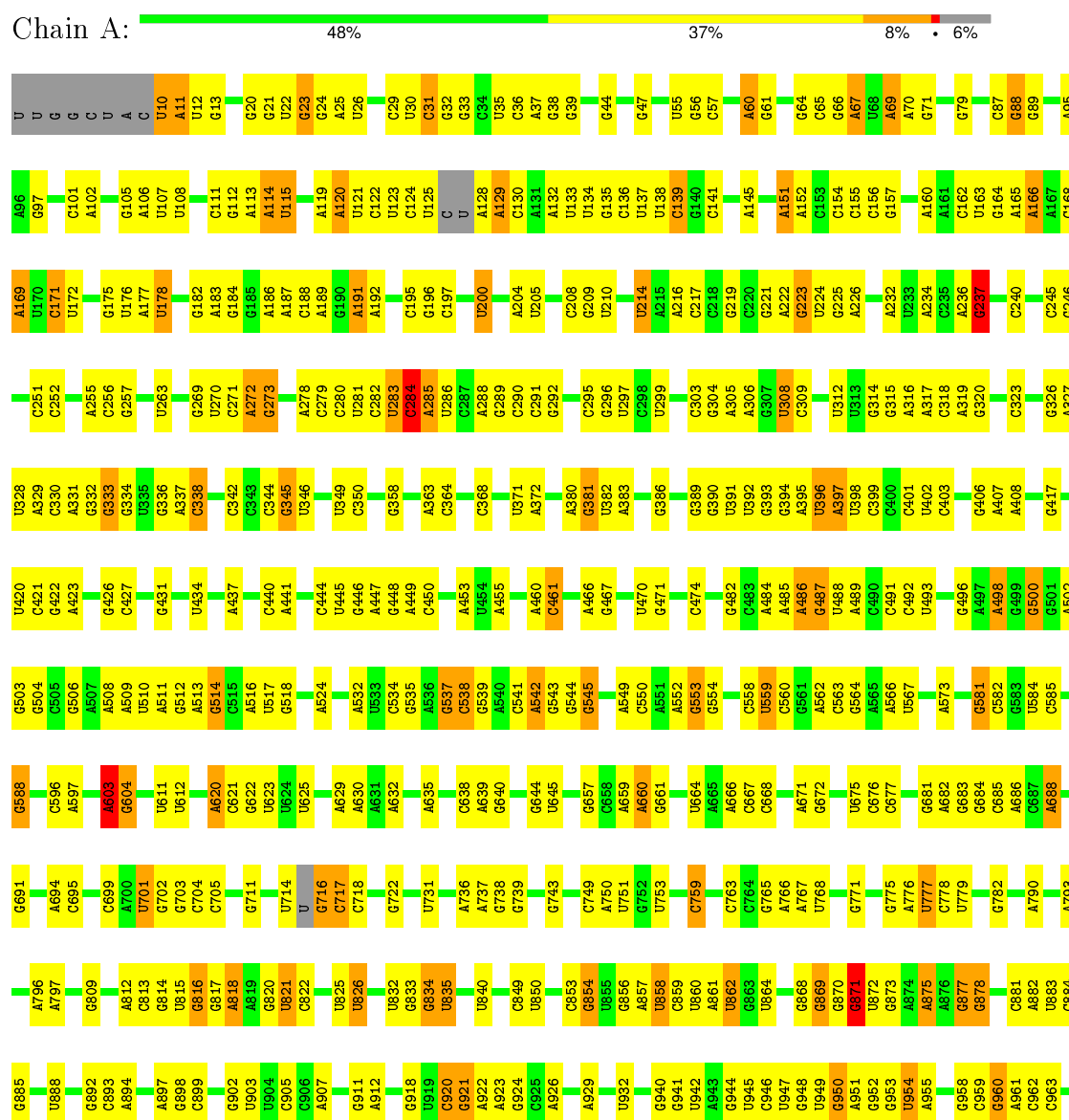
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	P	45	Total 45	O 45	0	0
37	Q	72	Total 72	O 72	0	0
37	R	57	Total 57	O 57	0	0
37	S	87	Total 87	O 87	0	0
37	T	34	Total 34	O 34	0	0
37	U	33	Total 33	O 33	0	0
37	V	27	Total 27	O 27	0	0
37	W	16	Total 16	O 16	0	0
37	X	68	Total 68	O 68	0	0
37	Y	27	Total 27	O 27	0	0
37	Z	100	Total 100	O 100	0	0
37	1	35	Total 35	O 35	0	0
37	2	57	Total 57	O 57	0	0
37	3	40	Total 40	O 40	0	0
37	4	72	Total 72	O 72	0	0

3 Residue-property plots

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

Note EDS was not executed.

• Molecule 1: 23S ribosomal RNA



C2248	C2249	G2250	G2251	A2252	A2255	G2256	A2258	C2262	G2263	A2264	G2265	A2266	G2267	G2270	G2271	G2272	U2276	U2277	U2278	G2279	A2280	G2281	U2282	G2289	U2290	C2291	G2292	G2293	A2300	A2301	A2302	U2308	C2309	A2310	G2311	G2312	C2313	C2314	C2315	G2316	G2317	U2320	A2321	U2322	G2323	G2324	C2325	U2326																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
C	G	C	G	U	A	G	C	C	U	A	C	C	G	G	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
G2121	C2122	A2123	C2126	U2127	G2128	U2133	G2134	A2135	G2136	A	C	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
C2029	U2032	G2033	U2034	C2035	A2038	A2039	G2040	G2041	G2063	A2064	A2065	U2066	U2067	U2068	U2069	U2070	U2071	U2072	U2073	U2074	A2081	A2082	A2083	A2084	A2085	C2088	A2089	G2090	G2091	G2092	G2093	G2094	A2095	G2096	G2097	A2100	A2101	G2102	A2103	C2104	C2105	C2106	G2110	G2111	C2114	U2115	U2116	U2117	A2118	C2119	U2120																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
A1942	C1943	G1944	G1945	G1946	G1947	G1951	U	A	A	C	C	U	A	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
A1859	U1860	C1861	C1862	C1863	C1864	A1865	A1866	C1867	A1868	A1869	C1872	G1873	U1874	U1875	U1876	U1877	U1878	U1879	U1880	U1881	U1882	U1883	U1884	U1885	U1886	U1887	U1888	U1889	U1890	U1891	U1892	U1893	U1894	U1895	U1896	U1897	U1898	U1899	U1900	U1901	U1902	U1903	U1904	U1905	U1906	U1907	U1908	U1909	U1910																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
C1768	C1769	U1770	U1771	C1772	C1773	C1774	C1775	C1776	C1777	C1778	C1779	C1780	C1781	C1782	C1783	C1784	C1785	C1786	C1787	C1788	C1789	C1790	C1791	C1792	C1793	C1794	C1795	C1796	C1797	C1798	C1799	C1800	C1801	C1802	C1803	C1804	C1805	C1806	C1807	C1808	C1809	C1810	C1811	C1812	C1813	C1814	C1815	C1816	C1817	C1818	C1819	C1820	C1821	C1822	C1823	C1824	C1825	C1826	C1827	C1828	C1829	C1830	C1831	C1832	C1833	C1834	C1835	C1836	C1837	C1838	C1839	C1840	C1841	C1842	C1843	C1844	C1845	C1846	C1847	C1848	C1849	C1850	C1851	C1852	C1853	C1854	C1855	C1856	C1857	C1858	C1859	C1860	C1861	C1862	C1863	C1864	C1865	C1866	C1867	C1868	C1869	C1870	C1871	C1872	C1873	C1874	C1875	C1876	C1877	C1878	C1879	C1880	C1881	C1882	C1883	C1884	C1885	C1886	C1887	C1888	C1889	C1890	C1891	C1892	C1893	C1894	C1895	C1896	C1897	C1898	C1899	C1900	C1901	C1902	C1903	C1904	C1905	C1906	C1907	C1908	C1909	C1910	C1911	C1912	C1913	C1914	C1915	C1916	C1917	C1918	C1919	C1920	C1921	C1922	C1923	C1924	C1925	C1926	C1927	C1928	C1929	C1930	C1931	C1932	C1933	C1934	C1935	C1936	C1937	C1938	C1939	C1940	C1941	C1942	C1943	C1944	C1945	C1946	C1947	C1948	C1949	C1950	C1951	C1952	C1953	C1954	C1955	C1956	C1957	C1958	C1959	C1960	C1961	C1962	C1963	C1964	C1965	C1966	C1967	C1968	C1969	C1970	C1971	C1972	C1973	C1974	C1975	C1976	C1977	C1978	C1979	C1980	C1981	C1982	C1983	C1984	C1985	C1986	C1987	C1988	C1989	C1990	C1991	C1992	C1993	C1994	C1995	C1996	C1997	C1998	C1999	C2000	C2001	C2002	C2003	C2004	C2005	C2006	C2007	C2008	C2009	C2010	C2011	C2012	C2013	C2014	C2015	C2016	C2017	C2018	C2019	C2020	C2021	C2022	C2023	C2024	C2025	C2026	C2027	C2028	C2029	C2030	C2031	C2032	C2033	C2034	C2035	C2036	C2037	C2038	C2039	C2040	C2041	C2042	C2043	C2044	C2045	C2046	C2047	C2048	C2049	C2050	C2051	C2052	C2053	C2054	C2055	C2056	C2057	C2058	C2059	C2060	C2061	C2062	C2063	C2064	C2065	C2066	C2067	C2068	C2069	C2070	C2071	C2072	C2073	C2074	C2075	C2076	C2077	C2078	C2079	C2080	C2081	C2082	C2083	C2084	C2085	C2086	C2087	C2088	C2089	C2090	C2091	C2092	C2093	C2094	C2095	C2096	C2097	C2098	C2099	C2100	C2101	C2102	C2103	C2104	C2105	C2106	C2107	C2108	C2109	C2110	C2111	C2112	C2113	C2114	C2115	C2116	C2117	C2118	C2119	C2120	C2121	C2122	C2123	C2124	C2125	C2126	C2127	C2128	C2129	C2130	C2131	C2132	C2133	C2134	C2135	C2136	C2137	C2138	C2139	C2140	C2141	C2142	C2143	C2144	C2145	C2146	C2147	C2148	C2149	C2150	C2151	C2152	C2153	C2154	C2155	C2156	C2157	C2158	C2159	C2160	C2161	C2162	C2163	C2164	C2165	C2166	C2167	C2168	C2169	C2170	C2171	C2172	C2173	C2174	C2175	C2176	C2177	C2178	C2179	C2180	C2181	C2182	C2183	C2184	C2185	C2186	C2187	C2188	C2189	C2190	C2191	C2192	C2193	C2194	C2195	C2196	C2197	C2198	C2199	C2200	C2201	C2202	C2203	C2204	C2205	C2206	C2207	C2208	C2209	C2210	C2211	C2212	C2213	C2214	C2215	C2216	C2217	C2218	C2219	C2220	C2221	C2222	C2223	C2224	C2225	C2226	C2227	C2228	C2229	C2230	C2231	C2232	C2233	C2234	C2235	C2236	C2237	C2238	C2239	C2240	C2241	C2242	C2243	C2244	C2245	C2246	C2247	C2248	C2249	C2250	C2251	C2252	C2253	C2254	C2255	C2256	C2257	C2258	C2259	C2260	C2261	C2262	C2263	C2264	C2265	C2266	C2267	C2268	C2269	C2270	C2271	C2272	C2273	C2274	C2275	C2276	C2277	C2278	C2279	C2280	C2281	C2282	C2283	C2284	C2285	C2286	C2287	C2288	C2289	C2290	C2291	C2292	C2293	C2294	C2295	C2296	C2297	C2298	C2299	C2300	C2301	C2302	C2303	C2304	C2305	C2306	C2307	C2308	C2309	C2310	C2311	C2312	C2313	C2314	C2315	C2316	C2317	C2318	C2319	C2320	C2321	C2322	C2323	C2324	C2325	C2326	C2327	C2328	C2329	C2330	C2331	C2332	C2333	C2334	C2335	C2336	C2337	C2338	C2339	C2340	C2341	C2342	C2343	C2344	C2345	C2346	C2347	C2348	C2349	C2350	C2351	C2352	C2353	C2354	C2355	C2356	C2357	C2358	C2359	C2360	C2361	C2362	C2363	C2364	C2365	C2366	C2367	C2368	C2369	C2370	C2371	C2372	C2373	C2374	C2375	C2376	C2377	C2378	C2379	C2380	C2381	C2382	C2383	C2384	C2385	C2386	C2387	C2388	C2389	C2390	C2391	C2392	C2393	C2394	C2395	C2396	C2397	C2398	C2399	C2400	C2401	C2402	C2403	C2404	C2405	C2406	C2407	C2408	C2409	C2410	C2411	C2412	C2413	C2414	C2415	C2416	C2417	C2418	C2419	C2420	C2421	C2422	C2423	C2424	C2425	C2426	C2427	C2428	C2429	C2430	C2431	C2432	C2433	C2434	C2435	C2436	C2437	C2438	C2439	C2440	C2441	C2442	C2443	C2444	C2445	C2446	C2447	C2448	C2449	C2450	C2451	C2452	C2453	C2454	C2455	C2456	C2457	C2458	C2459	C2460	C2461	C2462	C2463	C2464	C2465	C2466	C2467	C2468	C2469	C2470	C2471	C2472	C2473	C2474	C2475	C2476	C2477	C2478	C2479	C2480	C2481	C2482	C2483	C2484	C2485	C2486	C2487	C2488	C2489	C2490	C2491	C2492	C2493	C2494	C2495	C2496	C2497	C2498	C2499	C2500	C2501	C2502	C2503	C2504	C2505	C2506	C2507	C2508	C2509	C2510	C2511	C2512	C2513	C2514	C2515	C2516	C2517	C2518	C2519	C2520	C2521	C2522	C2523	C2524	C2525	C2526	C2527	C2528	C2529	C2530	C2531	C2532	C2533	C2534	C2535	C2536	C2537	C2538	C2539	C2540	C2541	C2542	C2543	C2544	C2545	C2546	C2547	C2548	C2549	C2550	C2551	C2552	C2553	C2554	C2555	C2556	C2557	C2558	C2559	C2560	C2561	C2562	C2563	C2564	C2565	C2566	C2567	C2568	C2569	C2570	C2571	C2572	C2573	C2574	C2575	C2576	C2577	C2578	C2579	C2580	C2581	C2582	C2583	C2584	C2585	C2586	C2587	C2588	C2589	C2590	C2591	C2592	C2593	C2594	C2595	C2596	C2597	C2598	C2599	C2600	C2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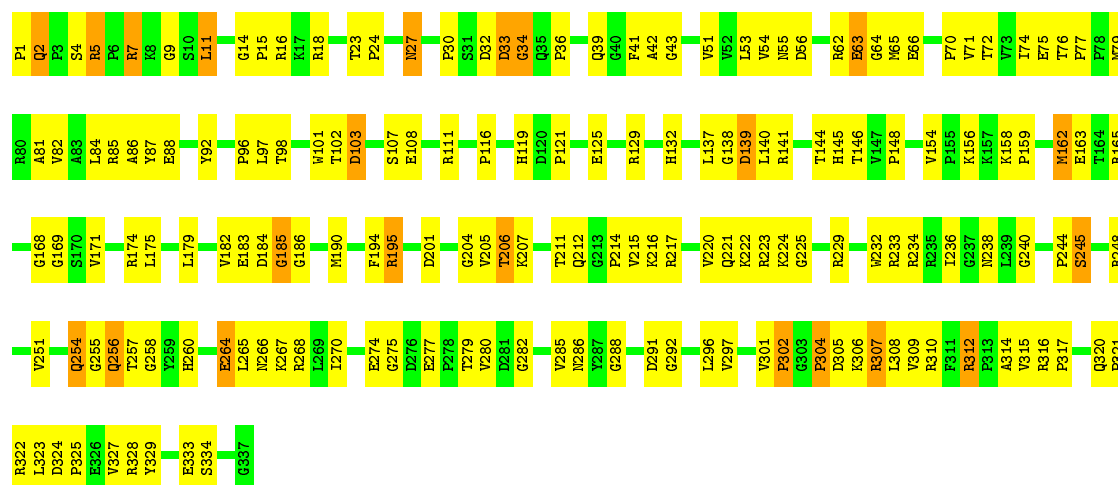
G3066	U3001
U3069	A3002
U3070	A3003
G3076	G3006
A3077	G3007
G3078	G3008
U3079	G3009
G3092	G3012
A3093	A3013
	G3014
U3099	G3019
G3100	G3020
G3101	G3021
G3102	G3022
A3103	U3023
A3104	U3024
A3105	G3025
G3106	G3026
G3107	G3027
G3108	U3028
	G3029
G3113	G3030
G3114	G3031
	G3032
G3122	U3033
	A3034
	G3035
	G3036
	G3037
	A3038
	U3039
	G3040
	G3041
	G3042
	G3043
	A3044
	A3045
	G3046
	A3047
	G3048
	G3049
	G3050
	A3051
	A3052
	G3053
	A3054
	U3055
	A3056
	A3057
	G3058
	G3059
	G3060
	G3061
	A3062
	G3063
	G3064
	G3065

- Molecule 3: 50S ribosomal protein L2P

V158	V159	G162	G163	R164	K171	A172	G173	M174	K175	H176	K178	M179	M186	P187	R190	G191	V192	A193	M194	N195	A196	V197	H198	H199	P200	F201	R206	Q207	K211	P212	I215	S216	R217	R223	K224	V225	A229	S230	K231	R232	T233	G234	G237	ASN	GLU				
Q81	V82	G83	V84	D85	I88	N92	T93	L94	P95	E98	I99	P100	E101	G102	V103	P104	V105	G106	N107	V108	A109	S110	D114	G115	G116	K117	F118	A119	R120	A121	S122	G123	V124	N125	A126	H131	D132	L140	P141	E144	R147	R153	A154	T155					
G1	R2	R3	G6	Q7	R8	R9	G10	R11	F16	R17	A18	P19	S20	H21	R22	A25	E29	E33	D34	G35	D36	V37	I38	A39	V42	V43	D44	I45	E46	H47	D48	P49	A50	R51	S52	A53	P54	V55	A56	A57	E51	D52	R65	R66	L67	I68	L69	G75	V76

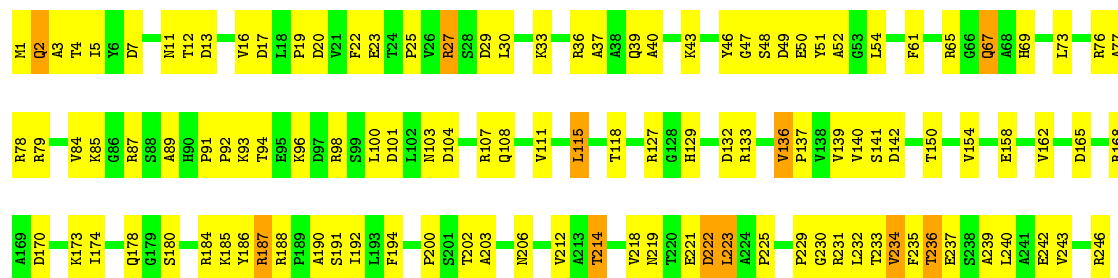
- Molecule 4: 50S ribosomal protein L3P

Chain D:  49% 45% 7%



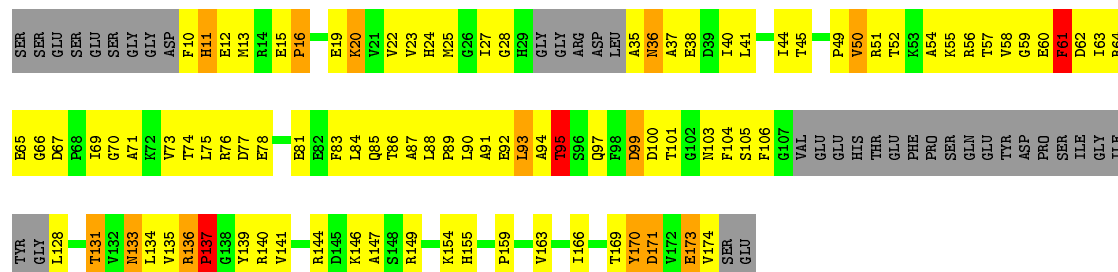
• Molecule 5: 50S ribosomal protein L4E

Chain E: 52% 43%



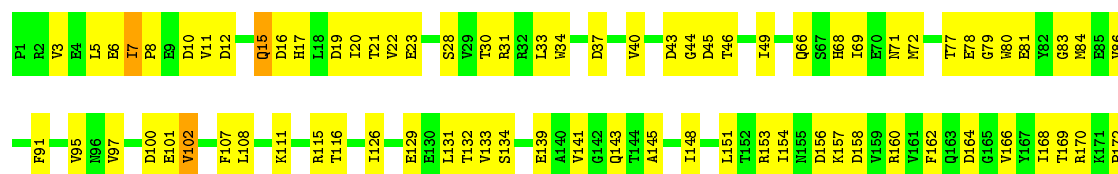
• Molecule 6: 50S ribosomal protein L5P

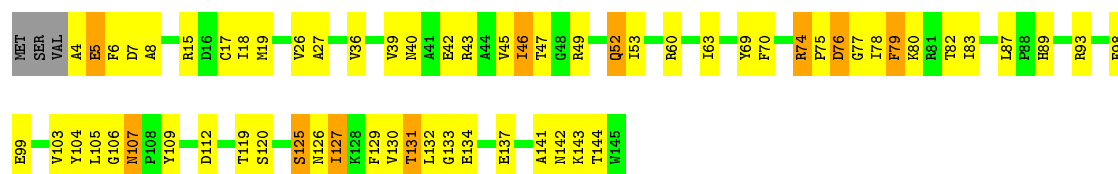
Chain F: 26% 45% 7% 20%



• Molecule 7: 50S ribosomal protein L6P

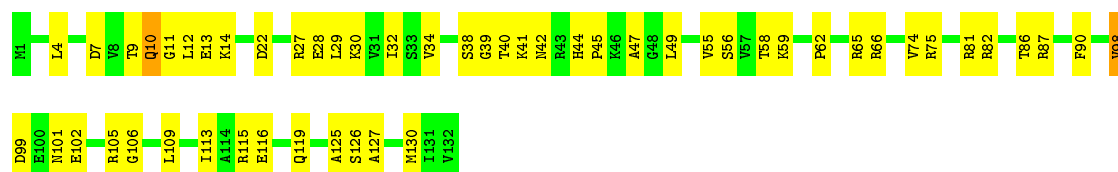
Chain G: 54% 42%





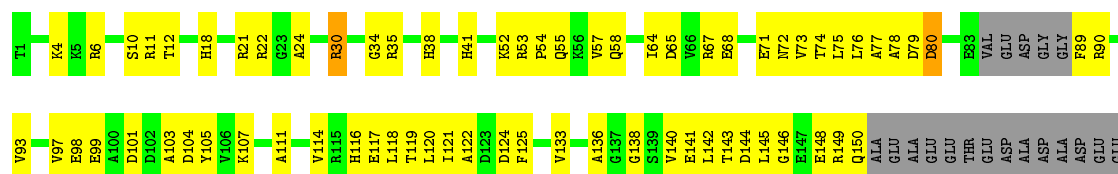
• Molecule 12: 50S ribosomal protein L14P

Chain L: 60% 39%



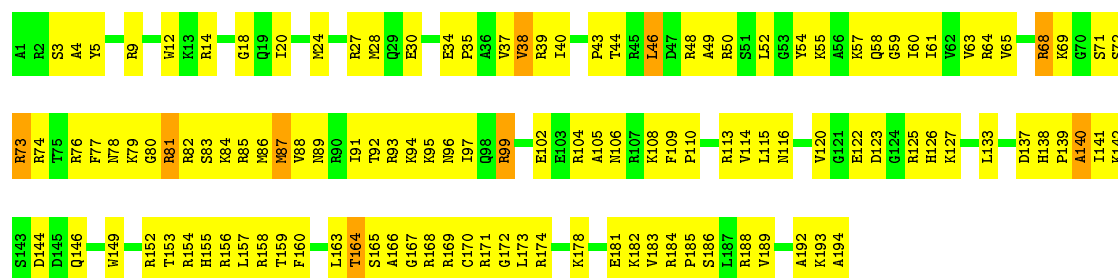
• Molecule 13: 50S ribosomal protein L15P

Chain M: 46% 41% 12%



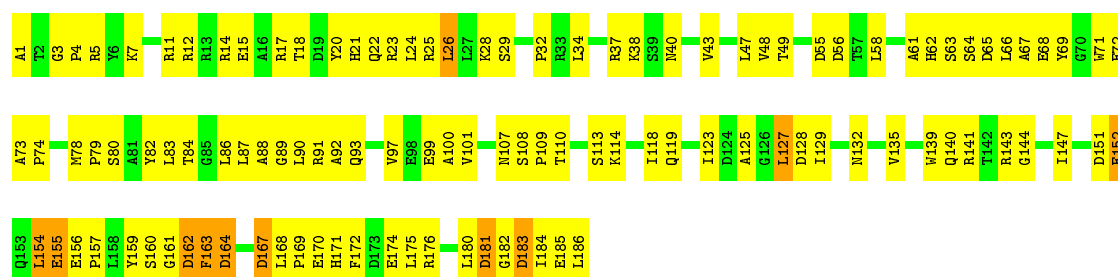
• Molecule 14: 50S ribosomal protein L15E

Chain N: 37% 59% 5%

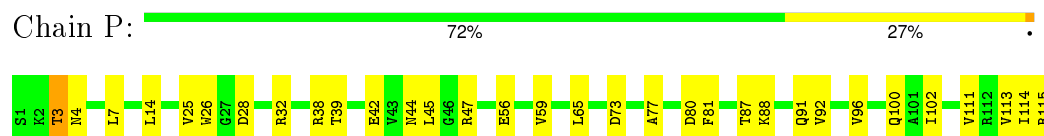


• Molecule 15: 50S ribosomal protein L18P

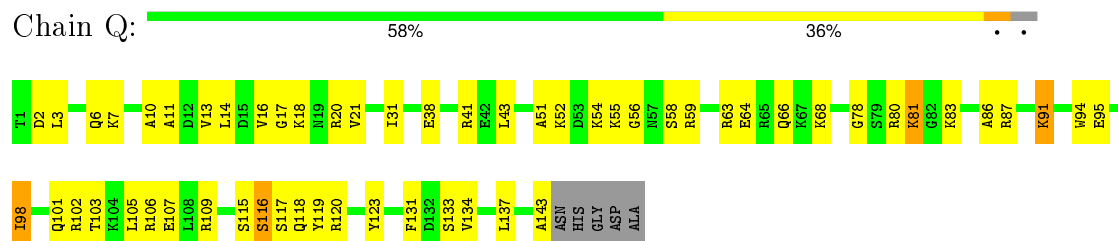
Chain O: 40% 54% 6%



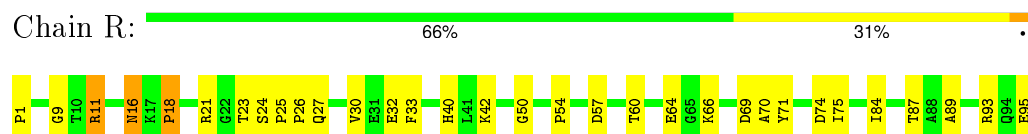
- Molecule 16: 50S ribosomal protein L18E



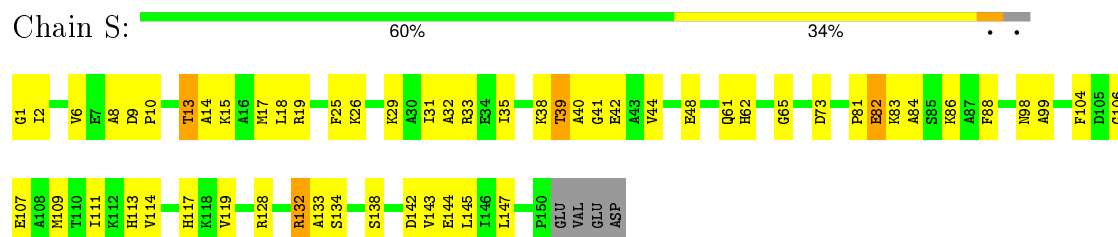
- Molecule 17: 50S ribosomal protein L19E



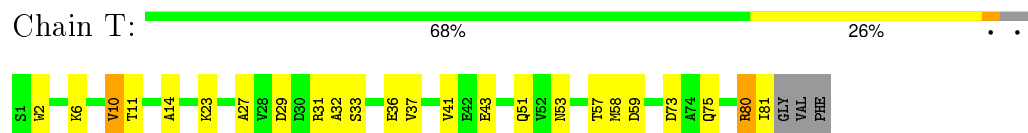
- Molecule 18: 50S ribosomal protein L21e



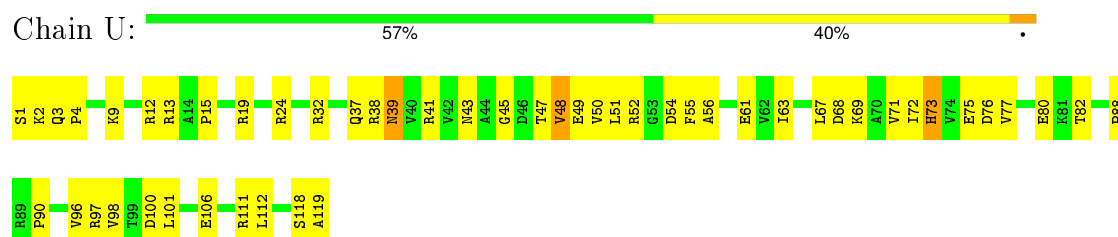
- Molecule 19: 50S ribosomal protein L22P



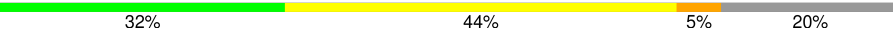
- Molecule 20: 50S ribosomal protein L23P

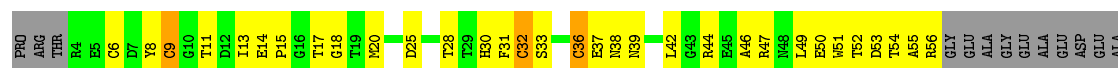


- Molecule 21: 50S ribosomal protein L24P



- Molecule 22: 50S ribosomal protein L24E

Chain V: 



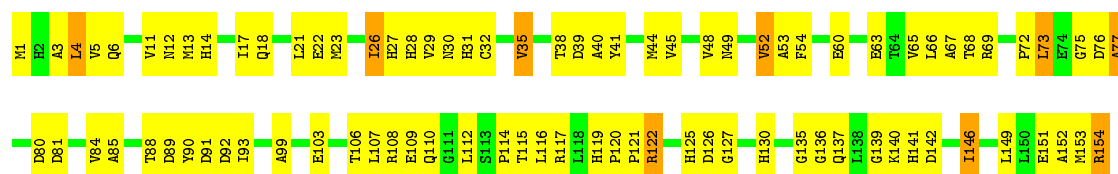
- Molecule 23: 50S ribosomal protein L29P

Chain W: 



- Molecule 24: 50S ribosomal protein L30P

Chain X: 



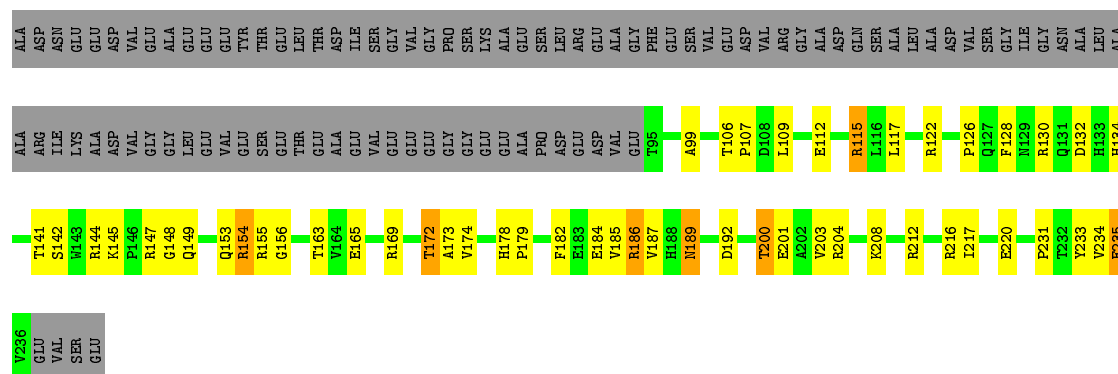
- Molecule 25: 50S ribosomal protein L31E

Chain Y: 

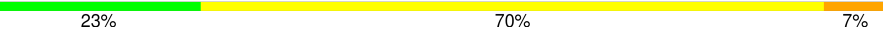


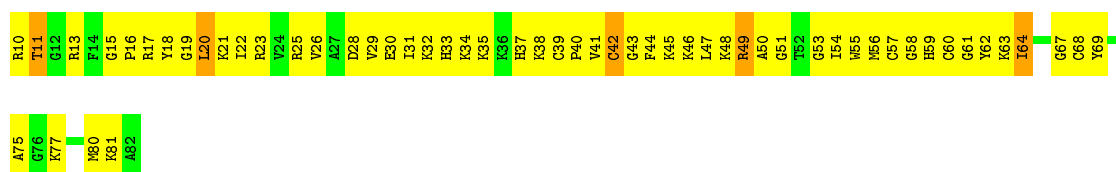
- Molecule 26: 50S ribosomal protein L32E

Chain Z: 



- Molecule 27: 50S ribosomal protein L37AE

Chain 1: 



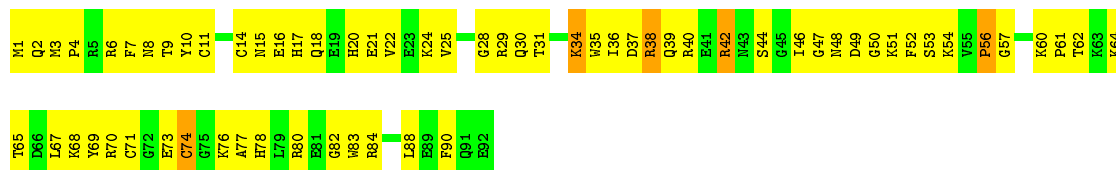
- Molecule 28: 50S ribosomal protein L37e



- Molecule 29: 50S ribosomal protein L39e



- Molecule 30: 50S ribosomal protein L44E



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.90 Å 300.47 Å 575.18 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	94.6 (20.00-3.00)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.201 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	98569	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, NA, K, CD, VIR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.57	9/66076 (0.0%)	0.76	37/103052 (0.0%)
2	B	0.81	10/2905 (0.3%)	0.91	17/4528 (0.4%)
3	C	0.44	0/1787	0.75	0/2409
4	D	0.41	0/2689	0.71	0/3652
5	E	0.48	0/1883	0.74	0/2551
6	F	0.40	0/1111	0.64	0/1498
7	G	0.44	0/1382	0.66	0/1880
8	H	0.40	0/896	0.63	0/1219
9	I	0.33	0/241	0.53	0/324
10	J	0.46	0/1246	0.83	2/1686 (0.1%)
11	K	0.46	0/1135	0.70	0/1530
12	L	0.43	0/1003	0.75	0/1351
13	M	0.42	0/1126	0.75	0/1504
14	N	0.63	0/1633	0.86	1/2180 (0.0%)
15	O	0.42	0/1473	0.71	0/1999
16	P	0.45	0/873	0.71	0/1181
17	Q	0.44	0/1143	0.64	0/1521
18	R	0.45	0/748	0.79	0/1005
19	S	0.45	0/1172	0.76	0/1578
20	T	0.41	0/648	0.65	0/875
21	U	0.38	0/957	0.70	0/1289
22	V	0.82	0/417	0.81	1/562 (0.2%)
23	W	0.40	0/502	0.61	0/675
24	X	0.50	0/1218	0.73	0/1655
25	Y	0.44	0/664	0.70	0/895
26	Z	0.46	0/1146	0.72	0/1536
27	1	0.77	0/575	0.82	0/763
28	2	0.54	0/437	0.78	0/578
29	3	0.42	0/398	0.63	0/527
30	4	0.98	0/771	0.81	0/1024
All	All	0.56	19/98255 (0.0%)	0.76	58/147027 (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
1	A	1	157
2	B	0	4
All	All	1	161

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2488	A	O5'-C5'	-8.71	1.28	1.42
2	B	3025	G	C2'-O2'	-7.62	1.31	1.41
2	B	3003	A	O5'-C5'	7.52	1.56	1.44
2	B	3024	U	O5'-C5'	7.15	1.55	1.44
2	B	3023	U	C4'-O4'	7.08	1.54	1.45

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP2-P-O3'	-18.66	64.14	105.20
1	A	1164	U	OP1-P-O3'	-18.19	65.19	105.20
1	A	1979	G	C2'-C3'-O3'	9.72	130.90	109.50
1	A	1563	G	C2'-C3'-O3'	9.58	130.58	109.50
1	A	1165	G	O5'-P-OP1	-8.38	98.16	105.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'

5 of 161 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	U	Sidechain
1	A	23	G	Sidechain
1	A	26	U	Sidechain
1	A	32	G	Sidechain
1	A	33	G	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	59017	0	29801	1306	0
2	B	2600	0	1326	85	0
3	C	1754	0	1763	144	0
4	D	2624	0	2533	195	0
5	E	1858	0	1816	146	0
6	F	1094	0	1085	135	0
7	G	1357	0	1266	79	0
8	H	885	0	854	73	0
9	I	240	0	231	23	0
10	J	1215	0	1215	168	0
11	K	1119	0	1098	70	0
12	L	993	0	1027	60	0
13	M	1114	0	1072	79	0
14	N	1605	0	1676	212	0
15	O	1444	0	1401	152	0
16	P	864	0	873	29	0
17	Q	1133	0	1127	68	0
18	R	734	0	729	27	0
19	S	1149	0	1122	68	0
20	T	641	0	605	26	0
21	U	949	0	923	52	0
22	V	410	0	368	48	0
23	W	499	0	511	30	0
24	X	1195	0	1137	115	0
25	Y	654	0	653	48	0
26	Z	1130	0	1133	62	0
27	1	563	0	601	83	0
28	2	430	0	426	30	0
29	3	393	0	406	22	0
30	4	755	0	732	89	0
31	A	38	0	34	3	0
32	4	1	0	0	0	0
32	A	109	0	0	0	0
32	B	1	0	0	0	0
32	C	2	0	0	0	0
32	D	1	0	0	0	0
32	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	1	0	0	0	0
34	4	1	0	0	0	0
34	A	71	0	0	0	0
34	B	2	0	0	0	0
34	C	1	0	0	0	0
34	E	1	0	0	0	0
34	J	2	0	0	0	0
34	K	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	R	1	0	0	0	0
34	S	2	0	0	0	0
34	T	1	0	0	0	0
34	U	1	0	0	0	0
35	4	1	0	0	1	0
35	A	8	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	K	3	0	0	1	0
35	L	1	0	0	0	0
35	M	1	0	0	2	0
35	N	1	0	0	2	0
35	O	1	0	0	1	0
35	P	1	0	0	0	0
35	S	1	0	0	0	0
35	Z	2	0	0	0	0
36	1	1	0	0	0	0
36	2	1	0	0	0	0
36	4	1	0	0	0	0
36	P	1	0	0	0	0
36	V	1	0	0	0	0
37	1	35	0	0	15	0
37	2	57	0	0	1	0
37	3	40	0	0	6	0
37	4	72	0	0	11	0
37	A	5881	0	0	302	0
37	B	146	0	0	21	0
37	C	135	0	0	15	0
37	D	141	0	0	33	0
37	E	178	0	0	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	F	49	0	0	17	0
37	G	43	0	0	10	0
37	H	30	0	0	11	0
37	I	21	0	0	7	0
37	J	76	0	0	23	0
37	K	55	0	0	6	0
37	L	64	0	0	16	0
37	M	85	0	0	21	0
37	N	141	0	0	35	0
37	O	67	0	0	20	0
37	P	45	0	0	10	0
37	Q	72	0	0	10	0
37	R	57	0	0	3	0
37	S	87	0	0	10	0
37	T	34	0	0	5	0
37	U	33	0	0	6	0
37	V	27	0	0	6	0
37	W	16	0	0	2	0
37	X	68	0	0	11	0
37	Y	27	0	0	5	0
37	Z	100	0	0	14	0
All	All	98569	0	59544	3401	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 23.

The worst 5 of 3401 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)
10:J:86:ARG:NH1	10:J:133:ILE:HG13	1.52	1.20
10:J:165:GLY:HA3	37:J:8397:HOH:O	1.39	1.18
27:1:39:CYS:SG	27:1:47:LEU:HD21	1.84	1.17
14:N:87:MET:HG2	30:4:46:ILE:HG21	1.25	1.15
21:U:71:VAL:HG11	21:U:90:PRO:HB3	1.31	1.11

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	235/239 (98%)	200 (85%)	29 (12%)	6 (3%)	7	33
4	D	335/337 (99%)	302 (90%)	22 (7%)	11 (3%)	5	26
5	E	244/246 (99%)	222 (91%)	22 (9%)	0	100	100
6	F	134/176 (76%)	95 (71%)	27 (20%)	12 (9%)	1	4
7	G	170/177 (96%)	157 (92%)	12 (7%)	1 (1%)	30	72
8	H	117/119 (98%)	104 (89%)	10 (8%)	3 (3%)	7	33
9	I	25/348 (7%)	23 (92%)	1 (4%)	1 (4%)	4	21
10	J	152/167 (91%)	130 (86%)	17 (11%)	5 (3%)	5	26
11	K	140/145 (97%)	127 (91%)	8 (6%)	5 (4%)	4	24
12	L	130/132 (98%)	120 (92%)	8 (6%)	2 (2%)	13	50
13	M	141/164 (86%)	120 (85%)	20 (14%)	1 (1%)	26	70
14	N	192/194 (99%)	165 (86%)	24 (12%)	3 (2%)	12	48
15	O	184/186 (99%)	164 (89%)	12 (6%)	8 (4%)	3	19
16	P	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
17	Q	141/148 (95%)	135 (96%)	5 (4%)	1 (1%)	26	70
18	R	93/95 (98%)	86 (92%)	3 (3%)	4 (4%)	3	19
19	S	148/154 (96%)	134 (90%)	13 (9%)	1 (1%)	26	70
20	T	79/84 (94%)	73 (92%)	6 (8%)	0	100	100
21	U	117/119 (98%)	110 (94%)	7 (6%)	0	100	100
22	V	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
23	W	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	5	27
24	X	152/154 (99%)	142 (93%)	8 (5%)	2 (1%)	15	53
25	Y	80/91 (88%)	71 (89%)	5 (6%)	4 (5%)	3	15
26	Z	140/240 (58%)	133 (95%)	7 (5%)	0	100	100
27	1	71/73 (97%)	61 (86%)	7 (10%)	3 (4%)	3	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	2	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
29	3	42/48 (88%)	41 (98%)	1 (2%)	0	100	100
30	4	90/92 (98%)	83 (92%)	5 (6%)	2 (2%)	8	38
All	All	3633/4235 (86%)	3265 (90%)	291 (8%)	77 (2%)	9	40

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	139	ASP
6	F	93	LEU
6	F	95	THR
6	F	173	GLU
8	H	101	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	179/181 (99%)	166 (93%)	13 (7%)	17	52
4	D	282/282 (100%)	264 (94%)	18 (6%)	22	59
5	E	193/193 (100%)	178 (92%)	15 (8%)	16	49
6	F	117/147 (80%)	106 (91%)	11 (9%)	11	39
7	G	152/155 (98%)	148 (97%)	4 (3%)	54	85
8	H	92/92 (100%)	91 (99%)	1 (1%)	80	94
9	I	27/283 (10%)	27 (100%)	0	100	100
10	J	122/122 (100%)	111 (91%)	11 (9%)	12	41
11	K	118/121 (98%)	107 (91%)	11 (9%)	11	39
12	L	106/106 (100%)	102 (96%)	4 (4%)	40	78
13	M	112/126 (89%)	108 (96%)	4 (4%)	42	79
14	N	166/166 (100%)	158 (95%)	8 (5%)	31	71
15	O	149/149 (100%)	144 (97%)	5 (3%)	44	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	93/93 (100%)	91 (98%)	2 (2%)	60	88
17	Q	113/116 (97%)	109 (96%)	4 (4%)	43	80
18	R	79/79 (100%)	75 (95%)	4 (5%)	29	69
19	S	117/121 (97%)	113 (97%)	4 (3%)	44	81
20	T	71/73 (97%)	69 (97%)	2 (3%)	51	84
21	U	105/105 (100%)	102 (97%)	3 (3%)	50	84
22	V	44/52 (85%)	42 (96%)	2 (4%)	34	74
23	W	51/56 (91%)	51 (100%)	0	100	100
24	X	130/130 (100%)	121 (93%)	9 (7%)	19	56
25	Y	66/73 (90%)	61 (92%)	5 (8%)	16	51
26	Z	120/195 (62%)	110 (92%)	10 (8%)	14	46
27	1	56/56 (100%)	49 (88%)	7 (12%)	6	24
28	2	46/46 (100%)	46 (100%)	0	100	100
29	3	42/44 (96%)	41 (98%)	1 (2%)	57	87
30	4	79/79 (100%)	73 (92%)	6 (8%)	16	51
All	All	3027/3441 (88%)	2863 (95%)	164 (5%)	27	66

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	52	GLN
13	M	117	GLU
27	1	32	LYS
11	K	76	ASP
11	K	131	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	116	HIS
18	R	40	HIS
29	3	18	ASN
14	N	58	GLN
15	O	153	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	248 (9%)	38 (1%)
2	B	121/122 (99%)	14 (11%)	4 (3%)
All	All	2868/3044 (94%)	262 (9%)	42 (1%)

5 of 262 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	A
1	A	31	C
1	A	60	A
1	A	67	A
1	A	69	A

5 of 42 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1352	A
1	A	1667	A
2	B	3023	U
1	A	1377	C
1	A	1474	C

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 232 ligands modelled in this entry, 231 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
31	VIR	A	9403	-	34,40,40	2.38	15 (44%)	37,55,55	2.17	10 (27%)

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
31	VIR	A	9403	-	-	0/42/58/58	0/1/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	9403	VIR	C28-C29	-6.50	1.15	1.32
31	A	9403	VIR	C17-C19	-3.06	1.46	1.50
31	A	9403	VIR	C13-C14	-3.00	1.46	1.51
31	A	9403	VIR	C1-C37	-2.62	1.38	1.47
31	A	9403	VIR	C16-C17	-2.49	1.50	1.54

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	9403	VIR	C28-C26-N25	-4.96	103.44	114.87
31	A	9403	VIR	C8-C6-N5	-3.21	110.64	118.55
31	A	9403	VIR	C24-N25-C26	-2.29	119.17	121.76
31	A	9403	VIR	C12-C8-C6	-2.20	122.14	129.47
31	A	9403	VIR	C31-C30-C32	2.18	115.25	111.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	9403	VIR	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.