



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 18, 2017 – 04:34 AM EDT

PDB ID : 5U4I
EMDB ID: : EMD-8505
Title : Structural Basis of Co-translational Quality Control by ArfA and RF2 Bound to Ribosome
Authors : Zeng, F.; Chen, Y.; Remis, J.; Shekhar, M.; Phillips, J.C.; Tajkhorshid, E.; Jin, H.
Deposited on : unknown
Resolution : 3.50 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

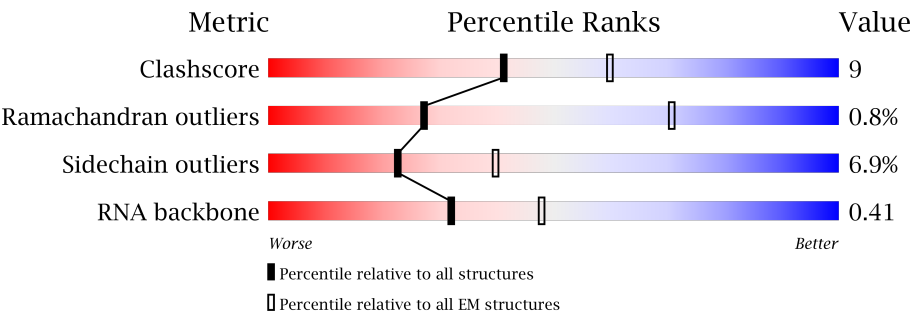
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.





















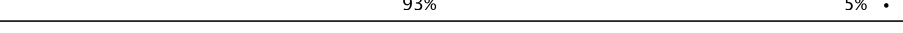






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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	A	2904	<div><div>40%</div><div>47%</div><div>13%</div></div>
2	B	118	<div><div>43%</div><div>47%</div><div>10%</div></div>
3	C	273	<div><div>78%</div><div>19%</div><div>..</div></div>
4	D	209	<div><div>83%</div><div>16%</div><div>.</div></div>
5	E	201	<div><div>84%</div><div>15%</div><div>.</div></div>
6	F	179	<div><div>82%</div><div>16%</div><div>..</div></div>
7	G	177	<div><div>86%</div><div>13%</div><div>.</div></div>
8	H	149	<div><div>88%</div><div>11%</div><div>.</div></div>






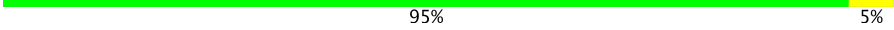


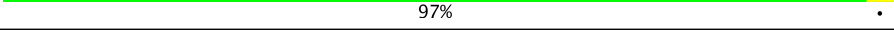
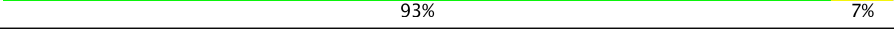

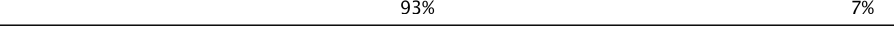

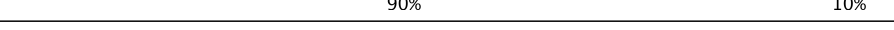



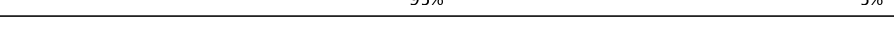



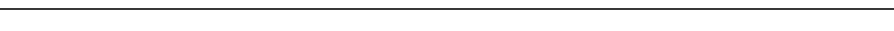


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Mol	Chain	Length	Quality of chain
9	J	142	 84% 14% ..
10	K	142	 92% 8% .
11	L	123	 80% 17% .
12	M	144	 83% 15% .
13	N	136	 85% 14% .
14	O	127	 73% 20% . 6%
15	P	117	 88% 11% .
16	Q	115	 89% 10% .
17	R	118	 80% 17% ..
18	S	103	 83% 15% ..
19	T	110	 79% 20% .
20	U	100	 83% 10% 7%
21	V	104	 79% 19% .
22	W	94	 82% 16% .
23	X	85	 75% 13% . 9%
24	Y	78	 76% 21% ..
25	Z	63	 87% 10% ..
26	0	59	 93% 5% .
27	1	57	 86% 11% ..
28	2	55	 73% 18% 9%
29	3	46	 89% 11%
30	4	65	 77% 22% .
31	5	38	 89% 11%
32	a	1533	 68% 32%
33	b	241	 87% 6% 7%

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Mol	Chain	Length	Quality of chain
34	c	233	
35	d	206	
36	e	167	
37	f	135	
38	g	179	
39	h	129	
40	i	130	
41	j	103	
42	k	117	
43	l	123	
44	m	118	
45	n	100	
46	o	88	
47	p	82	
48	q	84	
49	r	75	
50	s	82	
51	t	86	
52	u	71	
53	v	383	
54	w	57	
55	x	77	
55	y	77	
56	z	18	

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
1	PSU	A	2504	-	-	X	-

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 149495 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 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2904	Total	C	N	O	P	0	0
			62351	27820	11472	20155	2904		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	887	A	U	conflict	GB 42756

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	116	Total	C	N	O	S	0	0
			892	552	178	162			

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	117	Total	C	N	O	S	0	0
			947	604	192	151			

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	77	Total	C	N	O	S	0	0
			588	363	118	106	1		

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	0	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2	50	Total	C	N	O		0	0
			409	263	75	71			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	5	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1533	Total	C	N	O	P	0	0
			32906	14683	6036	10654	1533		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	527	A	G	conflict	GB 817573384

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	204	Total	C	N	O	S	0	0
			1633	1020	313	296	4		

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 45 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	65	Total	C	N	O	S	0	0
			539	341	100	97	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	15	GLU	ALA	conflict	UNP P0A7T7

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	82	Total	C	N	O	S	0	0
			658	421	125	110	2		

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 52 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	u	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 53 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	v	357	Total	C	N	O	S	0	0
			2836	1744	498	584	10		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	-17	HIS	-	expression tag	UNP P07012
v	-16	HIS	-	expression tag	UNP P07012
v	-15	HIS	-	expression tag	UNP P07012
v	-14	HIS	-	expression tag	UNP P07012
v	-13	HIS	-	expression tag	UNP P07012
v	-12	HIS	-	expression tag	UNP P07012
v	-11	SER	-	expression tag	UNP P07012
v	-10	ALA	-	expression tag	UNP P07012
v	-9	ALA	-	expression tag	UNP P07012
v	-8	LEU	-	expression tag	UNP P07012
v	-7	GLU	-	expression tag	UNP P07012
v	-6	VAL	-	expression tag	UNP P07012
v	-5	LEU	-	expression tag	UNP P07012
v	-4	PHE	-	expression tag	UNP P07012
v	-3	GLN	-	expression tag	UNP P07012
v	-2	GLY	-	expression tag	UNP P07012
v	-1	PRO	-	expression tag	UNP P07012
v	0	GLY	-	expression tag	UNP P07012

- Molecule 54 is a protein called Alternative ribosome-rescue factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	w	47	Total	C	N	O	S	0	0
			388	239	82	66	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
w	-1	GLY	-	expression tag	UNP P36675
w	0	SER	-	expression tag	UNP P36675

- Molecule 55 is a RNA chain called P-site or E-site fMet-tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace
55	x	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

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Mol	Chain	Residues	Atoms					AltConf	Trace
55	y	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	z	6	Total	C	N	O	P	0	0
			131	59	27	39	6		

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	B	4	Total	Mg	0
			4	4	
57	A	100	Total	Mg	0
			100	100	
57	a	20	Total	Mg	0
			20	20	

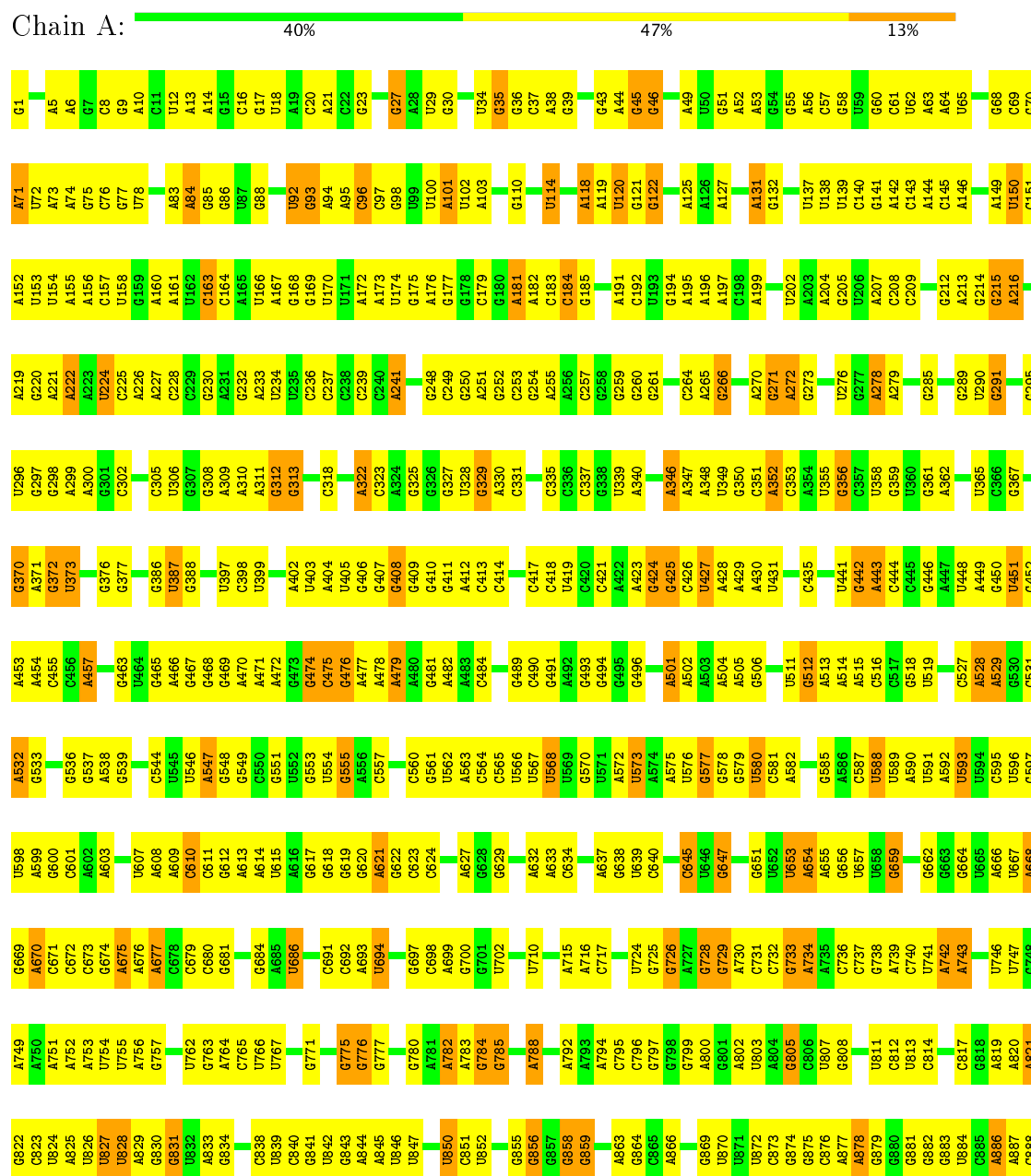
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	5	1	Total	Zn	0
			1	1	

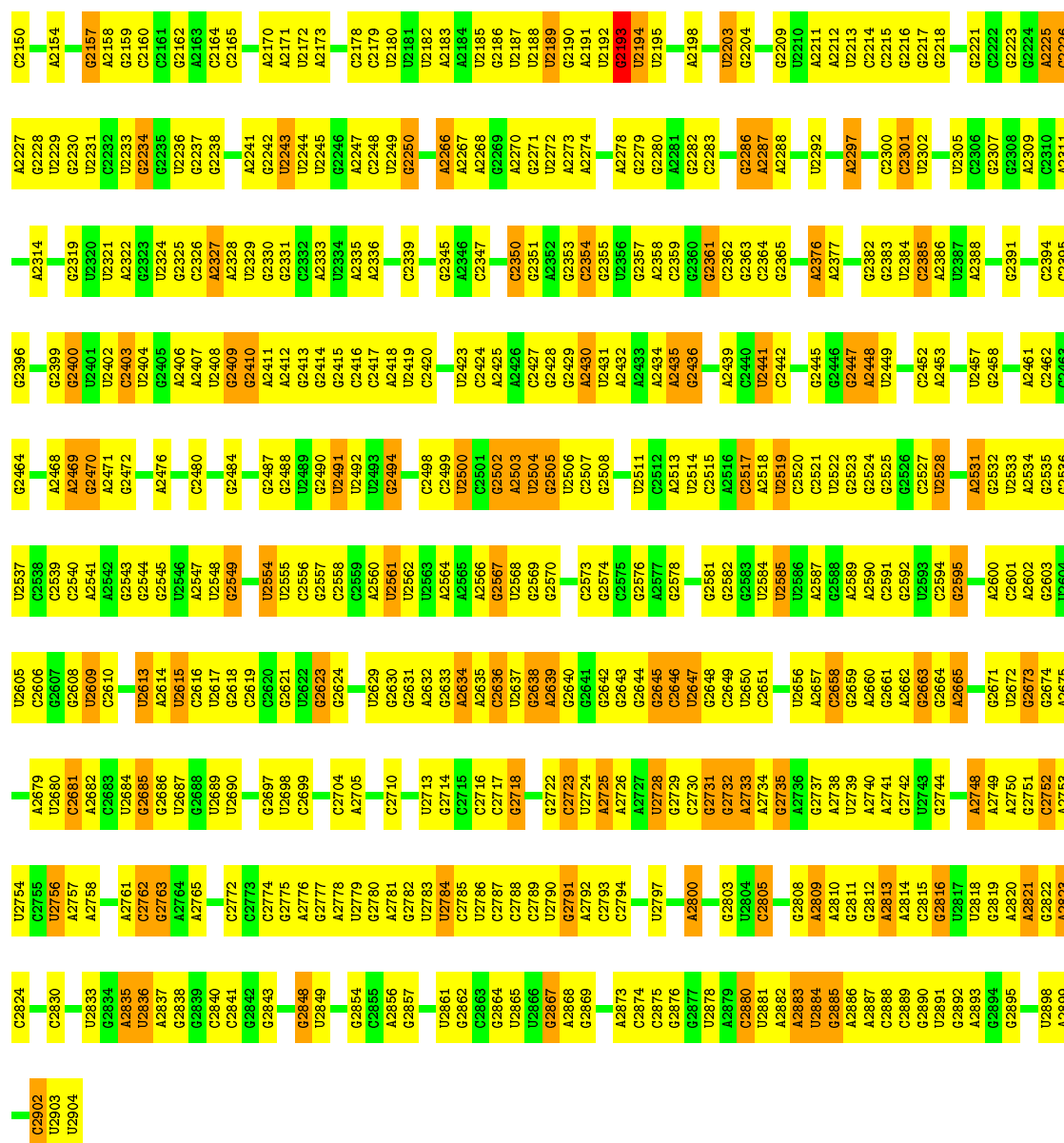
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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: 23S rRNA

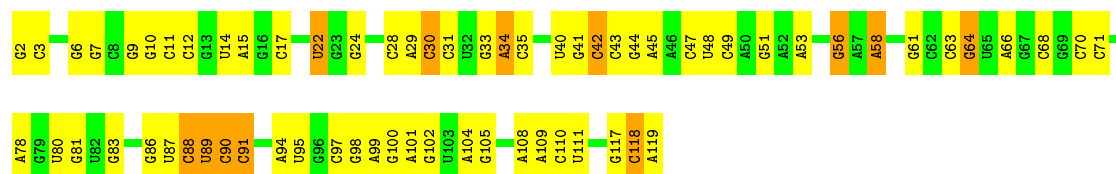


U2074	U2075	A2076	A2077	C2078	U2079	A2080	U2081	A2082	G2083	C2084	U2085	U2086	G2087	U2088	U2089	U2090	G2091	G2092	G2093	A2094	A2095	U2096	U2097	U2098	U2099	G2100	A2101	G2102	G2107	G2110	U2111	G2112	A2114	G2115	G2116	A2117	U2118	U2119	U2120	U2121	U2122	U2123	G2124	U2125	U2126	U2127	U2128	U2129	U2130	U2131	U2132	G2133	A2134	U2139	U2140	G2141	A2142	C2146	A2147	G2148	U2149																																																																																																																																																																																																																																																															
C1748	A1749	G1750	A1776	G1751	G1752	G1753	U1758	A1759	U1768	U1769	C1773	C1774	U1778	U1779	U1782	U1783	U1785	G1708	U1709	U1787	G1711	G1712	U1713	U1714	U1715	U1716	U1796	G1797	U1798	U1799	U1800	U1801	U1802	U1803	U1804	U1805	U1806	U1807	U1808	U1809	U1810	U1811	U1812	U1813	U1814	U1815	U1816	U1817	U1818	U1819	U1820	U1821	U1822	U1823	U1824	U1825	U1826	U1827	U1828	U1829																																																																																																																																																																																																																																																																
C1830	G1831	G1832	G1833	G1834	G1835	C1836	U1837	U1838	U1839	U1840	U1841	U1842	U1843	U1844	U1845	U1846	U1847	U1848	U1849	U1850	U1851	U1852	U1853	U1854	U1855	U1856	U1857	U1858	U1859	U1860	U1861	U1862	U1863	U1864	U1865	U1866	U1867	U1868	U1869	U1870	U1871	U1872	U1873	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	U1911	U1912	U1913	U1914	U1915	U1916	U1917	U1918	U1919	U1920	U1921	U1922	U1923																																																																																																																																																																																																																															
G1929	G1930	U1931	U1932	U1933	C1934	U1935	U1936	U1937	U1938	U1939	U1940	U1941	U1942	U1943	U1944	U1945	U1946	U1947	U1948	U1949	U1950	U1951	U1952	U1953	U1954	U1955	U1956	U1957	U1958	U1959	U1960	U1961	U1962	U1963	U1964	U1965	U1966	U1967	U1968	U1969	U1970	U1971	U1972	U1973	U1974	U1975	U1976	U1977	U1978	U1979	U1980	U1981	U1982	U1983	U1984	U1985	U1986	U1987	U1988	U1989	U1990	U1991	U1992	U1993	U1994	U1995	U1996	U1997	U1998	U1999	U2000	U2001	U2002	U2003	U2004	U2005	U2006	U2007	U2008	U2009	U2010	U2011	U2012	U2013	U2014	U2015	U2016	U2017	U2018	U2019	U2020	U2021	U2022	U2023	U2024	U2025	U2026	U2027	U2028	U2029	U2030	U2031	U2032	U2033	U2034	U2035	U2036	U2037	U2038	U2039	U2040	U2041	U2042	U2043	U2044	U2045	U2046	U2047	U2048	U2049	U2050	U2051	U2052	U2053	U2054	U2055	U2056	U2057	U2058	U2059	U2060	U2061	U2062	U2063	U2064	U2065	U2066	U2067	U2068	U2069	U2070	U2071	U2072	U2073																																																																																																																																																																												
C1043	C1044	C1045	A1046	G1047	A1048	A1049	A1050	G1051	C1052	C1053	G1054	G1055	G1056	A1057	U1058	U1059	U1060	U1061	G1062	U1063	U1064	U1065	U1066	U1067	G1068	A1069	A1070	G1071	C1072	C1073	G1074	C1075	C1076	A1077	U1078	U1079	U1080	U1081	U1082	U1083	A1084	U1085	A1086	G1087	A1088	A1089	U1090	A1091	A1092	A1093	A1094	A1095	A1096	U1097	A1098	U1099	U1100	C1102	U1103	U1104	U1105	G1106	U1107	U1108	U1109	U1110	U1111	G1112	U1113	U1114	U1115	U1116	U1117	U1118	U1119	U1120	U1121	U1122	U1123	U1124	U1125	U1126	U1127	U1128	U1129	U1130	U1131	U1132	U1133	U1134	U1135	U1136	U1137	U1138	U1139	U1140	U1141	U1142	U1143	U1144	U1145	U1146	U1147	U1148	U1149	U1150	U1151	U1152	U1153	U1154	U1155	U1156	U1157	U1158	U1159	U1160	U1161	U1162	U1163	U1164	U1165	U1166	U1167	U1168	U1169	U1170	U1171	U1172	U1173	U1174	U1175	U1176	U1177	U1178	U1179	U1180																																																																																																																																																																																				
A1269	C1270	G1271	A1272	U1273	U1274	A1275	A1276	G1277	C1278	G1279	G1280	A1281	U1282	U1283	U1284	U1285	U1286	A1287	U1288	U1289	C1290	U1291	C1292	U1293	U1294	U1295	U1296	U1297	C1298	U1299	U1300	A1301	A1302	U1303	U1304	U1305	U1306	U1307	U1308	U1309	U1310	U1311	U1312	U1313	U1314	U1315	U1316	U1317	U1318	U1319	U1320	A1321	U1322	U1323	U1324	U1325	U1326	U1327	U1328	U1329	U1330	U1331	U1332	U1333	U1334	U1335	U1336	U1337	U1338	U1339	U1340	U1341	U1342	U1343	U1344	U1345	U1346	U1347	U1348	U1349	U1350	U1351	U1352	U1353	U1354	U1355	U1356	U1357	U1358	U1359	U1360	U1361	U1362	U1363	U1364	U1365	U1366	U1367	U1368	U1369	U1370	U1371	U1372	U1373	U1374	U1375	U1376	U1377	U1378	U1379	U1380	U1381	U1382	U1383	U1384	U1385	U1386	U1387	U1388	U1389	U1390	U1391	U1392	U1393	U1394	U1395	U1396	U1397	U1398	U1399	U1400	U1401	U1402	U1403	U1404	U1405	U1406	U1407	U1408	U1409	U1410	U1411	U1412	U1413	U1414	U1415	U1416	U1417	U1418	U1419	U1420	U1421	U1422	U1423	U1424	U1425	U1426	U1427	U1428	U1429	U1430																																																																																																																																																											
A1431	G1432	A1433	G1434	G1435	G1436	G1437	U1438	U1439	U1440	U1441	U1442	U1443	U1444	U1445	U1446	U1447	U1448	U1449	U1450	U1451	U1452	U1453	U1454	U1455	U1456	U1457	U1458	U1459	U1460	U1461	U1462	U1463	U1464	U1465	U1466	U1467	U1468	U1469	U1470	U1471	U1472	U1473	U1474	U1475	U1476	U1477	U1478	U1479	U1480	U1481	U1482	U1483	U1484	U1485	U1486	U1487	U1488	U1489	U1490	U1491	U1492	U1493	U1494	U1495	U1496	U1497	U1498	U1499	U1500	U1501	U1502	U1503	U1504	U1505	U1506	U1507	U1508	U1509	U1510	U1511	U1512	U1513	U1514	U1515	U1516	U1517	U1518	U1519	U1520	U1521	U1522	U1523	U1524	U1525	U1526	U1527	U1528	U1529	U1530	U1531	U1532	U1533	U1534	U1535	U1536	U1537	U1538	U1539	U1540	U1541	U1542	U1543	U1544	U1545	U1546	U1547	U1548	U1549	U1550	U1551	U1552	U1553	U1554	U1555	U1556	U1557	U1558	U1559	U1560	U1561	U1562	U1563	U1564	U1565	U1566	U1567	U1568	U1569	U1570	U1571	U1572	U1573	U1574	U1575	U1576	U1577	U1578	U1579	U1580	U1581	U1582	U1583	U1584	U1585	U1586	U1587	U1588	U1589	U1590	U1591	U1592	U1593	U1594	U1595	U1596	U1597	U1598	U1599	U1600	U1601	U1602	U1603	U1604	U1605	U1606	U1607	U1608	U1609	U1610	U1611	U1612	U1613	U1614	U1615	U1616	U1617	U1618	U1619	U1620	U1621	U1622	U1623	U1624	U1625	U1626	U1627	U1628	U1629	U1630	U1631	U1632	U1633	U1634	U1635	U1636	U1637	U1638	U1639	U1640	U1641	U1642	U1643	U1644	U1645	U1646	U1647	U1648	U1649	U1650	U1651	U1652	U1653	U1654	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	U1671	U1672	U1673	U1674	U1675	U1676	U1677	U1678	U1679	U1680	U1681	U1682	U1683	U1684	U1685	U1686	U1687	U1688	U1689	U1690	U1691	U1692	U1693	U1694	U1695	U1696	U1697	U1698	U1699	U1700	U1701	U1702	U1703	U1704	U1705	U1706	U1707	U1708	U1709	U1710	U1711	U1712	U1713	U1714	U1715	U1716	U1717	U1718	U1719	U1720	U1721	U1722	U1723	U1724	U1725	U1726	U1727	U1728	U1729	U1730	U1731	U1732	U1733	U1734	U1735	U1736	U1737	U1738	U1739	U1740	U1741	U1742	U1743	U1744	U1745	U1746	U1747



• Molecule 2: 5S rRNA

Chain B: 43% 47% 10%



• Molecule 3: 50S ribosomal protein L2

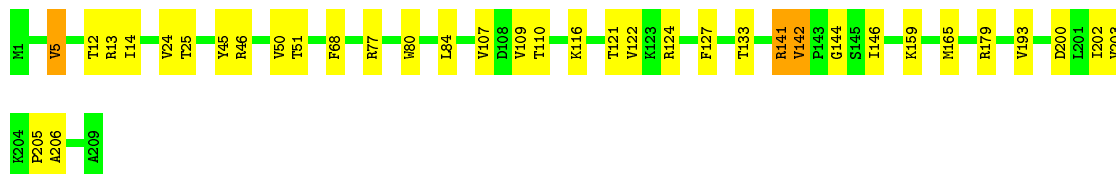
Chain C: 78% 19% 3%





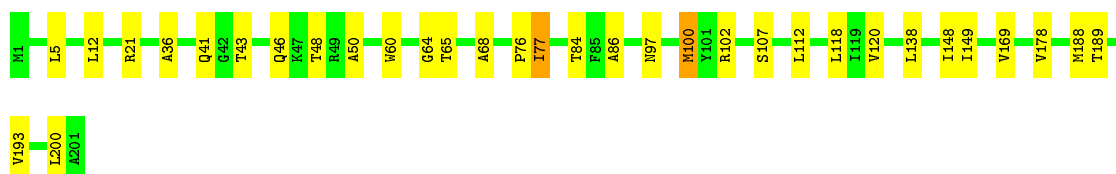
- Molecule 4: 50S ribosomal protein L3

Chain D: 83% 16% .



- Molecule 5: 50S ribosomal protein L4

Chain E: 84% 15% .



- Molecule 6: 50S ribosomal protein L5

Chain F: 82% 16% ..



- Molecule 7: 50S ribosomal protein L6

Chain G: 86% 13% .



- Molecule 8: 50S ribosomal protein L9

Chain H: 88% 11% .



- Molecule 9: 50S ribosomal protein L11

Chain J: 84% 14% ..



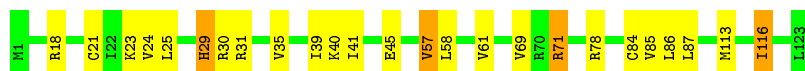
- Molecule 10: 50S ribosomal protein L13

Chain K:  92% 8% .




- Molecule 11: 50S ribosomal protein L14

Chain L:  80% 17% .




- Molecule 12: 50S ribosomal protein L15

Chain M:  83% 15% .



- Molecule 13: 50S ribosomal protein L16

Chain N:  85% 14% .




- Molecule 14: 50S ribosomal protein L17

Chain O:  73% 20% 6% .




- Molecule 15: 50S ribosomal protein L18

Chain P:  88% 11% .




- Molecule 16: 50S ribosomal protein L19

Chain Q:  89% 10% .




- Molecule 17: 50S ribosomal protein L20

Chain R:  80% 17% ..




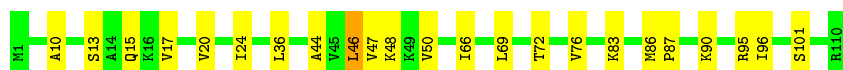
- Molecule 18: 50S ribosomal protein L21

Chain S:  83% 15% ..




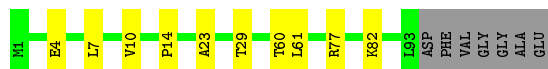
- Molecule 19: 50S ribosomal protein L22

Chain T:  79% 20% .




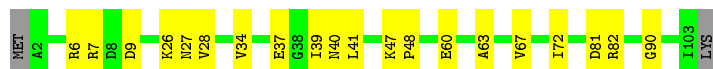
- Molecule 20: 50S ribosomal protein L23

Chain U:  83% 10% 7%




- Molecule 21: 50S ribosomal protein L24

Chain V:  79% 19% .



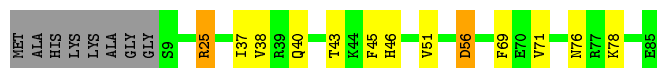
- Molecule 22: 50S ribosomal protein L25

Chain W:  82% 16% .



- Molecule 23: 50S ribosomal protein L27

Chain X:  75% 13% . 9%



- Molecule 24: 50S ribosomal protein L28

Chain Y:  76% 21% ..



- Molecule 25: 50S ribosomal protein L29

Chain Z: 87% 10% . .



- Molecule 26: 50S ribosomal protein L30

Chain 0: 93% 5% .



- Molecule 27: 50S ribosomal protein L32

Chain 1: 86% 11% . .



- Molecule 28: 50S ribosomal protein L33

Chain 2: 73% 18% 9%



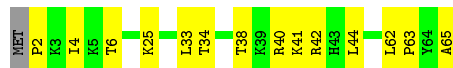
- Molecule 29: 50S ribosomal protein L34

Chain 3: 89% 11%



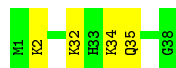
- Molecule 30: 50S ribosomal protein L35

Chain 4: 77% 22% .



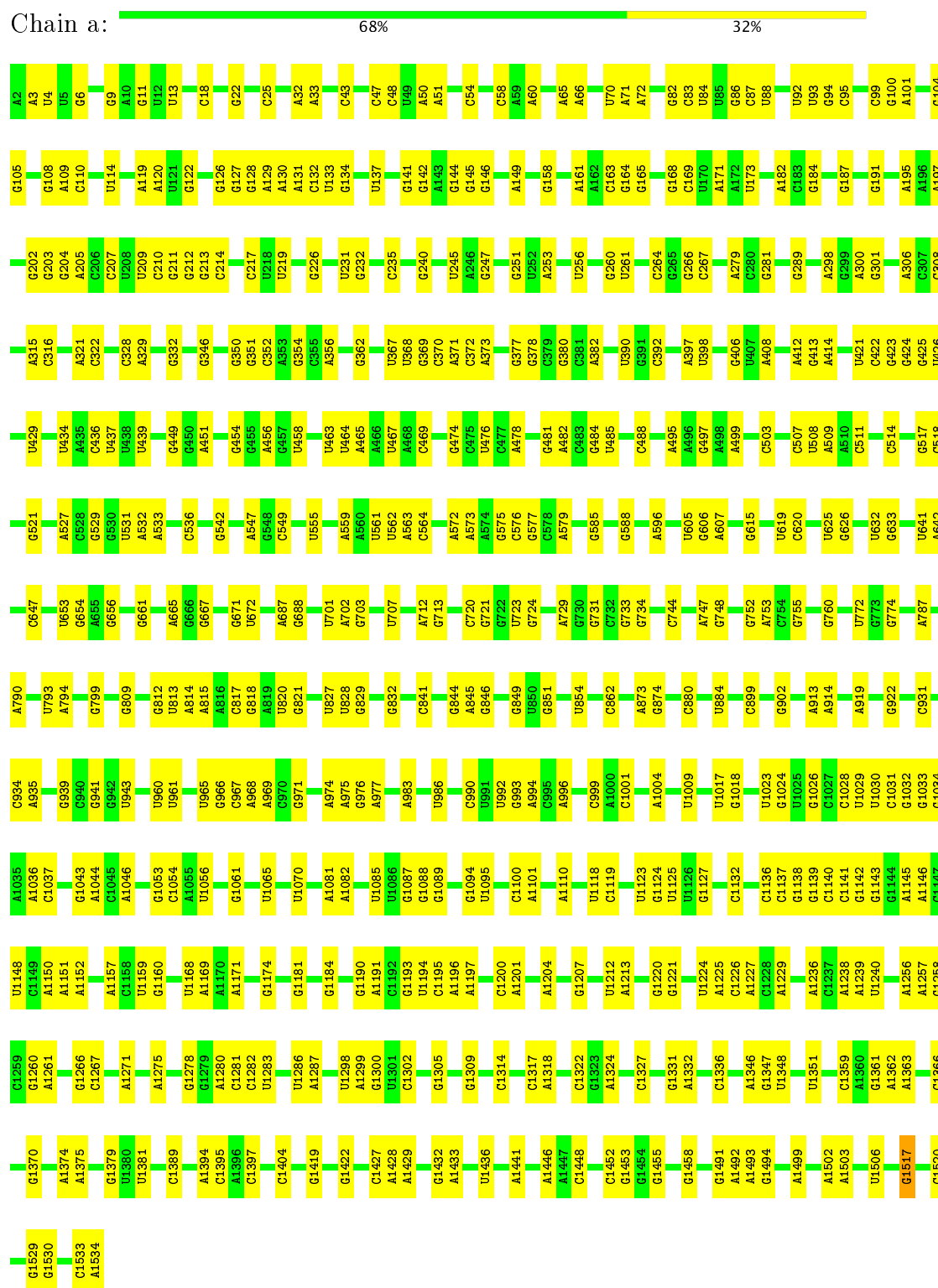
- Molecule 31: 50S ribosomal protein L36

Chain 5: 89% 11%



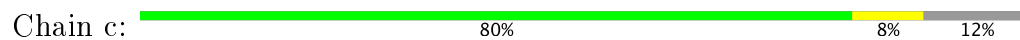
• Molecule 32: 16S rRNA

Chain a:





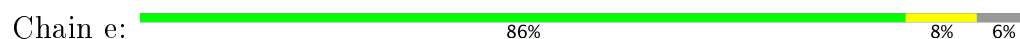
- Molecule 34: 30S ribosomal protein S3



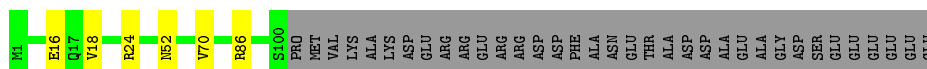
- Molecule 35: 30S ribosomal protein S4



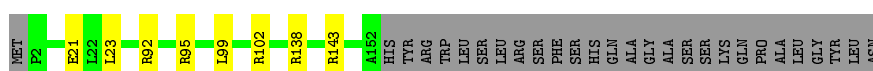
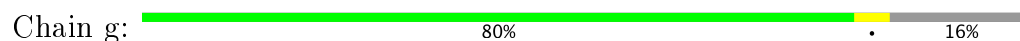
- Molecule 36: 30S ribosomal protein S5



- Molecule 37: 30S ribosomal protein S6



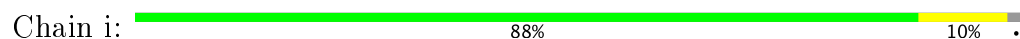
- Molecule 38: 30S ribosomal protein S7



- Molecule 39: 30S ribosomal protein S8



- Molecule 40: 30S ribosomal protein S9





- Molecule 41: 30S ribosomal protein S10

Chain j: 83% 13% 5%



- Molecule 42: 30S ribosomal protein S11

Chain k: 97%



- Molecule 43: 30S ribosomal protein S12

Chain l: 93% 7%



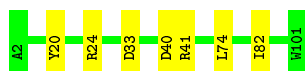
- Molecule 44: 30S ribosomal protein S13

Chain m: 91% 5% ..



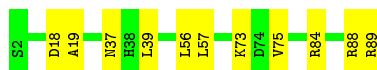
- Molecule 45: 30S ribosomal protein S14

Chain n: 93% 7%



- Molecule 46: 30S ribosomal protein S15

Chain o: 88% 13%




- Molecule 47: 30S ribosomal protein S16

Chain p: 90% 10%




- Molecule 48: 30S ribosomal protein S17

Chain q:  87% 8% 5%




- Molecule 49: 30S ribosomal protein S18

Chain r:  81% 5% 13%



- Molecule 50: 30S ribosomal protein S19

Chain s:  90% 9% .



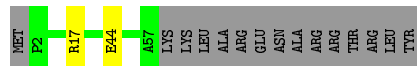
- Molecule 51: 30S ribosomal protein S20

Chain t:  95% 5%




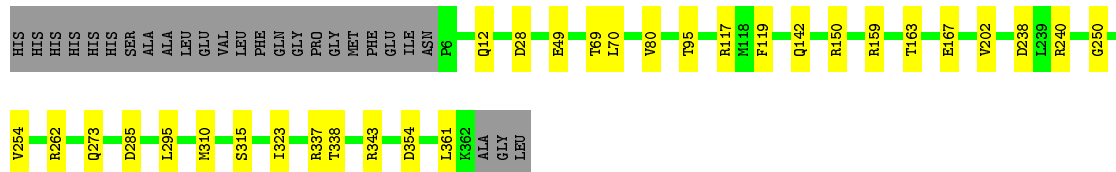
- Molecule 52: 30S ribosomal protein S21

Chain u:  76% . 21%



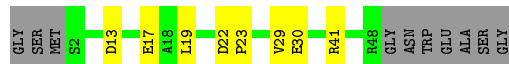
- Molecule 53: Peptide chain release factor 2

Chain v:  85% 8% 7%



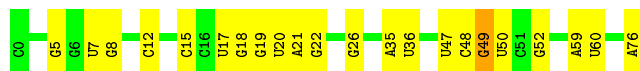
- Molecule 54: Alternative ribosome-rescue factor A

Chain w:  68% 14% 18%




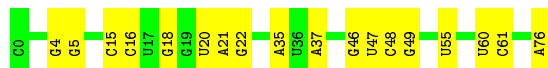
- Molecule 55: P-site or E-site fMet-tRNA(fMet)

Chain x:  71% 27%



- Molecule 55: P-site or E-site fMet-tRNA(fMet)

Chain y:  77% 23%



- Molecule 56: mRNA

Chain z:  28% 6% 67%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	155440	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	83822	Depositor
Image detector	GATAN K2 SUMMIT (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: 5MU, OMC, ZN, OMG, OMU, MA6, MG, MEQ, 2MG, 5MC, UR3, 4OC, 1MG, PSU

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	A	0.23	0/69434	0.65	2/108325 (0.0%)
10	K	0.37	0/1152	0.65	0/1551
11	L	0.35	0/955	0.62	0/1279
12	M	0.37	0/1062	0.64	0/1413
13	N	0.39	0/1093	0.66	0/1460
14	O	0.42	0/973	0.74	0/1301
15	P	0.36	0/902	0.67	0/1209
16	Q	0.37	0/929	0.64	0/1242
17	R	0.41	0/960	0.70	0/1278
18	S	0.39	0/829	0.62	0/1107
19	T	0.34	0/864	0.69	0/1156
2	B	0.23	0/2828	0.65	0/4410
20	U	0.36	0/744	0.67	0/994
21	V	0.40	0/787	0.61	0/1051
22	W	0.38	0/766	0.61	0/1025
23	X	0.38	0/595	0.62	0/787
24	Y	0.38	0/635	0.67	0/848
25	Z	0.33	0/502	0.69	1/667 (0.1%)
26	0	0.36	0/453	0.68	1/605 (0.2%)
27	1	0.36	0/450	0.64	0/599
28	2	0.40	0/416	0.57	0/554
29	3	0.41	0/380	0.73	0/498
3	C	0.36	0/2121	0.65	0/2852
30	4	0.36	0/513	0.67	0/676
31	5	0.33	0/303	0.62	0/397
32	a	0.23	0/36593	0.66	1/57081 (0.0%)
33	b	0.40	0/1784	0.62	0/2403
34	c	0.38	0/1651	0.66	0/2225
35	d	0.38	0/1655	0.68	0/2216
36	e	0.37	0/1169	0.65	0/1573
37	f	0.40	0/835	0.62	0/1128
38	g	0.38	0/1195	0.69	0/1602

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	h	0.36	0/989	0.65	0/1326
4	D	0.38	0/1586	0.61	0/2134
40	i	0.39	0/1034	0.70	0/1375
41	j	0.37	0/796	0.70	0/1077
42	k	0.38	0/893	0.60	0/1205
43	l	0.35	0/969	0.66	0/1300
44	m	0.62	2/892 (0.2%)	0.84	1/1193 (0.1%)
45	n	0.38	0/817	0.69	0/1088
46	o	0.37	0/722	0.68	0/964
47	p	0.39	0/659	0.64	0/884
48	q	0.38	0/657	0.66	0/881
49	r	0.40	0/548	0.63	0/736
5	E	0.36	0/1571	0.66	0/2113
50	s	0.46	1/675 (0.1%)	0.69	1/908 (0.1%)
51	t	0.37	0/676	0.67	0/895
52	u	0.43	0/472	0.73	0/627
53	v	0.38	0/2865	0.65	0/3858
54	w	0.35	0/394	0.63	0/519
55	x	0.24	0/1832	0.68	1/2855 (0.0%)
55	y	0.23	0/1832	0.65	0/2855
56	z	0.21	0/147	0.62	0/227
6	F	0.41	0/1434	0.65	0/1926
7	G	0.41	0/1343	0.64	0/1816
8	H	0.38	0/1122	0.63	0/1515
9	J	0.40	0/1046	0.61	0/1410
All	All	0.29	3/161499 (0.0%)	0.66	8/241199 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	m	90	ARG	CZ-NH1	13.28	1.50	1.33
44	m	90	ARG	CD-NE	5.57	1.55	1.46
50	s	55	ARG	CZ-NH1	5.15	1.39	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	m	90	ARG	NE-CZ-NH2	-14.43	113.09	120.30
50	s	55	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	A	2193	G	C2'-C3'-O3'	6.96	124.83	113.70
55	x	49	G	C2'-C3'-O3'	6.73	124.47	113.70
32	a	1517	G	C2'-C3'-O3'	6.38	123.91	113.70

There are no chirality outliers.

There are no planarity outliers.

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	62351	0	31373	1018	0
2	B	2529	0	1281	33	0
3	C	2082	0	2154	28	0
4	D	1565	0	1616	17	0
5	E	1552	0	1619	17	0
6	F	1410	0	1444	12	0
7	G	1323	0	1371	10	0
8	H	1111	0	1148	8	0
9	J	1032	0	1088	6	0
10	K	1129	0	1162	6	0
11	L	946	0	1023	13	0
12	M	1053	0	1129	12	0
13	N	1074	0	1157	10	0
14	O	960	0	1000	16	0
15	P	892	0	923	2	0
16	Q	917	0	962	4	0
17	R	947	0	1019	15	0
18	S	816	0	839	12	0
19	T	857	0	922	16	0
20	U	738	0	807	3	0
21	V	779	0	831	8	0
22	W	753	0	780	9	0
23	X	588	0	604	6	0
24	Y	625	0	652	9	0
25	Z	501	0	531	3	0
26	0	449	0	488	1	0
27	1	444	0	458	6	0
28	2	409	0	440	5	0
29	3	377	0	418	3	0
30	4	504	0	572	10	0
31	5	302	0	341	3	0
32	a	32906	0	16575	0	0
33	b	1753	0	1780	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	c	1624	0	1696	0	0
35	d	1633	0	1694	0	0
36	e	1156	0	1199	0	0
37	f	817	0	808	0	0
38	g	1181	0	1238	0	0
39	h	979	0	1031	0	0
40	i	1022	0	1070	0	0
41	j	786	0	828	0	0
42	k	877	0	887	0	0
43	l	955	0	1016	0	0
44	m	883	0	941	0	0
45	n	805	0	844	0	0
46	o	714	0	734	0	0
47	p	649	0	666	0	0
48	q	648	0	691	0	0
49	r	539	0	553	0	0
50	s	658	0	683	0	0
51	t	670	0	719	0	0
52	u	465	0	491	0	0
53	v	2836	0	2735	0	0
54	w	388	0	400	0	0
55	x	1640	0	837	0	0
55	y	1640	0	837	0	0
56	z	131	0	66	0	0
57	A	100	0	0	0	0
57	B	4	0	0	0	0
57	a	20	0	0	0	0
58	5	1	0	0	0	0
All	All	149495	0	101171	1250	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 9.

The worst 5 of 1250 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2244:U:N3	1:A:2435:A:N6	1.68	1.35
1:A:2013:A:N6	1:A:2613:U:H3	1.26	1.31
1:A:2067:G:O2'	1:A:2069:G:H8	1.16	1.28
1:A:2067:G:O2'	1:A:2069:G:C8	1.88	1.22
1:A:2500:U:O2	1:A:2504:PSU:N1	1.71	1.20

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	
3	C	269/273 (98%)	246 (91%)	20 (7%)	3 (1%)	17	59
4	D	207/209 (99%)	193 (93%)	13 (6%)	1 (0%)	32	73
5	E	199/201 (99%)	183 (92%)	14 (7%)	2 (1%)	18	61
6	F	175/179 (98%)	155 (89%)	16 (9%)	4 (2%)	7	43
7	G	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
8	H	147/149 (99%)	130 (88%)	15 (10%)	2 (1%)	13	53
9	J	139/142 (98%)	117 (84%)	16 (12%)	6 (4%)	3	28
10	K	140/142 (99%)	135 (96%)	4 (3%)	1 (1%)	25	68
11	L	121/123 (98%)	113 (93%)	8 (7%)	0	100	100
12	M	142/144 (99%)	130 (92%)	11 (8%)	1 (1%)	25	68
13	N	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
14	O	118/127 (93%)	105 (89%)	12 (10%)	1 (1%)	22	65
15	P	114/117 (97%)	103 (90%)	10 (9%)	1 (1%)	20	63
16	Q	112/115 (97%)	101 (90%)	11 (10%)	0	100	100
17	R	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
18	S	101/103 (98%)	90 (89%)	8 (8%)	3 (3%)	5	37
19	T	108/110 (98%)	102 (94%)	5 (5%)	1 (1%)	20	63
20	U	91/100 (91%)	83 (91%)	6 (7%)	2 (2%)	8	44
21	V	100/104 (96%)	82 (82%)	17 (17%)	1 (1%)	18	61
22	W	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
23	X	75/85 (88%)	68 (91%)	6 (8%)	1 (1%)	14	55
24	Y	75/78 (96%)	69 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Z	60/63 (95%)	56 (93%)	3 (5%)	1 (2%)	11	49
26	0	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	10	48
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	48/55 (87%)	44 (92%)	3 (6%)	1 (2%)	8	45
29	3	44/46 (96%)	44 (100%)	0	0	100	100
30	4	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
31	5	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
33	b	222/241 (92%)	207 (93%)	14 (6%)	1 (0%)	32	73
34	c	204/233 (88%)	192 (94%)	10 (5%)	2 (1%)	18	61
35	d	202/206 (98%)	192 (95%)	10 (5%)	0	100	100
36	e	155/167 (93%)	145 (94%)	8 (5%)	2 (1%)	14	55
37	f	98/135 (73%)	93 (95%)	4 (4%)	1 (1%)	18	61
38	g	149/179 (83%)	141 (95%)	8 (5%)	0	100	100
39	h	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
40	i	125/130 (96%)	112 (90%)	10 (8%)	3 (2%)	7	42
41	j	96/103 (93%)	87 (91%)	6 (6%)	3 (3%)	5	37
42	k	115/117 (98%)	103 (90%)	11 (10%)	1 (1%)	20	63
43	l	121/123 (98%)	112 (93%)	8 (7%)	1 (1%)	22	65
44	m	112/118 (95%)	105 (94%)	7 (6%)	0	100	100
45	n	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
46	o	86/88 (98%)	83 (96%)	2 (2%)	1 (1%)	15	57
47	p	80/82 (98%)	72 (90%)	8 (10%)	0	100	100
48	q	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
49	r	63/75 (84%)	62 (98%)	1 (2%)	0	100	100
50	s	80/82 (98%)	74 (92%)	5 (6%)	1 (1%)	14	55
51	t	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
52	u	54/71 (76%)	54 (100%)	0	0	100	100
53	v	354/383 (92%)	334 (94%)	19 (5%)	1 (0%)	44	80
54	w	45/57 (79%)	39 (87%)	5 (11%)	1 (2%)	8	44
All	All	6056/6398 (95%)	5615 (93%)	390 (6%)	51 (1%)	27	65

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	241	GLY
5	E	64	GLY
18	S	82	HIS
6	F	174	ASP
9	J	20	SER

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	
3	C	216/218 (99%)	198 (92%)	18 (8%)	13	46
4	D	164/164 (100%)	153 (93%)	11 (7%)	19	57
5	E	165/165 (100%)	159 (96%)	6 (4%)	40	74
6	F	148/150 (99%)	136 (92%)	12 (8%)	14	48
7	G	137/138 (99%)	132 (96%)	5 (4%)	40	74
8	H	114/114 (100%)	109 (96%)	5 (4%)	33	69
9	J	109/110 (99%)	103 (94%)	6 (6%)	25	62
10	K	116/116 (100%)	114 (98%)	2 (2%)	66	87
11	L	104/104 (100%)	96 (92%)	8 (8%)	15	50
12	M	103/103 (100%)	96 (93%)	7 (7%)	18	56
13	N	109/109 (100%)	103 (94%)	6 (6%)	25	62
14	O	100/103 (97%)	95 (95%)	5 (5%)	28	65
15	P	86/87 (99%)	78 (91%)	8 (9%)	10	41
16	Q	99/100 (99%)	93 (94%)	6 (6%)	22	60
17	R	89/90 (99%)	81 (91%)	8 (9%)	11	42
18	S	84/84 (100%)	81 (96%)	3 (4%)	40	74
19	T	93/93 (100%)	92 (99%)	1 (1%)	78	91
20	U	80/84 (95%)	78 (98%)	2 (2%)	53	81
21	V	83/85 (98%)	78 (94%)	5 (6%)	22	60
22	W	78/78 (100%)	69 (88%)	9 (12%)	6	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	X	59/63 (94%)	55 (93%)	4 (7%)	18	56
24	Y	67/68 (98%)	60 (90%)	7 (10%)	8	36
25	Z	54/55 (98%)	53 (98%)	1 (2%)	62	85
26	0	48/49 (98%)	48 (100%)	0	100	100
27	1	47/48 (98%)	45 (96%)	2 (4%)	33	70
28	2	45/49 (92%)	44 (98%)	1 (2%)	57	83
29	3	38/38 (100%)	38 (100%)	0	100	100
30	4	51/52 (98%)	51 (100%)	0	100	100
31	5	34/34 (100%)	34 (100%)	0	100	100
33	b	186/199 (94%)	172 (92%)	14 (8%)	16	51
34	c	170/190 (90%)	153 (90%)	17 (10%)	9	37
35	d	171/173 (99%)	157 (92%)	14 (8%)	13	47
36	e	119/126 (94%)	107 (90%)	12 (10%)	9	37
37	f	87/116 (75%)	82 (94%)	5 (6%)	24	61
38	g	124/147 (84%)	116 (94%)	8 (6%)	20	58
39	h	104/104 (100%)	98 (94%)	6 (6%)	23	61
40	i	105/107 (98%)	95 (90%)	10 (10%)	10	40
41	j	86/90 (96%)	76 (88%)	10 (12%)	6	30
42	k	90/90 (100%)	88 (98%)	2 (2%)	57	83
43	l	103/103 (100%)	96 (93%)	7 (7%)	18	56
44	m	92/96 (96%)	85 (92%)	7 (8%)	15	51
45	n	83/83 (100%)	76 (92%)	7 (8%)	13	46
46	o	76/76 (100%)	66 (87%)	10 (13%)	5	24
47	p	65/65 (100%)	57 (88%)	8 (12%)	5	27
48	q	74/78 (95%)	67 (90%)	7 (10%)	10	40
49	r	57/66 (86%)	53 (93%)	4 (7%)	18	55
50	s	72/72 (100%)	65 (90%)	7 (10%)	9	38
51	t	65/65 (100%)	61 (94%)	4 (6%)	21	59
52	u	48/61 (79%)	46 (96%)	2 (4%)	34	70
53	v	304/324 (94%)	274 (90%)	30 (10%)	9	38
54	w	40/46 (87%)	33 (82%)	7 (18%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5041/5228 (96%)	4695 (93%)	346 (7%)	23 55

5 of 346 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	b	114	LEU
36	e	31	PHE
53	v	150	ARG
33	b	204	ASP
34	c	176	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
21	V	46	GLN
35	d	36	GLN
53	v	214	HIS
22	W	49	ASN
36	e	73	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2903/2904 (99%)	855 (29%)	82 (2%)
2	B	117/118 (99%)	35 (29%)	1 (0%)
32	a	1529/1533 (99%)	490 (32%)	0
55	x	76/77 (98%)	22 (28%)	0
55	y	76/77 (98%)	18 (23%)	0
56	z	5/18 (27%)	1 (20%)	0
All	All	4706/4727 (99%)	1421 (30%)	83 (1%)

5 of 1421 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	13	A
1	A	14	A
1	A	23	G
1	A	27	G

5 of 83 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1088	A
1	A	1311	G
1	A	2638	G
1	A	1126	A
1	A	1190	G

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

28 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	A	1835	1	19,26,27	1.30	2 (10%)	20,38,41	2.42	7 (35%)
1	PSU	A	1911	1	16,21,22	1.15	1 (6%)	20,30,33	3.56	6 (30%)
1	PSU	A	1917	1	16,21,22	1.13	1 (6%)	20,30,33	3.66	8 (40%)
1	5MU	A	1939	1	14,22,23	0.96	1 (7%)	16,32,35	2.88	5 (31%)
1	5MC	A	1962	1	15,22,23	1.58	1 (6%)	17,32,35	1.00	0
1	OMG	A	2251	1,55	18,26,27	1.34	3 (16%)	22,38,41	2.00	6 (27%)
1	2MG	A	2445	1	19,26,27	1.30	2 (10%)	20,38,41	2.38	7 (35%)
1	PSU	A	2457	1	16,21,22	1.36	1 (6%)	20,30,33	3.69	7 (35%)
1	OMC	A	2498	1,57	15,22,23	0.84	1 (6%)	19,31,34	1.24	2 (10%)
1	PSU	A	2504	1	16,21,22	1.39	1 (6%)	20,30,33	3.68	9 (45%)
1	OMU	A	2552	1	14,22,23	0.89	0	18,31,34	2.12	2 (11%)
1	PSU	A	2580	1	16,21,22	1.37	2 (12%)	20,30,33	3.52	8 (40%)
1	PSU	A	2605	1	16,21,22	1.23	1 (6%)	20,30,33	3.32	7 (35%)
1	1MG	A	745	1	18,26,27	1.44	3 (16%)	18,39,42	1.74	3 (16%)
1	PSU	A	746	1,57	16,21,22	1.29	1 (6%)	20,30,33	3.47	5 (25%)
1	5MU	A	747	1	14,22,23	0.87	1 (7%)	16,32,35	2.62	5 (31%)
1	PSU	A	955	1	16,21,22	1.13	1 (6%)	20,30,33	3.52	6 (30%)
32	2MG	a	1207	32	19,26,27	1.51	3 (15%)	20,38,41	2.51	8 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	4OC	a	1402	32	16,23,24	0.77	0	19,32,35	1.20	3 (15%)
32	5MC	a	1407	32	15,22,23	1.62	2 (13%)	17,32,35	1.04	1 (5%)
32	UR3	a	1498	32	14,22,23	1.03	1 (7%)	16,32,35	0.99	1 (6%)
32	2MG	a	1516	32	19,26,27	1.36	2 (10%)	20,38,41	2.40	8 (40%)
32	MA6	a	1518	32	16,26,27	1.17	1 (6%)	18,38,41	2.69	5 (27%)
32	MA6	a	1519	32	16,26,27	1.19	1 (6%)	18,38,41	2.50	7 (38%)
32	PSU	a	516	32	16,21,22	1.06	1 (6%)	20,30,33	3.68	8 (40%)
32	2MG	a	966	32	19,26,27	1.47	3 (15%)	20,38,41	2.45	7 (35%)
32	5MC	a	967	32	15,22,23	1.64	1 (6%)	17,32,35	1.00	1 (5%)
53	MEQ	v	252	53	9,9,10	0.47	0	7,10,12	0.91	0

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	A	1835	1	-	0/5/27/28	0/3/3/3
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1917	1	-	0/7/25/26	0/2/2/2
1	5MU	A	1939	1	-	0/3/25/26	0/2/2/2
1	5MC	A	1962	1	-	0/3/25/26	0/2/2/2
1	OMG	A	2251	1,55	-	0/5/27/28	0/3/3/3
1	2MG	A	2445	1	-	0/5/27/28	0/3/3/3
1	PSU	A	2457	1	-	0/7/25/26	0/2/2/2
1	OMC	A	2498	1,57	-	0/5/27/28	0/2/2/2
1	PSU	A	2504	1	-	0/7/25/26	0/2/2/2
1	OMU	A	2552	1	-	0/5/27/28	0/2/2/2
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
1	1MG	A	745	1	-	0/3/25/26	0/3/3/3
1	PSU	A	746	1,57	-	0/7/25/26	0/2/2/2
1	5MU	A	747	1	-	0/3/25/26	0/2/2/2
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
32	2MG	a	1207	32	-	0/5/27/28	0/3/3/3
32	4OC	a	1402	32	-	0/7/29/30	0/2/2/2
32	5MC	a	1407	32	-	0/3/25/26	0/2/2/2
32	UR3	a	1498	32	-	0/3/25/26	0/2/2/2
32	2MG	a	1516	32	-	0/5/27/28	0/3/3/3
32	MA6	a	1518	32	-	0/7/29/30	0/3/3/3
32	MA6	a	1519	32	-	0/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PSU	a	516	32	-	0/7/25/26	0/2/2/2
32	2MG	a	966	32	-	0/5/27/28	0/3/3/3
32	5MC	a	967	32	-	0/3/25/26	0/2/2/2
53	MEQ	v	252	53	-	0/7/9/11	0/0/0/0

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2504	PSU	C5-C1'	-4.42	1.48	1.52
1	A	2457	PSU	C5-C1'	-4.30	1.48	1.52
1	A	2580	PSU	C5-C1'	-3.91	1.48	1.52
1	A	746	PSU	C5-C1'	-3.76	1.49	1.52
1	A	2605	PSU	C5-C1'	-3.29	1.49	1.52

The worst 5 of 142 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1911	PSU	N1-C2-N3	-9.86	121.31	128.40
1	A	1917	PSU	N1-C2-N3	-9.85	121.32	128.40
32	a	516	PSU	N1-C2-N3	-9.66	121.45	128.40
1	A	955	PSU	N1-C2-N3	-9.13	121.83	128.40
1	A	746	PSU	N1-C2-N3	-9.02	121.91	128.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1835	2MG	2	0
1	A	1939	5MU	1	0
1	A	1962	5MC	1	0
1	A	2504	PSU	14	0
1	A	2605	PSU	1	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 125 ligands modelled in this entry, 125 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.