



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 30, 2017 – 03:28 PM EST

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 : 2016-12-04
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 : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

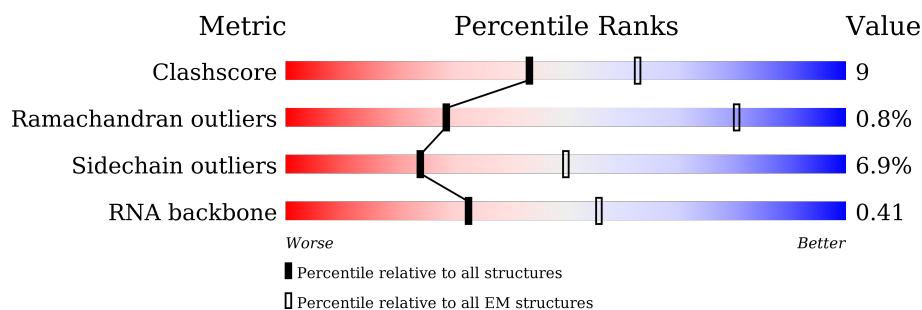
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	2904	40% 47% 13%
2	B	118	43% 47% 10%
3	C	273	78% 19% ..
4	D	209	83% 16% .
5	E	201	84% 15% .
6	F	179	82% 16% ..
7	G	177	86% 13% .
8	H	149	88% 11% .













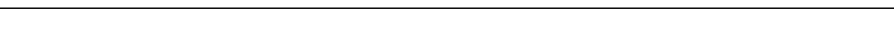
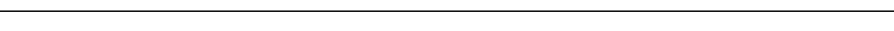
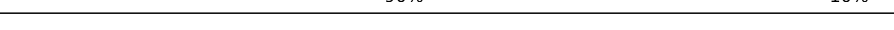



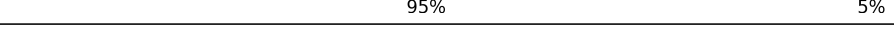





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Mol	Chain	Length	Quality of chain
9	J	142	 84% 14% ..
10	K	142	 92% 8% .
11	L	123	 80% 17% .
12	M	144	 83% 15% .
13	N	136	 85% 14% .
14	O	127	 73% 20% . 6%
15	P	117	 88% 11% .
16	Q	115	 89% 10% .
17	R	118	 80% 17% ..
18	S	103	 83% 15% ..
19	T	110	 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		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		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	

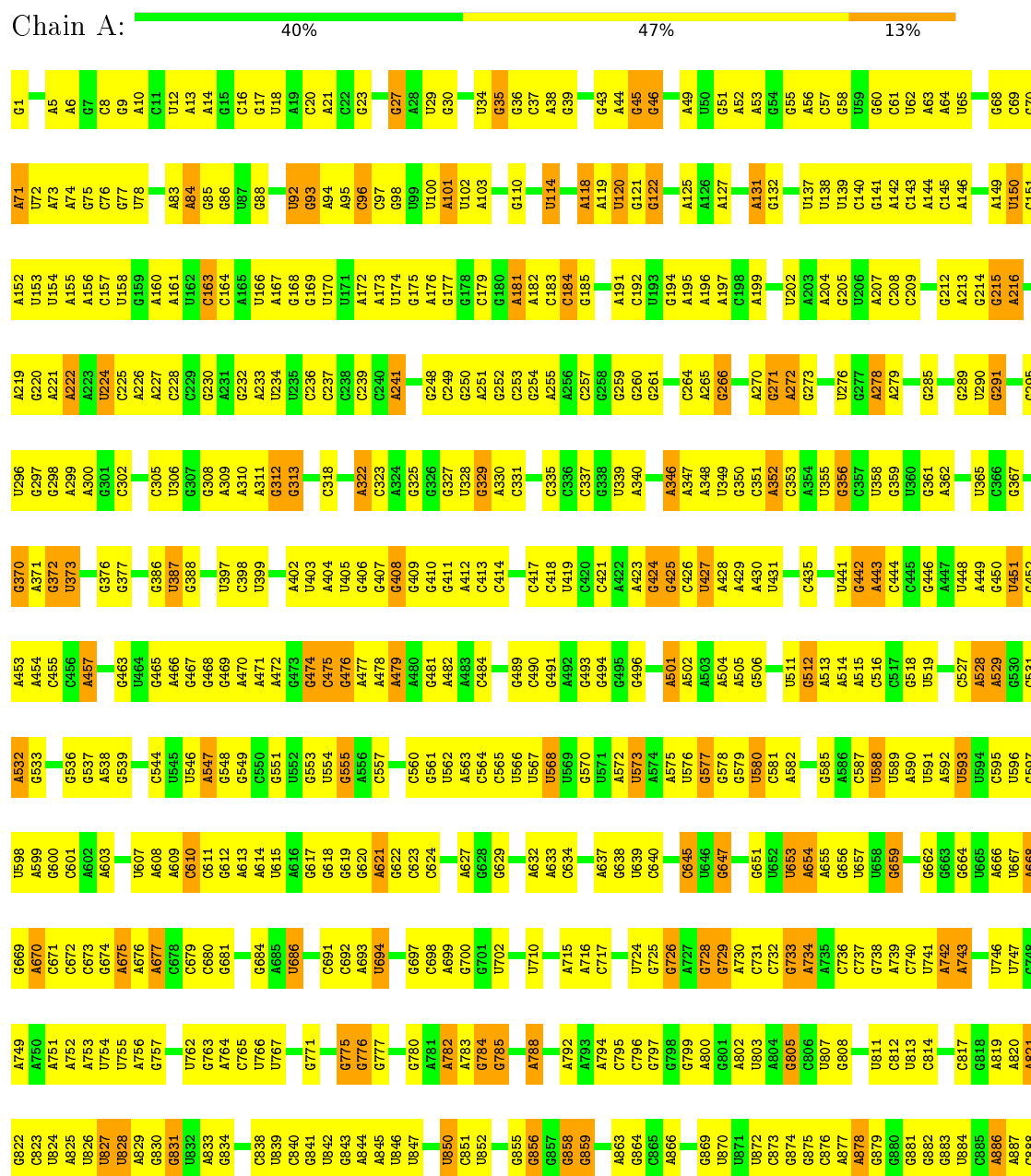
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

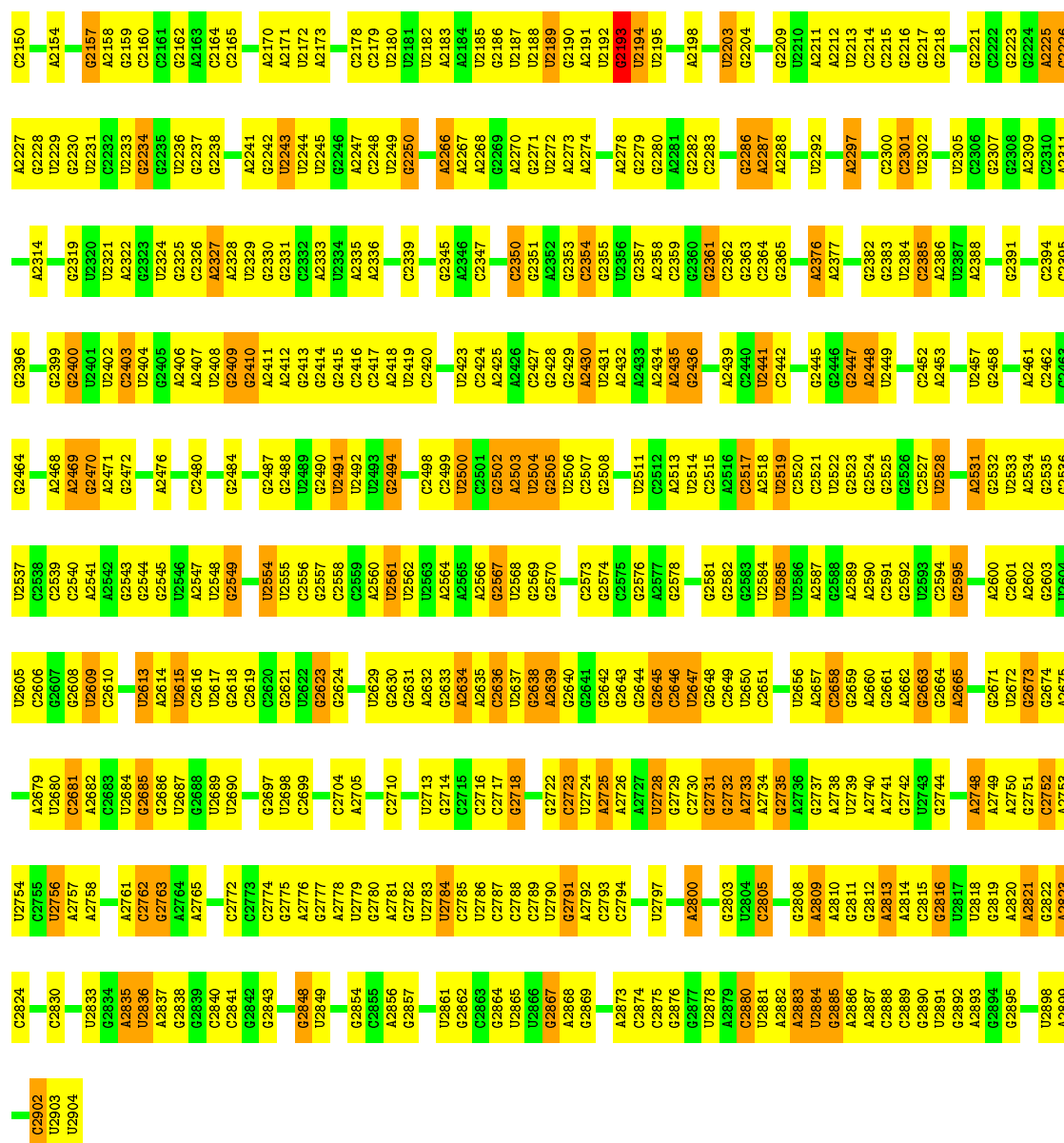
3 Residue-property plots

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

• Molecule 1: 23S rRNA

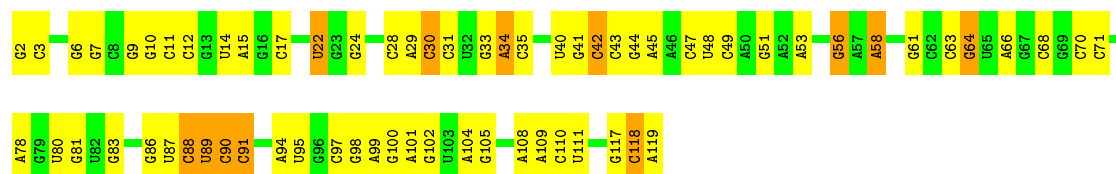


U2074	U2075	U2076	U2077	U2078	U2079	A2080	U2081	U2082	G2083	G2084	U2085	U2086	G2087	U2088	U2089	U2090	G2091	G2092	G2093	G2094	A2095	U2096	U2097	U2098	U2099	G2100	G2101	G2102	G2103	U2104	U2105	U2106	U2107	U2108	U2109	U2110	U2111	U2112	U2113	U2114	U2115	U2116	U2117	U2118	U2119	G2120	U2121	U2122	U2123	U2124	U2125	U2126	U2127	U2128	U2129	U2130	U2131	U2132	U2133	U2134	U2135	U2136	U2137	U2138	U2139	U2140	U2141	U2142	U2143	U2144	U2145	U2146	U2147	U2148	U2149																																																																																						
C1748	A1749	G1750	G1751	G1752	G1753	U1754	U1755	A1756	U1757	U1758	U1759	U1760	U1761	U1762	U1763	U1764	U1765	U1766	U1767	U1768	U1769	U1770	U1771	U1772	U1773	U1774	U1775	U1776	U1777	U1778	U1779	U1780	U1781	U1782	U1783	U1784	U1785	U1786	U1787	U1788	U1789	U1790	U1791	U1792	U1793	U1794	U1795	U1796	U1797	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																																																																																
G1830	G1831	G1832	G1833	G1834	G1835	G1836	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																																																																				
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U1181	G1182	U1183	U1184	U1185	U1186	U1187	U1188	U1189	U1190	U1191	U1192	U1193	U1194	U1195	U1196	U1197	U1198	U1199	U1200	U1201	U1202	U1203	U1204	U1205	U1206	U1207	U1208	U1209	U1210	U1211	U1212	U1213	U1214	U1215	U1216	U1217	U1218	U1219	U1220	U1221	U1222	U1223	U1224	U1225	U1226	U1227	U1228	U1229	U1230	U1231	U1232	U1233	U1234	U1235	U1236	U1237	U1238	U1239	U1240	U1241	U1242	U1243	U1244	U1245	U1246	U1247	U1248	U1249	U1250	U1251	U1252	U1253	U1254	U1255	U1256	U1257	U1258	U1259	U1260	U1261	U1262	U1263	U1264	U1265	U1266																																																																												
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C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C9																																																																																							



• Molecule 2: 5S rRNA

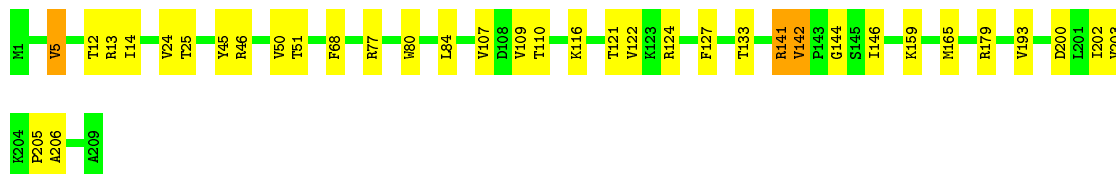
Chain B: 43% 47% 10%





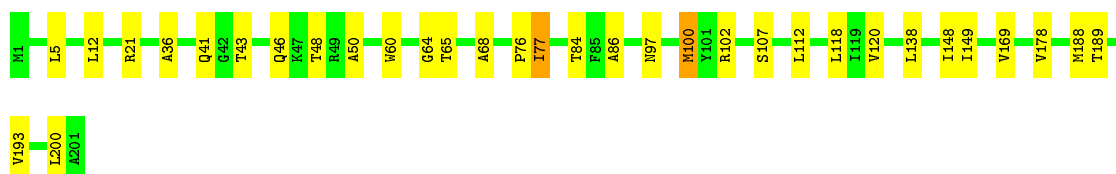
• Molecule 4: 50S ribosomal protein L3

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% .



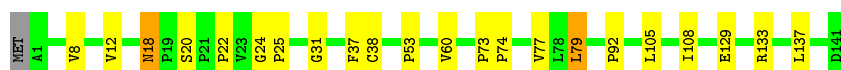
• Molecule 8: 50S ribosomal protein L9

Chain H: 88% 11% .



• Molecule 9: 50S ribosomal protein L11

Chain J: 84% 14% ..




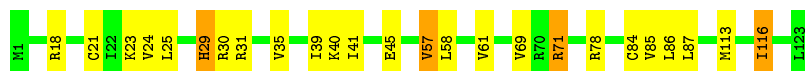
- Molecule 10: 50S ribosomal protein L13

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% .




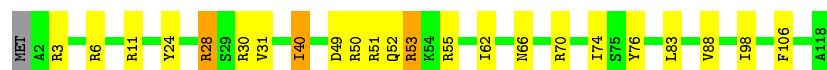
- Molecule 16: 50S ribosomal protein L19

Chain Q:  89% 10% .




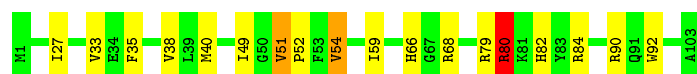
- Molecule 17: 50S ribosomal protein L20

Chain R:  80% 17% ..




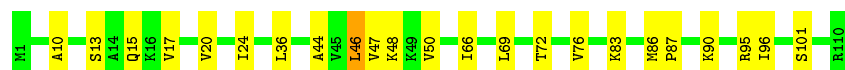
- Molecule 18: 50S ribosomal protein L21

Chain S:  83% 15% ..




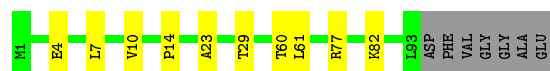
- Molecule 19: 50S ribosomal protein L22

Chain T:  79% 20% .




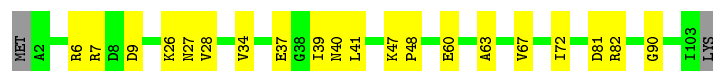
- Molecule 20: 50S ribosomal protein L23

Chain U:  83% 10% 7%




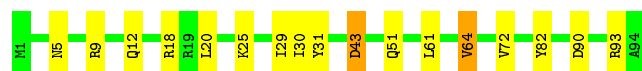
- Molecule 21: 50S ribosomal protein L24

Chain V:  79% 19% .



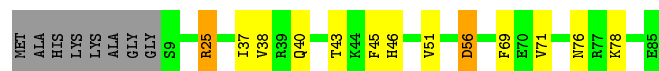
- Molecule 22: 50S ribosomal protein L25

Chain W:  82% 16% .



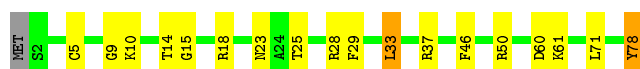
- Molecule 23: 50S ribosomal protein L27

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%



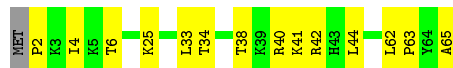
- Molecule 29: 50S ribosomal protein L34

Chain 3: 89% 11%



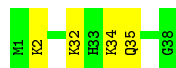
- Molecule 30: 50S ribosomal protein L35

Chain 4: 77% 22% .



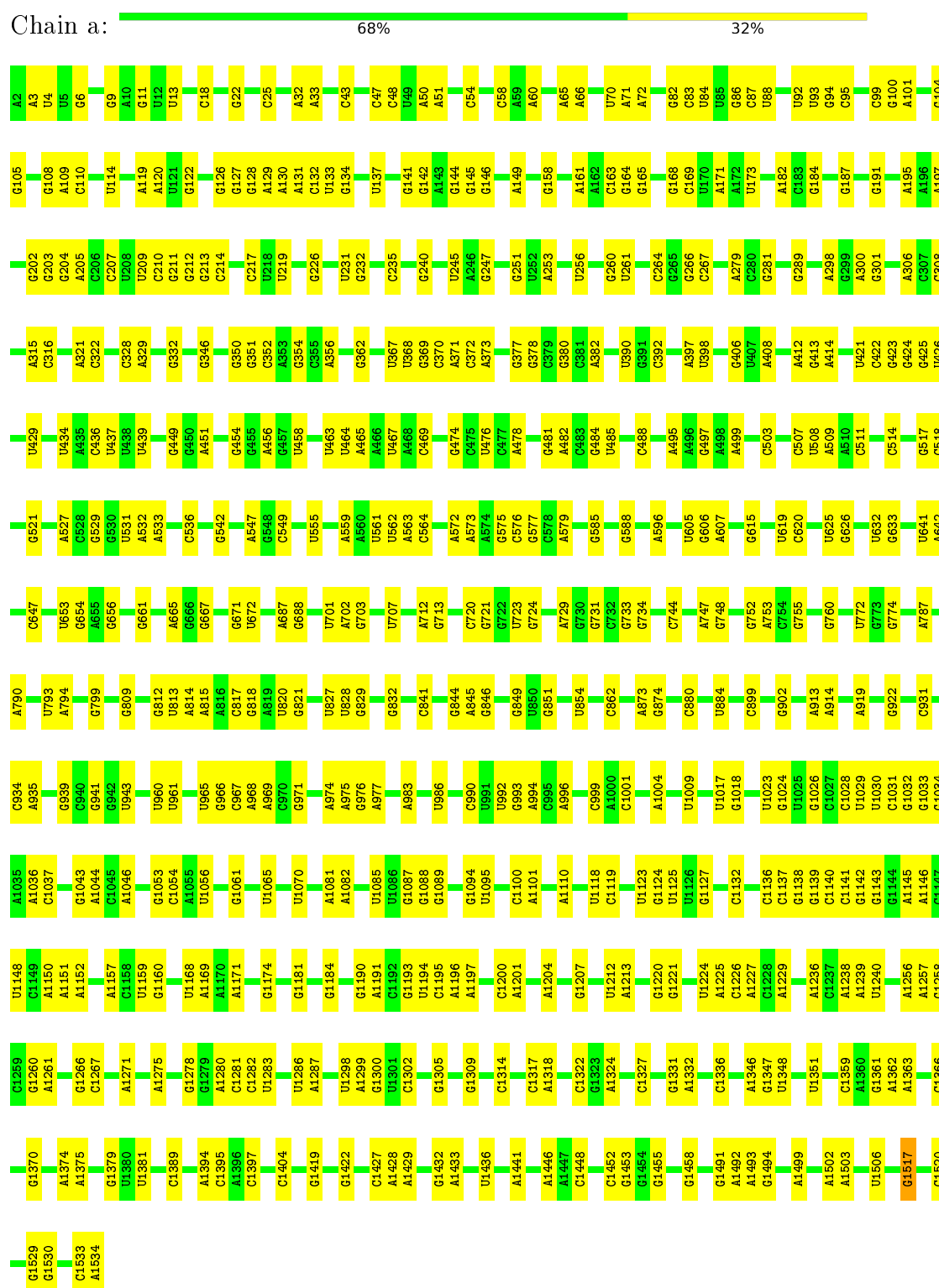
- Molecule 31: 50S ribosomal protein L36

Chain 5: 89% 11%



• Molecule 32: 16S rRNA

Chain a:



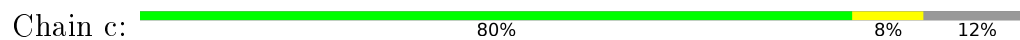
• Molecule 33: 30S ribosomal protein S2

Chain b:





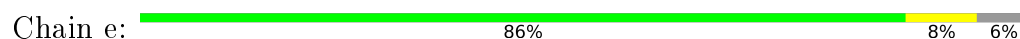
- Molecule 34: 30S ribosomal protein S3



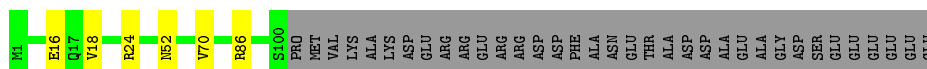
- Molecule 35: 30S ribosomal protein S4



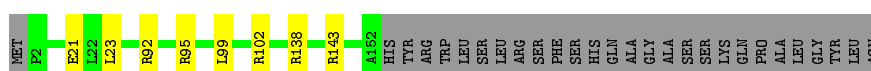
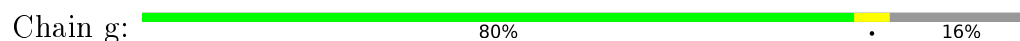
- Molecule 36: 30S ribosomal protein S5



- Molecule 37: 30S ribosomal protein S6



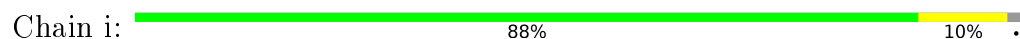
- Molecule 38: 30S ribosomal protein S7



- 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%



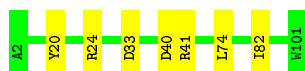
- Molecule 44: 30S ribosomal protein S13

Chain m: 91% 5% . .



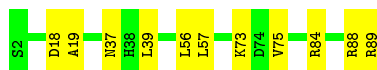
- Molecule 45: 30S ribosomal protein S14

Chain n: 93% 7%



- Molecule 46: 30S ribosomal protein S15

Chain o: 88% 13%




- Molecule 47: 30S ribosomal protein S16

Chain p: 90% 10%




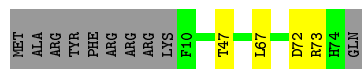
- Molecule 48: 30S ribosomal protein S17

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% .




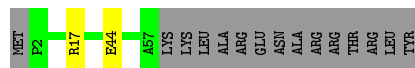
- Molecule 51: 30S ribosomal protein S20

Chain t:  95% 5%




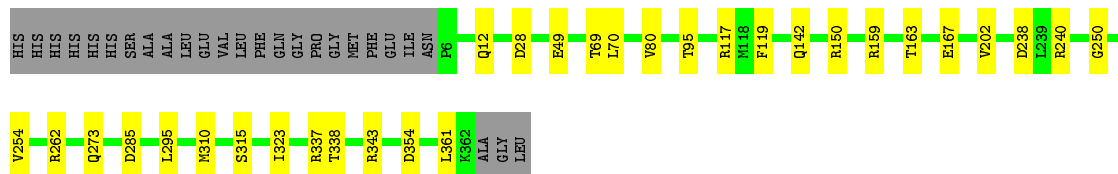
- Molecule 52: 30S ribosomal protein S21

Chain u:  76% . 21%



- Molecule 53: Peptide chain release factor 2

Chain v:  85% 8% 7%



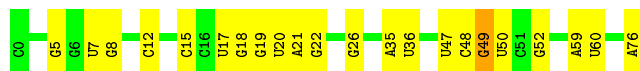
- Molecule 54: Alternative ribosome-rescue factor A

Chain w:  68% 14% 18%




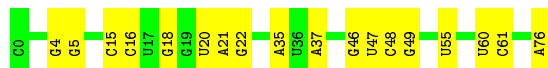
- Molecule 55: P-site or E-site fMet-tRNA(fMet)

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, Not provided	Depositor
Number of particles used	155440	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	83822	Depositor
Image detector	Not provided	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	63
4	D	207/209 (99%)	193 (93%)	13 (6%)	1 (0%)	34	78
5	E	199/201 (99%)	183 (92%)	14 (7%)	2 (1%)	19	66
6	F	175/179 (98%)	155 (89%)	16 (9%)	4 (2%)	8	48
7	G	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
8	H	147/149 (99%)	130 (88%)	15 (10%)	2 (1%)	14	58
9	J	139/142 (98%)	117 (84%)	16 (12%)	6 (4%)	3	31
10	K	140/142 (99%)	135 (96%)	4 (3%)	1 (1%)	26	72
11	L	121/123 (98%)	113 (93%)	8 (7%)	0	100	100
12	M	142/144 (99%)	130 (92%)	11 (8%)	1 (1%)	26	72
13	N	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
14	O	118/127 (93%)	105 (89%)	12 (10%)	1 (1%)	24	70
15	P	114/117 (97%)	103 (90%)	10 (9%)	1 (1%)	21	68
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	42
19	T	108/110 (98%)	102 (94%)	5 (5%)	1 (1%)	21	68
20	U	91/100 (91%)	83 (91%)	6 (7%)	2 (2%)	8	49
21	V	100/104 (96%)	82 (82%)	17 (17%)	1 (1%)	19	66
22	W	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
23	X	75/85 (88%)	68 (91%)	6 (8%)	1 (1%)	15	60
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	54
26	0	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	11	53
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	48/55 (87%)	44 (92%)	3 (6%)	1 (2%)	9	50
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%)	34	78
34	c	204/233 (88%)	192 (94%)	10 (5%)	2 (1%)	19	66
35	d	202/206 (98%)	192 (95%)	10 (5%)	0	100	100
36	e	155/167 (93%)	145 (94%)	8 (5%)	2 (1%)	15	60
37	f	98/135 (73%)	93 (95%)	4 (4%)	1 (1%)	19	66
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	47
41	j	96/103 (93%)	87 (91%)	6 (6%)	3 (3%)	5	41
42	k	115/117 (98%)	103 (90%)	11 (10%)	1 (1%)	21	68
43	l	121/123 (98%)	112 (93%)	8 (7%)	1 (1%)	24	70
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%)	16	61
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%)	15	60
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%)	46	84
54	w	45/57 (79%)	39 (87%)	5 (11%)	1 (2%)	8	49
All	All	6056/6398 (95%)	5615 (93%)	390 (6%)	51 (1%)	29	70

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%)	14	50
4	D	164/164 (100%)	153 (93%)	11 (7%)	20	61
5	E	165/165 (100%)	159 (96%)	6 (4%)	42	77
6	F	148/150 (99%)	136 (92%)	12 (8%)	15	52
7	G	137/138 (99%)	132 (96%)	5 (4%)	42	77
8	H	114/114 (100%)	109 (96%)	5 (4%)	35	73
9	J	109/110 (99%)	103 (94%)	6 (6%)	27	67
10	K	116/116 (100%)	114 (98%)	2 (2%)	68	89
11	L	104/104 (100%)	96 (92%)	8 (8%)	16	54
12	M	103/103 (100%)	96 (93%)	7 (7%)	20	60
13	N	109/109 (100%)	103 (94%)	6 (6%)	27	67
14	O	100/103 (97%)	95 (95%)	5 (5%)	30	69
15	P	86/87 (99%)	78 (91%)	8 (9%)	11	45
16	Q	99/100 (99%)	93 (94%)	6 (6%)	23	64
17	R	89/90 (99%)	81 (91%)	8 (9%)	12	46
18	S	84/84 (100%)	81 (96%)	3 (4%)	42	77
19	T	93/93 (100%)	92 (99%)	1 (1%)	80	92
20	U	80/84 (95%)	78 (98%)	2 (2%)	55	84
21	V	83/85 (98%)	78 (94%)	5 (6%)	24	64
22	W	78/78 (100%)	69 (88%)	9 (12%)	7	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	X	59/63 (94%)	55 (93%)	4 (7%)	20	60
24	Y	67/68 (98%)	60 (90%)	7 (10%)	9	39
25	Z	54/55 (98%)	53 (98%)	1 (2%)	65	87
26	0	48/49 (98%)	48 (100%)	0	100	100
27	1	47/48 (98%)	45 (96%)	2 (4%)	35	74
28	2	45/49 (92%)	44 (98%)	1 (2%)	60	85
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%)	17	55
34	c	170/190 (90%)	153 (90%)	17 (10%)	9	41
35	d	171/173 (99%)	157 (92%)	14 (8%)	14	51
36	e	119/126 (94%)	107 (90%)	12 (10%)	9	40
37	f	87/116 (75%)	82 (94%)	5 (6%)	25	66
38	g	124/147 (84%)	116 (94%)	8 (6%)	21	62
39	h	104/104 (100%)	98 (94%)	6 (6%)	25	65
40	i	105/107 (98%)	95 (90%)	10 (10%)	11	43
41	j	86/90 (96%)	76 (88%)	10 (12%)	7	33
42	k	90/90 (100%)	88 (98%)	2 (2%)	60	85
43	l	103/103 (100%)	96 (93%)	7 (7%)	20	60
44	m	92/96 (96%)	85 (92%)	7 (8%)	16	55
45	n	83/83 (100%)	76 (92%)	7 (8%)	14	50
46	o	76/76 (100%)	66 (87%)	10 (13%)	5	27
47	p	65/65 (100%)	57 (88%)	8 (12%)	6	29
48	q	74/78 (95%)	67 (90%)	7 (10%)	11	43
49	r	57/66 (86%)	53 (93%)	4 (7%)	19	59
50	s	72/72 (100%)	65 (90%)	7 (10%)	10	42
51	t	65/65 (100%)	61 (94%)	4 (6%)	23	63
52	u	48/61 (79%)	46 (96%)	2 (4%)	36	74
53	v	304/324 (94%)	274 (90%)	30 (10%)	10	41
54	w	40/46 (87%)	33 (82%)	7 (18%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5041/5228 (96%)	4695 (93%)	346 (7%)	24 59

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	18,26,27	1.25	2 (11%)	21,38,41	2.43	7 (33%)
1	PSU	A	1911	1	15,21,22	1.16	1 (6%)	16,30,33	2.25	4 (25%)
1	PSU	A	1917	1	15,21,22	1.15	1 (6%)	16,30,33	2.35	5 (31%)
1	5MU	A	1939	1	13,22,23	0.85	0	16,32,35	3.17	4 (25%)
1	5MC	A	1962	1	14,22,23	1.53	1 (7%)	17,32,35	0.97	1 (5%)
1	OMG	A	2251	1,55	18,26,27	1.28	2 (11%)	21,38,41	1.80	5 (23%)
1	2MG	A	2445	1	18,26,27	1.23	2 (11%)	21,38,41	2.42	8 (38%)
1	PSU	A	2457	1	15,21,22	1.33	1 (6%)	16,30,33	2.56	4 (25%)
1	OMC	A	2498	1,57	15,22,23	0.74	1 (6%)	20,31,34	1.82	3 (15%)
1	PSU	A	2504	1	15,21,22	1.38	1 (6%)	16,30,33	2.56	6 (37%)
1	OMU	A	2552	1	14,22,23	0.78	0	19,31,34	1.77	2 (10%)
1	PSU	A	2580	1	15,21,22	1.35	2 (13%)	16,30,33	2.44	5 (31%)
1	PSU	A	2605	1	15,21,22	1.23	1 (6%)	16,30,33	2.19	4 (25%)
1	1MG	A	745	1	17,26,27	1.44	3 (17%)	19,39,42	1.25	3 (15%)
1	PSU	A	746	1,57	15,21,22	1.27	1 (6%)	16,30,33	2.12	2 (12%)
1	5MU	A	747	1	13,22,23	0.84	1 (7%)	16,32,35	3.03	5 (31%)
1	PSU	A	955	1	15,21,22	1.12	1 (6%)	16,30,33	2.23	4 (25%)
32	2MG	a	1207	32	18,26,27	1.44	2 (11%)	21,38,41	2.49	7 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	4OC	a	1402	32	15,23,24	0.72	0	21,32,35	1.96	4 (19%)
32	5MC	a	1407	32	14,22,23	1.57	2 (14%)	17,32,35	1.06	1 (5%)
32	UR3	a	1498	32	13,22,23	0.99	1 (7%)	18,32,35	0.99	0
32	2MG	a	1516	32	18,26,27	1.29	2 (11%)	21,38,41	2.44	8 (38%)
32	MA6	a	1518	32	18,26,27	1.13	1 (5%)	15,38,41	2.48	3 (20%)
32	MA6	a	1519	32	18,26,27	1.16	1 (5%)	15,38,41	2.60	6 (40%)
32	PSU	a	516	32	15,21,22	1.06	1 (6%)	16,30,33	2.40	5 (31%)
32	2MG	a	966	32	18,26,27	1.40	2 (11%)	21,38,41	2.44	7 (33%)
32	5MC	a	967	32	14,22,23	1.58	1 (7%)	17,32,35	1.00	1 (5%)
53	MEQ	v	252	53	7,9,10	0.42	0	8,10,12	0.93	1 (12%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	a	1519	32	-	0/7/29/30	0/3/3/3
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 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2504	PSU	C5-C1'	-4.39	1.48	1.52
1	A	2457	PSU	C5-C1'	-4.27	1.48	1.52
1	A	2580	PSU	C5-C1'	-3.88	1.48	1.52
1	A	746	PSU	C5-C1'	-3.73	1.49	1.52
1	A	2605	PSU	C5-C1'	-3.26	1.49	1.52

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	747	5MU	C5-C4-N3	-8.28	118.40	125.35
1	A	1939	5MU	C5-C4-N3	-8.00	118.64	125.35
32	a	1518	MA6	N3-C2-N1	-6.81	123.52	128.87
32	a	1519	MA6	N3-C2-N1	-6.68	123.62	128.87
1	A	2457	PSU	C5-C1'-C2'	-5.16	106.67	115.44

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.