



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2025 – 06:32 pm GMT

PDB ID : 7OII
EMDB ID : EMD-12930
Title : CspA-70 cotranslational folding intermediate 2
Authors : Agirrezabala, X.; Samatova, E.; Macher, M.; Liutkute, M.; Gil-Carton, D.;
Novacek, J.; Valle, M.; Rodnina, M.V.
Deposited on : 2021-05-11
Resolution : 3.00 Å(reported)
Based on initial model : 6ORE

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

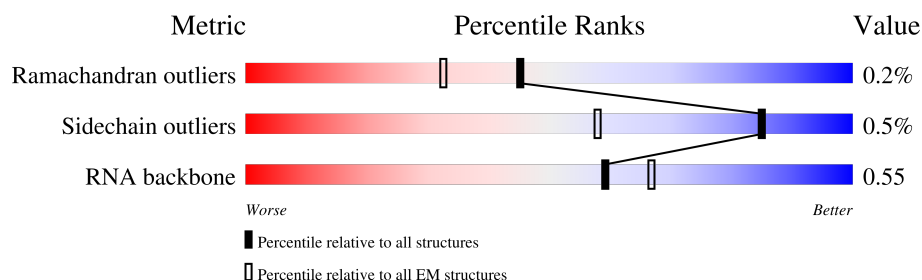
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



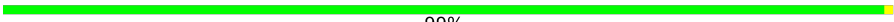
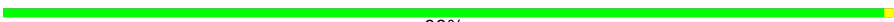












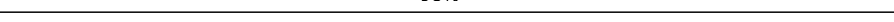
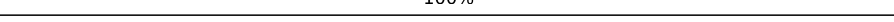
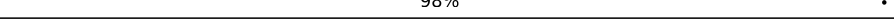
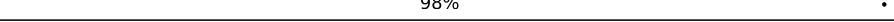
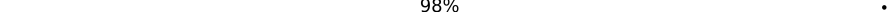
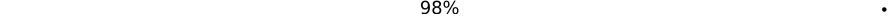
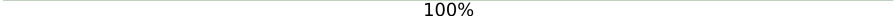
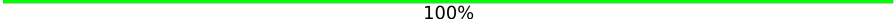
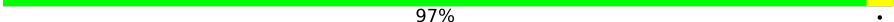
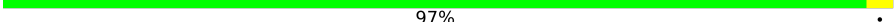

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	1	2903	71% 27% .
2	2	1534	77% 22% .
3	3	120	82% 17% .
4	C	271	100%
5	D	209	98% .
6	E	201	100%
7	F	177	99% .
8	G	175	99% .
9	H	149	98% .















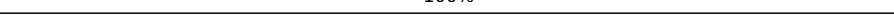
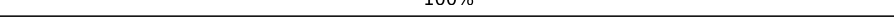
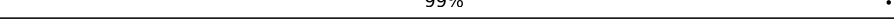
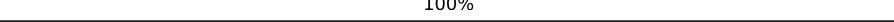
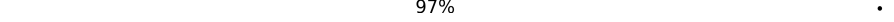


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Mol	Chain	Length	Quality of chain
10	I	142	 99% .
11	J	123	 99% .
12	K	144	 99% .
13	L	136	 99% .
14	M	119	 99% .
15	N	116	 100%
16	O	114	 100%
17	P	117	 99% .
18	Q	103	 98% .
19	R	110	 99% .
20	S	94	 100%
21	T	103	 99% .
22	U	94	 99% .
23	V	84	 98% .
24	W	77	 100%
25	X	62	 98% .
26	Y	58	 98% .
27	Z	66	 98% .
28	a	56	 98% .
29	b	52	 100%
30	c	46	 100%
31	d	64	 97% .
32	e	38	 97% .
33	f	225	 100%
34	g	208	 99% .

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Mol	Chain	Length	Quality of chain
35	h	205	 100%
36	i	156	 97% .
37	j	104	 100%
38	k	151	 100%
39	l	129	 100%
40	m	127	 98% .
41	n	99	 98% ..
42	o	117	 99% .
43	p	123	 99% .
44	q	116	 100%
45	r	100	 100%
46	s	88	 100%
47	t	82	 100%
48	u	80	 100%
49	v	66	 100%
50	w	83	 99% .
51	x	86	 100%
52	y	70	 97% .
53	4	6	 67% 33%
54	z	85	 52% 34% 14%
55	B	39	 100%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 145171 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	1	2903	Total	C	N	O	P	0	0
			62336	27816	11470	20147	2903		

- Molecule 2 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1534	Total	C	N	O	P	0	0
			32929	14693	6041	10661	1534		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 4 is a protein called 50S ribosomal protein L2.

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

- Molecule 5 is a protein called 50S ribosomal protein L3.

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

- Molecule 6 is a protein called 50S ribosomal protein L4.

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

- Molecule 7 is a protein called 50S ribosomal protein L5.

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

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 9 is a protein called 50S ribosomal protein L9.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	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	J	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	K	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	L	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	M	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	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	O	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	P	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	Q	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	R	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	S	94	Total	C	N	O	S	0	0
			746	470	140	134	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
21	T	103	Total	C	N	O	0	0
			788	498	148	142		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	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	V	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	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	X	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	Y	58	Total	C	N	O	S	0	0
			448	281	87	78	2		

- Molecule 27 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 28 is a protein called 50S ribosomal protein L32.

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

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	52	Total	C	N	O	S	0	0
			426	275	78	73			

- Molecule 30 is a protein called 50S ribosomal protein L34.

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

- Molecule 31 is a protein called 50S ribosomal protein L35.

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

- Molecule 32 is a protein called 50S ribosomal protein L36.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	225	Total	C	N	O	S	0	0
			1760	1113	316	323	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	208	Total	C	N	O	S	0	0
			1636	1036	307	290	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	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	l	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	m	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	n	99	Total	C	N	O	S	0	0
			790	495	151	143	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	o	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	p	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	116	Total	C	N	O	S	0	0
			900	558	181	158	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	r	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	s	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	t	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	u	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	v	66	Total	C	N	O	S	0	0
			544	344	102	97	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	w	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	x	86	Total	C	N	O	S	0	0
			669	414	138	114	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	y	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	4	6	Total	C	N	O	P	0	0
			122	55	17	44	6		

- Molecule 54 is a RNA chain called tRNA-Leu.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	z	85	Total	C	N	O	P	0	0
			1830	822	328	595	85		

- Molecule 55 is a protein called Cold-shock DNA-binding protein family.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	B	39	Total	C	N	O	0	0
			250	159	43	48		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	ILE	VAL	conflict	UNP A0A1H2D2H5

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	1	282	Total 282	Mg 282	0
56	2	119	Total 119	Mg 119	0
56	3	8	Total 8	Mg 8	0
56	C	1	Total 1	Mg 1	0
56	D	1	Total 1	Mg 1	0
56	M	1	Total 1	Mg 1	0
56	P	1	Total 1	Mg 1	0
56	a	2	Total 2	Mg 2	0
56	h	1	Total 1	Mg 1	0
56	q	1	Total 1	Mg 1	0
56	4	1	Total 1	Mg 1	0
56	z	4	Total 4	Mg 4	0

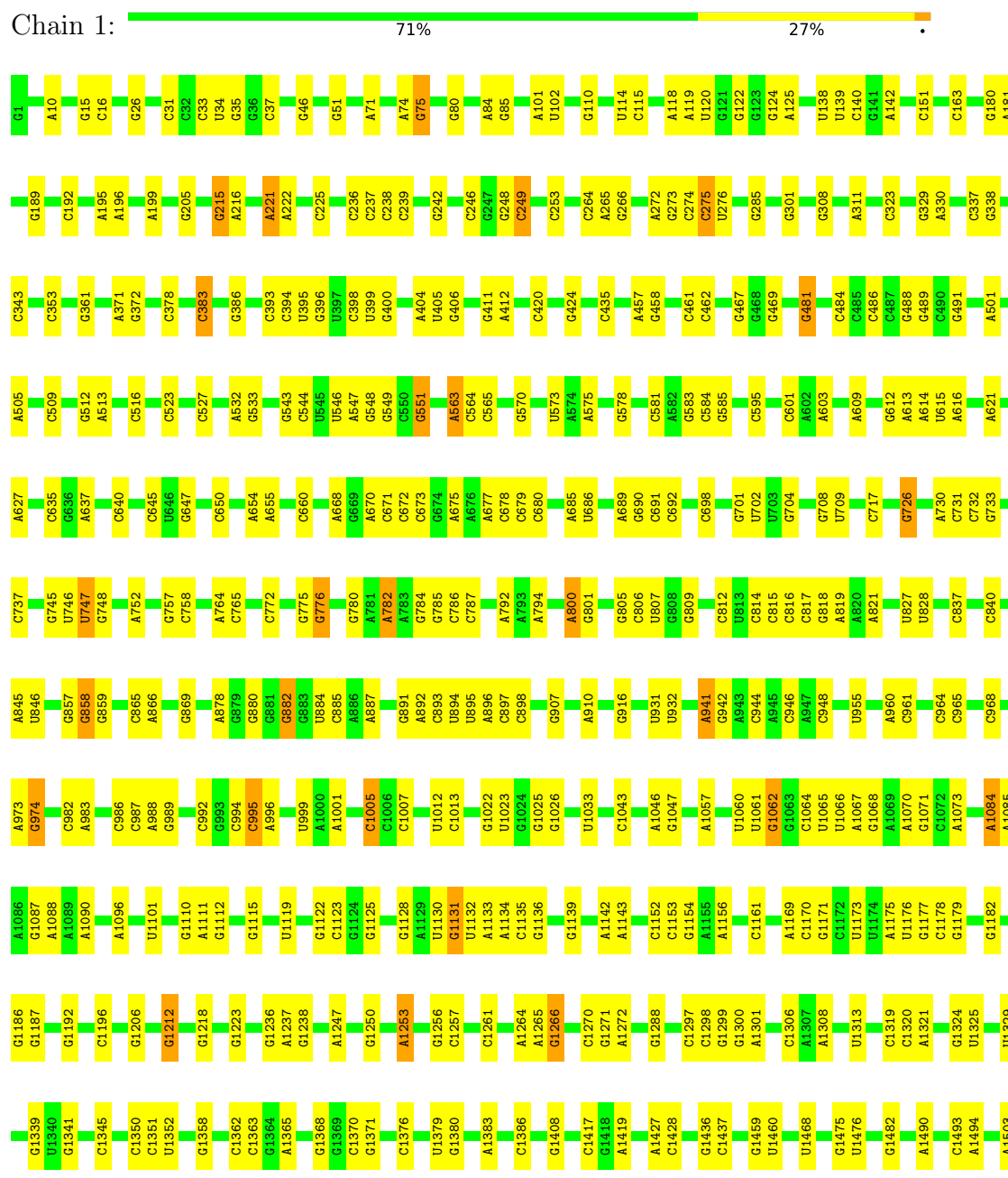
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	Z	1	Total 1	Zn 1	0
57	e	1	Total 1	Zn 1	0

3 Residue-property plots

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

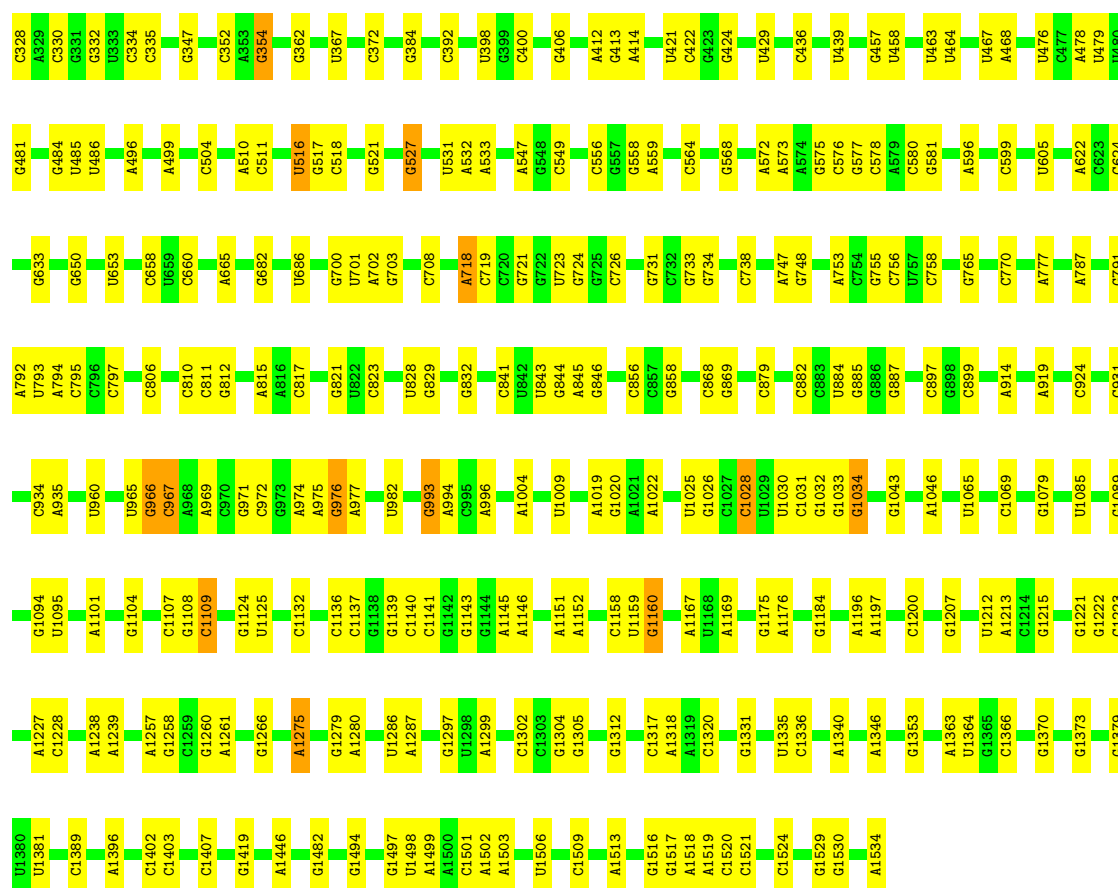


A1504	A1618	C1793	U1923	U2022	A2114	A2225	C2347	A2476	U2586	C2730	A2879
A1508	G1619	A1794	C1924	C2023	G2115	U2229	C2350	U2477	C2591	A2733	C2880
A1509	C1625	C1795	C1929	G2024	G2116	U2239	C2357	U2478	C2592	A2734	A2883
G1510	G1631	C1800	G1930	C2025	A2117	C2232	G2361	C2480	U2593	G2744	U2884
A1515	A1634	A1801	G1939	G2029	A2118	G2238	G2365	U2491	C2594	A2748	G2885
G1521	A1638	A1808	C1934	A2030	G2121	G2239	C2364	C2496	G2597	G2751	C2888
G1524	C1639	G1811	A1936	A2031	G2122	U2243	G2365	A2497	C2601	U2756	U2891
G1529	C1646	A1815	A1937	A2032	A2121	U2244	A2376	C2498	A2602	A2757	G2894
G1530	U1647	C1816	A1938	U2034	G2125	C2248	G2382	G2502	U2605	A2785	U2898
A1532	U1648	C1822	U1940	C2036	U2131	U2249	G2383	A2503	G2607	G2777	U2903
A1536	U1649	A1828	C1941	C2043	U2132	G2250	U2384	U2504	G2608	A2778	G2903
G1537	G1651	G1829	C1947	C2044	A2134	G2252	C2385	U2505	U2609	G2791	G2908
U1554	A1652	A1832	G1950	C2045	U2139	C2260	U2402	C2506	C2611	G2792	U2909
C1557	G1653	C1833	G1955	C2050	G2140	C2263	A2406	C2510	U2613	A2793	G2910
C1558	U1657	U1834	C1958	G2053	A2142	C2264	C2417	U2512	U2629	U2797	C2911
U1559	C1658	C1836	C1961	C2054	C2145	G2271	U2423	U2513	C2645	A2798	A2799
C1564	A1668	A1847	C1962	C2056	A2147	C2275	A2424	C2515	G2663	G2811	G2811
C1565	U1669	A1848	C1967	A2060	A2158	A2278	A2425	A2518	A2675	C2815	C2815
C1566	C1670	A1853	A1970	G2061	G2160	A2279	A2426	U2519	U2676	U2818	U2818
G1567	G1673	G1857	U1971	C2063	C2161	C2283	G2428	C2520	G2677	G2819	G2819
G1568	C1675	A1858	U1972	C2064	G2162	A2284	G2429	C2521	C2678	A2820	A2820
A1569	G1697	U1865	G1973	C2065	A2163	C2285	A2430	G2529	C2681	A2823	A2823
A1571	C1731	C1974	C1974	C2066	C2165	G2287	U2431	G2535	C2682	C2824	C2824
A1572	G1715	C1868	C1985	C2069	A2169	A2288	A2435	C2538	C2683	G2825	G2825
G1573	C1728	G1869	C1986	C2072	G2170	U2305	C2440	C2539	G2688	U2833	U2833
U1578	U1729	C1870	C1990	C2073	A2171	G2308	U2441	C2540	U2689	G2834	G2834
A1579	C1730	A1871	U1991	U2074	U2172	A2309	C2442	G2547	U2690	A2835	A2835
A1580	G1732	A1872	G1992	U2075	A2173	A2314	G2443	C2551	C2704	U2836	U2836
A1583	C1738	C1894	C1993	G2083	C2178	G2319	G2445	U2552	G2709	C2841	C2841
G1587	G1756	C1895	C1996	C2081	A2183	G2319	G2446	G2553	C2710	G2848	G2848
U1589	C1761	A1899	C1997	U2092	U2189	A2322	A2448	U2554	G2714	C2853	C2853
A1590	C1904	C2000	C2001	A2094	G2190	G2323	A2450	C2558	C2715	U2858	U2858
A1603	C1905	C2002	G2002	A2095	U2192	G2325	A2451	C2559	C2716	C2862	C2862
C1604	G1906	C1906	C2006	G2100	G2193	C2326	G2454	A2566	G2717	C2867	C2867
C1605	A1773	G1907	C2007	A2101	U2195	A2327	U2457	G2567	G2719	U2861	U2861
A1608	U1782	U1911	C2008	G2102	A2198	A2333	G2458	A2572	A2721	C2863	C2863
C1612	C1788	A1912	A2009	G2107	G2204	U2334	C2465	C2574	G2722	G2867	G2867
C1615	A1789	A1913	U2011	G2110	A2211	A2335	C2466	C2575	U2724	A2872	A2872
A1616	C1790	C1914	G2012	U2111	G2211	A2336	G2470	U2580	A2726	A2873	A2873
A1617	G1792	31D1915	A2013	G2112	A2211	G2345					
		A1916	A2014	U2113		A2346					

• Molecule 2: 16S rRNA

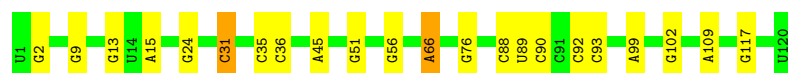
Chain 2:  77% 22%

A1	A7	A8	G9	G15	A16	U17	C18	G21	G22	C23	G31	A32	C36	G39	C47	C48	U49	A50	A51	C52	A53	C54	A66	C67	G68	G69	U70	A71	A72	C73	A74	G75	G76	A81	G82	C83	U84	U85	G86	C87	U92	C106	A109	A120	U121
A130	A131	G141	G144	A149	A160	C163	G164	C169	G177	A181	A182	A197	G204	C207	C210	G211	G212	G226	U245	A246	G247	G251	G266	C267	C271	A279	G289	C290	C295	A306	C312	G319	A320	C322											



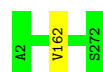
- Molecule 3: 5S rRNA

Chain 3: 82% 17% .



- Molecule 4: 50S ribosomal protein L2

Chain C: 100%



- Molecule 5: 50S ribosomal protein L3

Chain D: 98%



- Molecule 6: 50S ribosomal protein L4

Chain E: 100%



- Molecule 7: 50S ribosomal protein L5

Chain F:  99%



- Molecule 8: 50S ribosomal protein L6

Chain G:  99%



- Molecule 9: 50S ribosomal protein L9

Chain H:  98%



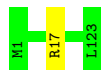
- Molecule 10: 50S ribosomal protein L13

Chain I:  99%



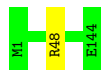
- Molecule 11: 50S ribosomal protein L14

Chain J:  99%



- Molecule 12: 50S ribosomal protein L15

Chain K:  99%



- Molecule 13: 50S ribosomal protein L16

Chain L:  99%



- Molecule 14: 50S ribosomal protein L17

Chain M:  99%



- Molecule 15: 50S ribosomal protein L18

Chain N:  100%

There are no outlier residues recorded for this chain.

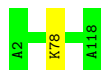
- Molecule 16: 50S ribosomal protein L19

Chain O:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: 50S ribosomal protein L20

Chain P:  99%



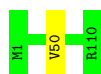
- Molecule 18: 50S ribosomal protein L21

Chain Q:  98%



- Molecule 19: 50S ribosomal protein L22

Chain R:  99%



- Molecule 20: 50S ribosomal protein L23

Chain S:  100%

There are no outlier residues recorded for this chain.

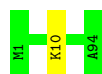
- Molecule 21: 50S ribosomal protein L24

Chain T:  99%



- Molecule 22: 50S ribosomal protein L25

Chain U:  99%



- Molecule 23: 50S ribosomal protein L27

Chain V:  98%



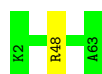
- Molecule 24: 50S ribosomal protein L28

Chain W:  100%

There are no outlier residues recorded for this chain.

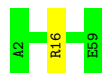
- Molecule 25: 50S ribosomal protein L29

Chain X:  98%



- Molecule 26: 50S ribosomal protein L30

Chain Y:  98%



- Molecule 27: 50S ribosomal protein L31

Chain Z:  98%



- Molecule 28: 50S ribosomal protein L32

Chain a:  98%



- Molecule 29: 50S ribosomal protein L33

Chain b:  100%

There are no outlier residues recorded for this chain.

- Molecule 30: 50S ribosomal protein L34

Chain c:  100%

There are no outlier residues recorded for this chain.

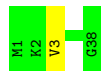
- Molecule 31: 50S ribosomal protein L35

Chain d:  97%



- Molecule 32: 50S ribosomal protein L36

Chain e:  97%



- Molecule 33: 30S ribosomal protein S2

Chain f:  100%

There are no outlier residues recorded for this chain.

- Molecule 34: 30S ribosomal protein S3

Chain g:  99%



- Molecule 35: 30S ribosomal protein S4

Chain h:  100%

There are no outlier residues recorded for this chain.

- Molecule 36: 30S ribosomal protein S5

Chain i:  97%



- Molecule 37: 30S ribosomal protein S6

Chain j:  100%

There are no outlier residues recorded for this chain.

- Molecule 38: 30S ribosomal protein S7

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 39: 30S ribosomal protein S8

Chain l:  100%

There are no outlier residues recorded for this chain.

- Molecule 40: 30S ribosomal protein S9

Chain m:  98%



- Molecule 41: 30S ribosomal protein S10

Chain n:  98%



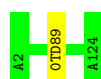
- Molecule 42: 30S ribosomal protein S11

Chain o:  99%



- Molecule 43: 30S ribosomal protein S12

Chain p:  99%



- Molecule 44: 30S ribosomal protein S13

Chain q:  100%

There are no outlier residues recorded for this chain.

- Molecule 45: 30S ribosomal protein S14

Chain r:  100%

There are no outlier residues recorded for this chain.

- Molecule 46: 30S ribosomal protein S15

Chain s:  100%

There are no outlier residues recorded for this chain.

- Molecule 47: 30S ribosomal protein S16

Chain t:  100%

There are no outlier residues recorded for this chain.

- Molecule 48: 30S ribosomal protein S17

Chain u:  100%

There are no outlier residues recorded for this chain.

- Molecule 49: 30S ribosomal protein S18

Chain v:  100%

There are no outlier residues recorded for this chain.

- Molecule 50: 30S ribosomal protein S19

Chain w:  99%



- Molecule 51: 30S ribosomal protein S20

Chain x:  100%

There are no outlier residues recorded for this chain.

- Molecule 52: 30S ribosomal protein S21

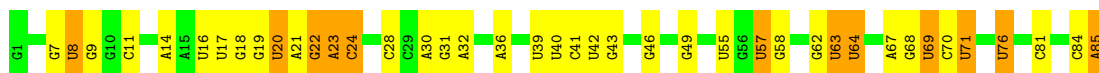
Chain y:  97%



- Molecule 53: mRNA



- Molecule 54: tRNA-Leu



- Molecule 55: Cold-shock DNA-binding protein family



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	23782	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (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: G7M, 5MC, OMU, OMC, MG, 5MU, ZN, 0TD, UR3, 3TD, 2MG, 1MG, PSU, 4OC, 2MA, MA6, 6MZ, OMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	1.63	238/69286 (0.3%)	1.27	240/108087 (0.2%)
2	2	1.45	60/36590 (0.2%)	1.19	59/57074 (0.1%)
3	3	1.39	3/2872 (0.1%)	1.16	8/4478 (0.2%)
4	C	1.06	1/2121 (0.0%)	0.71	0/2852
5	D	1.07	1/1586 (0.1%)	0.72	1/2134 (0.0%)
6	E	0.96	0/1571	0.69	1/2113 (0.0%)
7	F	0.75	0/1434	0.68	0/1926
8	G	0.71	0/1333	0.64	0/1805
9	H	0.51	0/1122	0.79	0/1515
10	I	1.03	1/1152 (0.1%)	0.67	0/1551
11	J	0.98	0/955	0.74	0/1279
12	K	0.98	0/1062	0.76	0/1413
13	L	1.01	0/1093	0.69	0/1460
14	M	1.00	0/964	0.73	0/1289
15	N	0.89	0/902	0.68	0/1209
16	O	1.03	0/929	0.68	0/1242
17	P	1.19	0/960	0.75	0/1278
18	Q	1.02	0/829	0.70	0/1107
19	R	1.02	1/864 (0.1%)	0.73	0/1156
20	S	0.98	0/752	0.65	0/1005
21	T	0.89	0/796	0.66	0/1062
22	U	0.88	0/766	0.66	0/1025
23	V	1.04	0/642	0.70	0/848
24	W	0.99	0/635	0.71	0/848
25	X	0.76	0/502	0.74	1/667 (0.1%)
26	Y	0.93	0/452	0.73	1/605 (0.2%)
27	Z	0.64	1/531 (0.2%)	0.67	0/709
28	a	1.02	1/450 (0.2%)	0.74	0/599
29	b	0.83	0/433	0.62	0/576
30	c	1.03	0/380	0.78	0/498
31	d	1.05	0/513	0.74	0/676

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	e	1.05	1/303 (0.3%)	0.75	0/397
33	f	0.65	0/1791	0.66	0/2413
34	g	0.82	0/1663	0.66	0/2241
35	h	0.80	0/1665	0.64	0/2227
36	i	0.95	2/1165 (0.2%)	0.73	0/1568
37	j	0.76	0/867	0.67	0/1171
38	k	0.73	0/1195	0.68	0/1602
39	l	0.93	0/989	0.70	0/1326
40	m	0.82	0/1034	0.71	0/1375
41	n	0.74	0/800	0.79	1/1082 (0.1%)
42	o	0.80	0/893	0.68	0/1205
43	p	0.94	0/960	0.72	0/1286
44	q	0.71	0/909	0.69	0/1215
45	r	0.80	0/817	0.66	0/1088
46	s	0.80	0/722	0.68	0/964
47	t	0.90	0/659	0.67	0/884
48	u	0.81	0/657	0.71	0/881
49	v	0.84	0/553	0.69	0/743
50	w	0.69	0/680	0.62	0/915
51	x	0.78	0/675	0.69	0/895
52	y	0.71	0/597	0.66	0/792
53	4	1.64	1/134 (0.7%)	1.42	0/205
54	z	1.47	9/1768 (0.5%)	1.33	14/2759 (0.5%)
55	B	0.55	0/255	0.62	0/347
All	All	1.40	320/156228 (0.2%)	1.13	326/233667 (0.1%)

The worst 5 of 320 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	z	32	A	N9-C4	-8.67	1.32	1.37
1	1	2442	C	N1-C6	-7.47	1.32	1.37
54	z	84	C	N1-C6	-7.46	1.32	1.37
1	1	1999	C	N1-C6	-7.20	1.32	1.37
1	1	673	C	N1-C6	-7.17	1.32	1.37

The worst 5 of 326 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1670	C	C5-C4-N4	-9.67	113.43	120.20
1	1	1670	C	N3-C4-C5	9.66	125.76	121.90
1	1	2719	G	C2-N3-C4	-9.16	107.32	111.90
1	1	2193	G	C4-N9-C1'	9.01	138.21	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1509	A	O4'-C1'-N9	8.55	115.04	108.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	C	269/271 (99%)	256 (95%)	13 (5%)	0	100	100
5	D	207/209 (99%)	201 (97%)	3 (1%)	3 (1%)	9	37
6	E	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
7	F	175/177 (99%)	164 (94%)	10 (6%)	1 (1%)	22	57
8	G	173/175 (99%)	162 (94%)	11 (6%)	0	100	100
9	H	147/149 (99%)	135 (92%)	10 (7%)	2 (1%)	9	37
10	I	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
11	J	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
12	K	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
13	L	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
14	M	117/119 (98%)	114 (97%)	3 (3%)	0	100	100
15	N	114/116 (98%)	111 (97%)	3 (3%)	0	100	100
16	O	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
17	P	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
18	Q	101/103 (98%)	94 (93%)	5 (5%)	2 (2%)	6	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	R	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
20	S	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
21	T	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
22	U	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
23	V	82/84 (98%)	73 (89%)	7 (8%)	2 (2%)	5	25
24	W	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
25	X	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
26	Y	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
27	Z	64/66 (97%)	59 (92%)	5 (8%)	0	100	100
28	a	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
29	b	50/52 (96%)	50 (100%)	0	0	100	100
30	c	44/46 (96%)	44 (100%)	0	0	100	100
31	d	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
32	e	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
33	f	223/225 (99%)	211 (95%)	12 (5%)	0	100	100
34	g	206/208 (99%)	197 (96%)	9 (4%)	0	100	100
35	h	203/205 (99%)	200 (98%)	3 (2%)	0	100	100
36	i	154/156 (99%)	144 (94%)	10 (6%)	0	100	100
37	j	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
38	k	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
39	l	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
40	m	125/127 (98%)	117 (94%)	8 (6%)	0	100	100
41	n	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
42	o	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
43	p	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
44	q	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
45	r	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
46	s	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
47	t	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
48	u	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
49	v	64/66 (97%)	64 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	w	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
51	x	84/86 (98%)	84 (100%)	0	0	100	100
52	y	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
55	B	37/39 (95%)	29 (78%)	8 (22%)	0	100	100
All	All	5653/5754 (98%)	5440 (96%)	203 (4%)	10 (0%)	45	77

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	152	PRO
5	D	153	GLY
5	D	154	LYS
9	H	90	LEU
23	V	5	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	C	216/216 (100%)	216 (100%)	0	100	100
5	D	164/164 (100%)	163 (99%)	1 (1%)	84	93
6	E	165/165 (100%)	165 (100%)	0	100	100
7	F	148/148 (100%)	148 (100%)	0	100	100
8	G	136/136 (100%)	135 (99%)	1 (1%)	81	91
9	H	114/114 (100%)	113 (99%)	1 (1%)	75	89
10	I	116/116 (100%)	116 (100%)	0	100	100
11	J	104/104 (100%)	103 (99%)	1 (1%)	73	88
12	K	103/103 (100%)	102 (99%)	1 (1%)	73	88
13	L	109/109 (100%)	108 (99%)	1 (1%)	75	89
14	M	99/99 (100%)	98 (99%)	1 (1%)	73	88
15	N	86/86 (100%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	O	99/99 (100%)	99 (100%)	0	100	100
17	P	89/89 (100%)	88 (99%)	1 (1%)	70	87
18	Q	84/84 (100%)	84 (100%)	0	100	100
19	R	93/93 (100%)	93 (100%)	0	100	100
20	S	81/81 (100%)	81 (100%)	0	100	100
21	T	84/84 (100%)	83 (99%)	1 (1%)	67	86
22	U	78/78 (100%)	77 (99%)	1 (1%)	65	85
23	V	62/62 (100%)	62 (100%)	0	100	100
24	W	67/67 (100%)	67 (100%)	0	100	100
25	X	54/54 (100%)	54 (100%)	0	100	100
26	Y	48/48 (100%)	48 (100%)	0	100	100
27	Z	59/59 (100%)	59 (100%)	0	100	100
28	a	47/47 (100%)	47 (100%)	0	100	100
29	b	47/47 (100%)	47 (100%)	0	100	100
30	c	38/38 (100%)	38 (100%)	0	100	100
31	d	51/51 (100%)	49 (96%)	2 (4%)	27	61
32	e	34/34 (100%)	34 (100%)	0	100	100
33	f	187/187 (100%)	187 (100%)	0	100	100
34	g	171/171 (100%)	169 (99%)	2 (1%)	67	86
35	h	172/172 (100%)	172 (100%)	0	100	100
36	i	119/119 (100%)	117 (98%)	2 (2%)	56	81
37	j	91/91 (100%)	91 (100%)	0	100	100
38	k	124/124 (100%)	124 (100%)	0	100	100
39	l	104/104 (100%)	104 (100%)	0	100	100
40	m	105/105 (100%)	103 (98%)	2 (2%)	52	79
41	n	86/86 (100%)	84 (98%)	2 (2%)	45	75
42	o	90/90 (100%)	89 (99%)	1 (1%)	70	87
43	p	102/102 (100%)	102 (100%)	0	100	100
44	q	94/94 (100%)	94 (100%)	0	100	100
45	r	83/83 (100%)	83 (100%)	0	100	100
46	s	76/76 (100%)	76 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	t	65/65 (100%)	65 (100%)	0	100	100
48	u	74/74 (100%)	74 (100%)	0	100	100
49	v	57/57 (100%)	57 (100%)	0	100	100
50	w	72/72 (100%)	71 (99%)	1 (1%)	62	83
51	x	65/65 (100%)	65 (100%)	0	100	100
52	y	60/60 (100%)	58 (97%)	2 (3%)	33	67
55	B	16/28 (57%)	16 (100%)	0	100	100
All	All	4688/4700 (100%)	4664 (100%)	24 (0%)	85	94

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	i	29	ARG
40	m	106	ARG
40	m	25	ASN
41	n	5	ARG
14	M	80	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
8	G	38	ASN
9	H	128	HIS
31	d	31	HIS
33	f	36	ASN
50	w	69	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2898/2903 (99%)	494 (17%)	10 (0%)
2	2	1529/1534 (99%)	255 (16%)	5 (0%)
3	3	119/120 (99%)	16 (13%)	0
53	4	5/6 (83%)	1 (20%)	0
54	z	84/85 (98%)	26 (30%)	0
All	All	4635/4648 (99%)	792 (17%)	15 (0%)

5 of 792 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	15	G
1	1	34	U
1	1	35	G
1	1	46	G

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	1475	G
2	2	1109	C
1	1	2189	U
2	2	1145	A
2	2	86	G

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

46 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	PSU	1	2457	1	18,21,22	1.18	2 (11%)	22,30,33	2.20	5 (22%)
1	6MZ	1	2030	1	18,25,26	1.89	4 (22%)	16,36,39	3.27	3 (18%)
1	5MC	1	1962	1	18,22,23	3.04	7 (38%)	26,32,35	1.26	5 (19%)
2	2MG	2	1516	2	18,26,27	2.21	7 (38%)	16,38,41	1.47	4 (25%)
1	PSU	1	1911	1	18,21,22	0.90	0	22,30,33	1.87	3 (13%)
2	MA6	2	1518	2	18,26,27	1.31	1 (5%)	19,38,41	3.44	2 (10%)
54	5MU	z	40	54	19,22,23	1.38	5 (26%)	28,32,35	2.27	11 (39%)
1	PSU	1	1917	1	18,21,22	1.01	1 (5%)	22,30,33	2.13	5 (22%)
54	5MU	z	57	54	19,22,23	4.54	7 (36%)	28,32,35	3.71	9 (32%)
1	PSU	1	955	1	18,21,22	1.08	1 (5%)	22,30,33	1.99	5 (22%)
1	2MG	1	1835	1	18,26,27	2.04	7 (38%)	16,38,41	1.45	3 (18%)
2	2MG	2	1207	2	18,26,27	2.22	7 (38%)	16,38,41	1.35	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	G7M	2	527	2	20,26,27	2.23	9 (45%)	17,39,42	1.11	1 (5%)
2	4OC	2	1402	2	20,23,24	2.69	8 (40%)	26,32,35	1.08	1 (3%)
2	2MG	2	966	2	18,26,27	2.27	7 (38%)	16,38,41	1.32	3 (18%)
1	OMC	1	2498	56,1	19,22,23	2.51	6 (31%)	26,31,34	0.96	0
1	G7M	1	2069	1	20,26,27	2.17	8 (40%)	17,39,42	1.29	2 (11%)
1	6MZ	1	1618	1	18,25,26	1.89	5 (27%)	16,36,39	3.26	3 (18%)
1	5MU	1	1939	56,1	19,22,23	4.39	7 (36%)	28,32,35	3.71	10 (35%)
2	5MC	2	967	2	18,22,23	3.27	7 (38%)	26,32,35	1.12	2 (7%)
54	5MU	z	20	56,54	19,22,23	4.78	7 (36%)	28,32,35	3.73	9 (32%)
1	PSU	1	2504	1	18,21,22	0.98	1 (5%)	22,30,33	1.85	4 (18%)
54	5MU	z	39	54	19,22,23	1.44	5 (26%)	28,32,35	2.17	9 (32%)
2	MA6	2	1519	2	18,26,27	1.37	1 (5%)	19,38,41	3.65	2 (10%)
54	5MU	z	71	54	19,22,23	1.34	5 (26%)	28,32,35	2.21	9 (32%)
1	OMU	1	2552	1	19,22,23	2.74	6 (31%)	26,31,34	1.67	6 (23%)
1	PSU	1	2580	56,1	18,21,22	1.14	1 (5%)	22,30,33	2.23	6 (27%)
54	5MU	z	69	54	19,22,23	6.60	6 (31%)	28,32,35	28.78	14 (50%)
54	5MU	z	42	54,2	19,22,23	4.34	7 (36%)	28,32,35	3.84	11 (39%)
54	5MU	z	63	54	19,22,23	1.45	6 (31%)	28,32,35	2.45	13 (46%)
54	5MU	z	55	54	19,22,23	4.68	7 (36%)	28,32,35	3.48	9 (32%)
1	5MU	1	747	1	19,22,23	4.50	7 (36%)	28,32,35	3.78	9 (32%)
1	1MG	1	745	1	18,26,27	2.61	5 (27%)	19,39,42	1.62	4 (21%)
2	PSU	2	516	56,2	18,21,22	0.97	1 (5%)	22,30,33	1.88	3 (13%)
54	5MU	z	76	54	19,22,23	1.43	6 (31%)	28,32,35	2.14	9 (32%)
1	2MG	1	2445	1	18,26,27	2.15	7 (38%)	16,38,41	1.25	4 (25%)
54	5MU	z	8	54	19,22,23	4.51	7 (36%)	28,32,35	3.93	9 (32%)
1	OMG	1	2251	54,1	18,26,27	2.01	7 (38%)	19,38,41	1.44	4 (21%)
1	2MA	1	2503	56,1	19,25,26	2.87	7 (36%)	21,37,40	1.64	4 (19%)
1	3TD	1	1915	1	18,22,23	4.04	7 (38%)	22,32,35	1.54	3 (13%)
1	PSU	1	746	56,1	18,21,22	1.04	2 (11%)	22,30,33	1.74	3 (13%)
2	UR3	2	1498	2	19,22,23	2.41	6 (31%)	26,32,35	1.04	2 (7%)
43	0TD	p	89	43	7,9,10	1.49	1 (14%)	6,11,13	1.92	2 (33%)
54	5MU	z	64	54	19,22,23	1.44	6 (31%)	28,32,35	2.32	7 (25%)
2	5MC	2	1407	2	18,22,23	3.12	7 (38%)	26,32,35	0.90	1 (3%)
1	PSU	1	2605	1	18,21,22	1.05	1 (5%)	22,30,33	1.92	4 (18%)

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	PSU	1	2457	1	-	0/7/25/26	0/2/2/2
1	6MZ	1	2030	1	-	2/5/27/28	0/3/3/3
1	5MC	1	1962	1	-	0/7/25/26	0/2/2/2
2	2MG	2	1516	2	-	0/5/27/28	0/3/3/3
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
2	MA6	2	1518	2	-	3/7/29/30	0/3/3/3
54	5MU	z	40	54	-	2/7/25/26	0/2/2/2
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
54	5MU	z	57	54	-	2/7/25/26	0/2/2/2
1	PSU	1	955	1	-	0/7/25/26	0/2/2/2
1	2MG	1	1835	1	-	2/5/27/28	0/3/3/3
2	2MG	2	1207	2	-	0/5/27/28	0/3/3/3
2	G7M	2	527	2	-	3/3/25/26	0/3/3/3
2	4OC	2	1402	2	-	2/9/29/30	0/2/2/2
2	2MG	2	966	2	-	0/5/27/28	0/3/3/3
1	OMC	1	2498	56,1	-	0/9/27/28	0/2/2/2
1	G7M	1	2069	1	-	1/3/25/26	0/3/3/3
1	6MZ	1	1618	1	-	3/5/27/28	0/3/3/3
1	5MU	1	1939	56,1	-	0/7/25/26	0/2/2/2
2	5MC	2	967	2	-	2/7/25/26	0/2/2/2
54	5MU	z	20	56,54	-	4/7/25/26	0/2/2/2
1	PSU	1	2504	1	-	2/7/25/26	0/2/2/2
54	5MU	z	39	54	-	4/7/25/26	0/2/2/2
2	MA6	2	1519	2	-	5/7/29/30	0/3/3/3
54	5MU	z	71	54	-	3/7/25/26	0/2/2/2
1	OMU	1	2552	1	-	0/9/27/28	0/2/2/2
1	PSU	1	2580	56,1	-	0/7/25/26	0/2/2/2
54	5MU	z	69	54	-	2/7/25/26	1/2/2/2
54	5MU	z	42	54,2	-	0/7/25/26	0/2/2/2
54	5MU	z	63	54	-	2/7/25/26	0/2/2/2
54	5MU	z	55	54	-	0/7/25/26	0/2/2/2
1	5MU	1	747	1	-	0/7/25/26	0/2/2/2
1	1MG	1	745	1	-	0/3/25/26	0/3/3/3
2	PSU	2	516	56,2	-	2/7/25/26	0/2/2/2
54	5MU	z	76	54	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	1	2445	1	-	2/5/27/28	0/3/3/3
54	5MU	z	8	54	-	2/7/25/26	0/2/2/2
1	OMG	1	2251	54,1	-	0/5/27/28	0/3/3/3
1	2MA	1	2503	56,1	-	2/3/25/26	0/3/3/3
1	3TD	1	1915	1	-	3/7/25/26	0/2/2/2
1	PSU	1	746	56,1	-	1/7/25/26	0/2/2/2
2	UR3	2	1498	2	-	1/7/25/26	0/2/2/2
43	0TD	p	89	43	-	3/7/12/14	-
54	5MU	z	64	54	-	2/7/25/26	0/2/2/2
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2

The worst 5 of 235 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	z	69	5MU	C6-C5	23.78	1.73	1.34
1	1	1915	3TD	C6-C5	11.71	1.49	1.35
54	z	57	5MU	C2-N1	11.02	1.56	1.38
54	z	20	5MU	C2-N1	10.76	1.55	1.38
54	z	20	5MU	C6-N1	10.47	1.55	1.38

The worst 5 of 240 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	z	69	5MU	C6-C5-C4	-115.15	21.76	118.03
54	z	69	5MU	C5-C4-N3	-87.09	40.98	115.31
54	z	69	5MU	C6-N1-C2	-29.10	91.84	121.30
54	z	69	5MU	O4-C4-C5	-25.79	95.01	124.90
54	z	69	5MU	N3-C2-N1	-18.31	90.58	114.89

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2	516	PSU	O4'-C1'-C5-C4
2	2	516	PSU	O4'-C1'-C5-C6
2	2	527	G7M	C3'-C4'-C5'-O5'
2	2	967	5MC	O4'-C4'-C5'-O5'
2	2	967	5MC	C3'-C4'-C5'-O5'

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	z	69	5MU	C2-C4-C5-C6-N1-N3

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 424 ligands modelled in this entry, 424 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.