



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 01:08 am BST

PDB ID : 3CCJ  
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation C2534U  
Authors : Blaha, G.; Gurel, G.  
Deposited on : 2008-02-26  
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

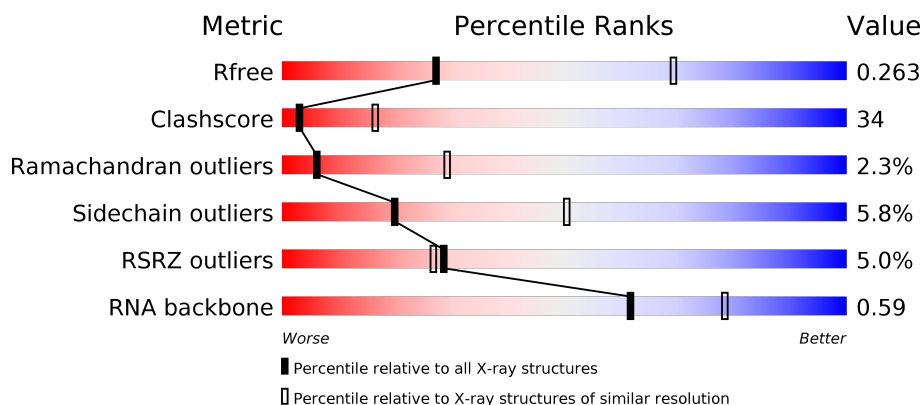
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	240	<div> <div>49%</div> <div>45%</div> <div>..</div> </div>
2	B	338	<div> <div>46%</div> <div>50%</div> <div>.</div> </div>
3	C	246	<div> <div>56%</div> <div>39%</div> <div>.</div> </div>
4	D	177	<div> <div>17%</div> <div>39%</div> <div>37%</div> <div>21%</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	

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Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	0	8066	-	-	-	X
33	CL	0	8812	-	-	X	-
33	CL	0	8813	-	-	X	-
33	CL	0	8822	-	-	-	X
33	CL	3	8804	-	-	X	-
33	CL	J	8801	-	-	X	-
33	CL	M	8818	-	-	X	-
33	CL	N	8807	-	-	X	-
34	SR	0	8957	-	-	-	X
34	SR	0	8979	-	-	-	X
34	SR	0	8982	-	-	-	X
34	SR	0	9004	-	-	-	X
34	SR	0	9006	-	-	-	X
34	SR	3	8999	-	-	-	X
34	SR	B	8987	-	-	-	X
35	NA	0	8509	-	-	-	X
35	NA	0	8545	-	-	-	X
35	NA	0	8560	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	L	8568	-	-	-	X
35	NA	R	8575	-	-	-	X

## 2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 99122 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1753	1072	352	324	5			

- Molecule 2 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1860	1130	345	384	1			

- Molecule 4 is a protein called 50S ribosomal protein L5P.

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

- Molecule 5 is a protein called 50S ribosomal protein L6P.

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

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 7 is a protein called 50S ribosomal protein L10E.

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

- Molecule 8 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 9 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 10 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 12 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	L	145	Total	C	N	O	0	0	0
			1118	670	222	226			

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 15 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	115	Total	C	N	O		0	0	0
			865	529	161	175				

- Molecule 16 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	143	Total	C	N	O		0	0	0
			1136	683	229	224				

- Molecule 17 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	95	Total	C	N	O		0	0	0
			735	450	141	144				

- Molecule 18 is a protein called 50S ribosomal protein L22P.

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

- Molecule 19 is a protein called 50S ribosomal protein L23P.

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

- Molecule 20 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	119	Total	C	N	O		0	0	0
			950	568	180	202				

- Molecule 21 is a protein called 50S ribosomal protein L24e.

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

- Molecule 22 is a protein called 50S ribosomal protein L29P.

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

- Molecule 23 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 24 is a protein called 50S ribosomal protein L31e.

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

- Molecule 25 is a protein called 50S ribosomal protein L32e.

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

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59020	26349	10872	19054	2745			

- Molecule 31 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	85	Total	Mg	0	0
			85	85		
32	Y	2	Total	Mg	0	0
			2	2		
32	K	1	Total	Mg	0	0
			1	1		
32	A	2	Total	Mg	0	0
			2	2		
32	T	1	Total	Mg	0	0
			1	1		
32	9	2	Total	Mg	0	0
			2	2		

- Molecule 33 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	8	Total	Cl	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	J	4	Total 4	Cl 4	0	0
33	Q	1	Total 1	Cl 1	0	0
33	B	1	Total 1	Cl 1	0	0
33	A	1	Total 1	Cl 1	0	0
33	N	1	Total 1	Cl 1	0	0
33	O	1	Total 1	Cl 1	0	0
33	R	1	Total 1	Cl 1	0	0
33	Y	1	Total 1	Cl 1	0	0
33	L	1	Total 1	Cl 1	0	0
33	3	1	Total 1	Cl 1	0	0
33	M	1	Total 1	Cl 1	0	0

- Molecule 34 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	93	Total 93	Sr 93	0	0
34	J	1	Total 1	Sr 1	0	0
34	1	2	Total 2	Sr 2	0	0
34	B	2	Total 2	Sr 2	0	0
34	3	2	Total 2	Sr 2	0	0
34	A	2	Total 2	Sr 2	0	0
34	2	1	Total 1	Sr 1	0	0
34	R	1	Total 1	Sr 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	9	2	Total 2	Sr 2	0	0
34	S	1	Total 1	Sr 1	0	0
34	F	1	Total 1	Sr 1	0	0

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	63	Total 63	Na 63	0	0
35	J	1	Total 1	Na 1	0	0
35	Q	1	Total 1	Na 1	0	0
35	B	1	Total 1	Na 1	0	0
35	C	1	Total 1	Na 1	0	0
35	R	3	Total 3	Na 3	0	0
35	9	2	Total 2	Na 2	0	0
35	L	1	Total 1	Na 1	0	0
35	S	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0

- Molecule 36 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	1	Total 1	K 1	0	0
36	M	1	Total 1	K 1	0	0

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	O	1	Total Cd 1 1	0	0
37	Z	1	Total Cd 1 1	0	0
37	1	1	Total Cd 1 1	0	0
37	3	1	Total Cd 1 1	0	0
37	U	1	Total Cd 1 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	A	122	Total O 122 122	0	0
38	B	158	Total O 158 158	0	0
38	C	176	Total O 176 176	0	0
38	D	51	Total O 51 51	0	0
38	E	51	Total O 51 51	0	0
38	F	27	Total O 27 27	0	0
38	G	15	Total O 15 15	0	0
38	H	73	Total O 73 73	0	0
38	I	3	Total O 3 3	0	0
38	J	55	Total O 55 55	0	0
38	K	61	Total O 61 61	0	0
38	L	99	Total O 99 99	0	0
38	M	148	Total O 148 148	0	0
38	N	56	Total O 56 56	0	0
38	O	42	Total O 42 42	0	0

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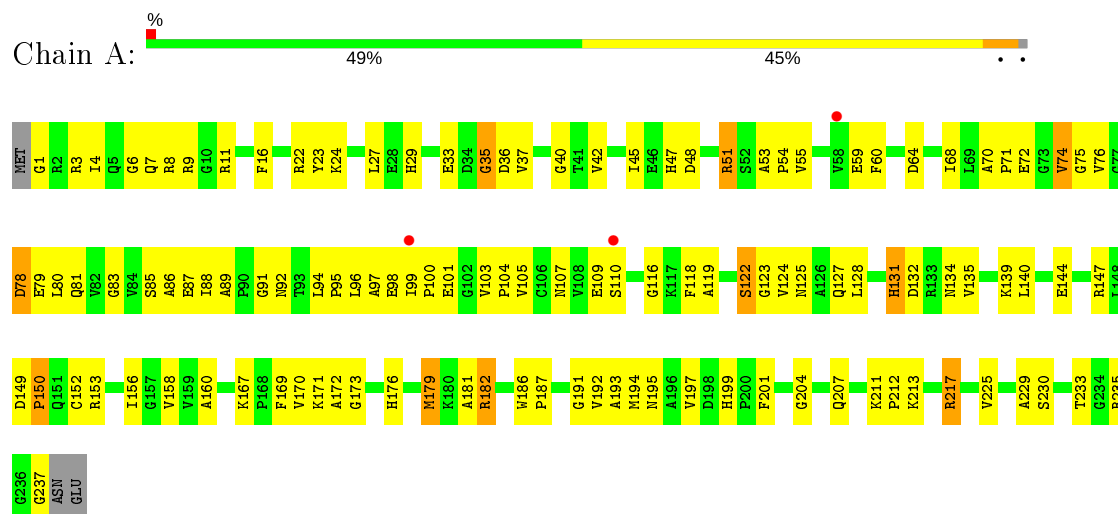
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	P	56	Total 56	O 56	0	0
38	Q	58	Total 58	O 58	0	0
38	R	78	Total 78	O 78	0	0
38	S	37	Total 37	O 37	0	0
38	T	41	Total 41	O 41	0	0
38	U	34	Total 34	O 34	0	0
38	V	10	Total 10	O 10	0	0
38	W	71	Total 71	O 71	0	0
38	X	28	Total 28	O 28	0	0
38	Y	102	Total 102	O 102	0	0
38	Z	33	Total 33	O 33	0	0
38	1	53	Total 53	O 53	0	0
38	2	48	Total 48	O 48	0	0
38	3	80	Total 80	O 80	0	0
38	0	5813	Total 5813	O 5813	0	0
38	9	144	Total 144	O 144	0	0

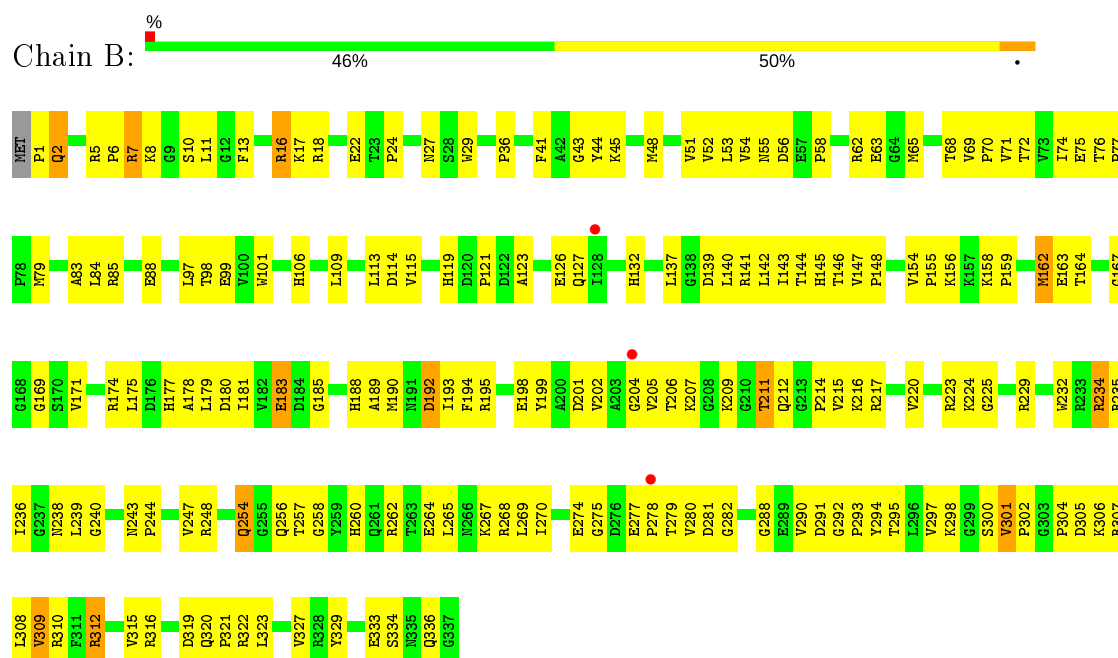
### 3 Residue-property plots

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

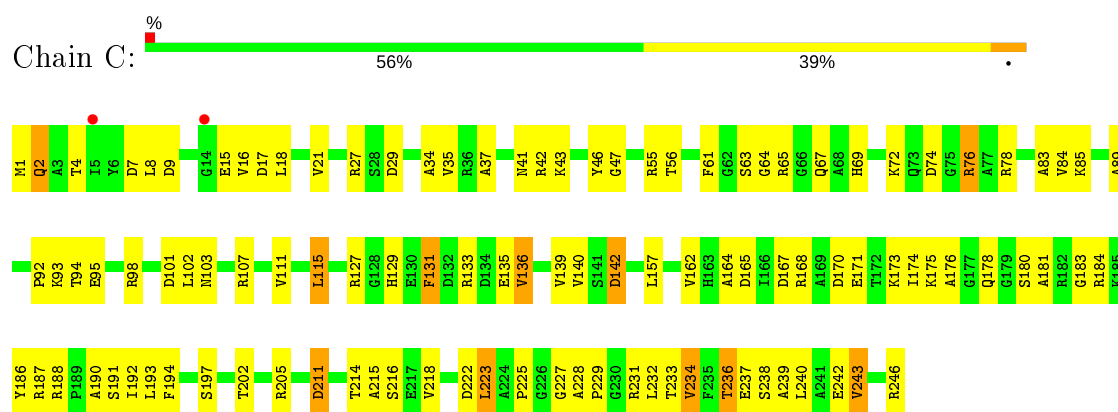
#### • Molecule 1: 50S ribosomal protein L2P



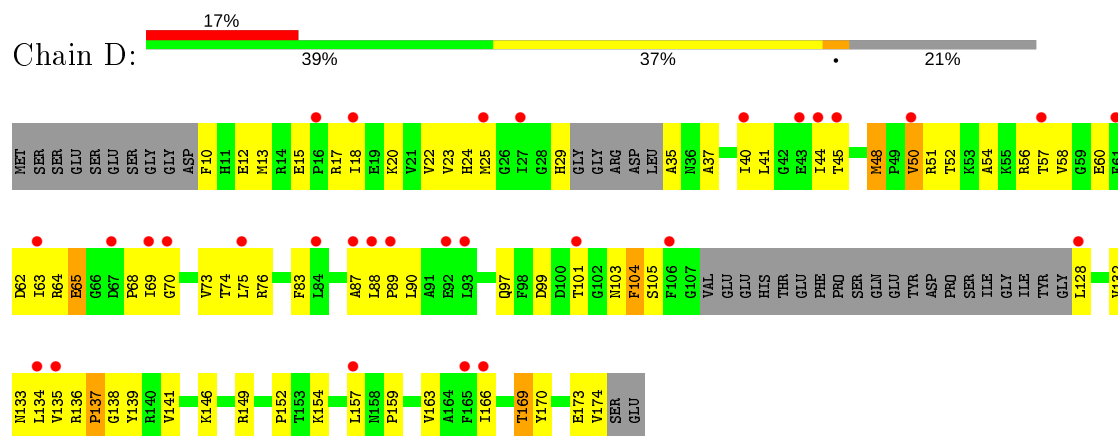
#### • Molecule 2: 50S ribosomal protein L3P



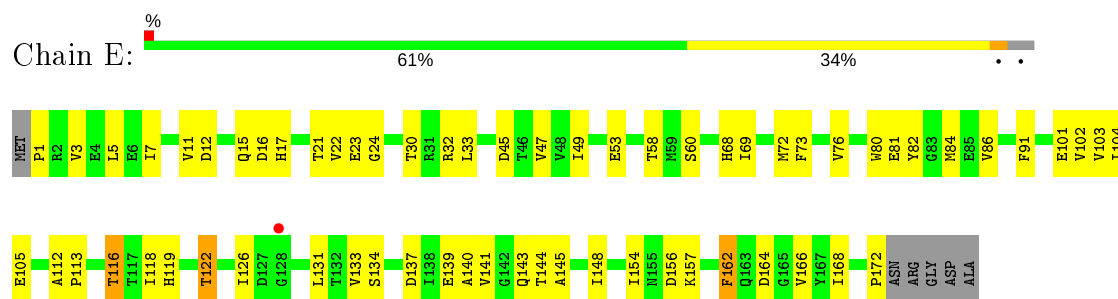
#### • Molecule 3: 50S ribosomal protein L4P



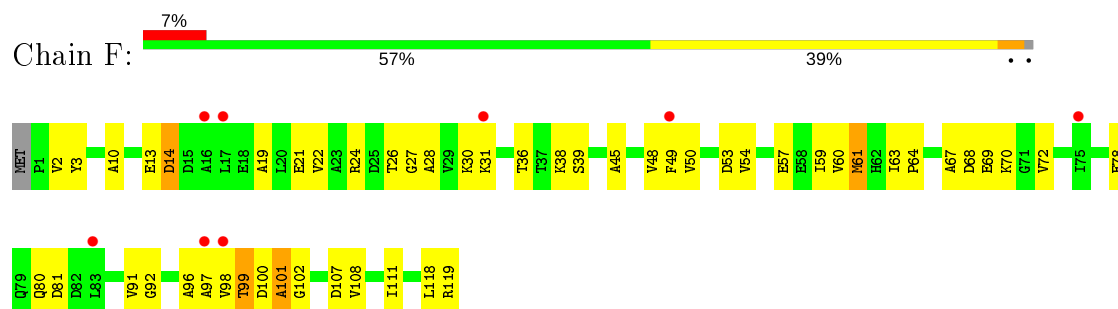
• Molecule 4: 50S ribosomal protein L5P



• Molecule 5: 50S ribosomal protein L6P

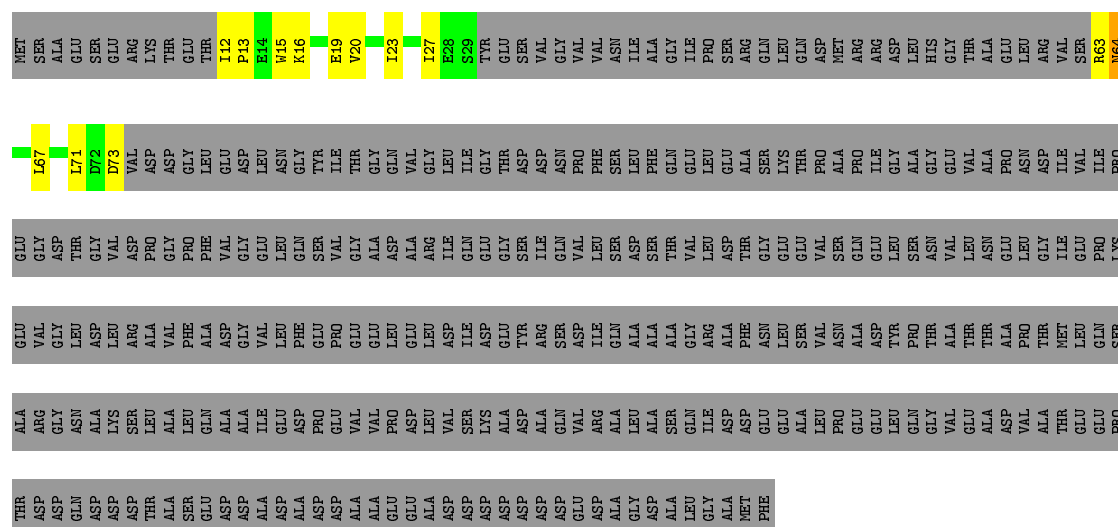


• Molecule 6: 50S ribosomal protein L7Ae



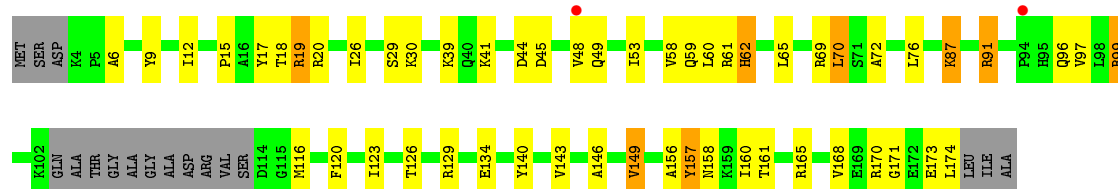
• Molecule 7: 50S ribosomal protein L10E

Chain G:  5% 92%



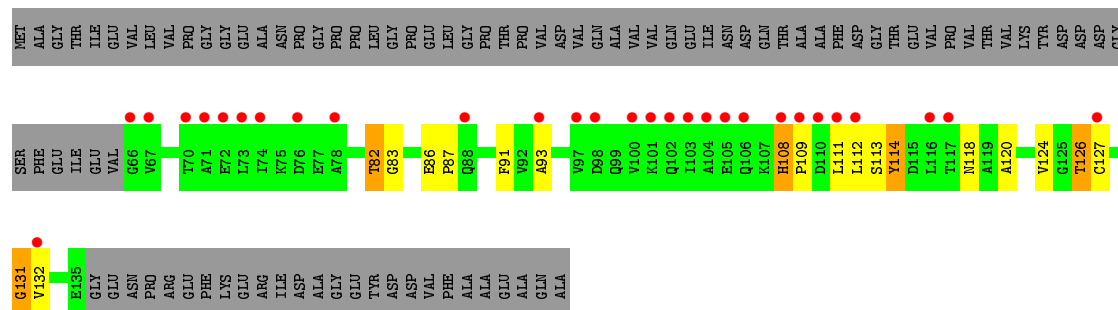
• Molecule 8: 50S ribosomal protein L10e

Chain H:  60% 26% 5% 10%



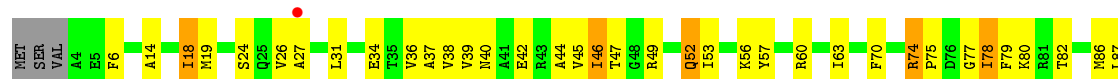
• Molecule 9: 50S ribosomal protein L11P

Chain I:  18% 31% 9% 57%

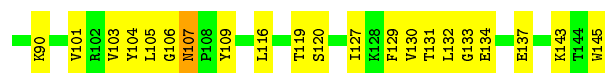


• Molecule 10: 50S ribosomal protein L13P

Chain J:  59% 35% 6%



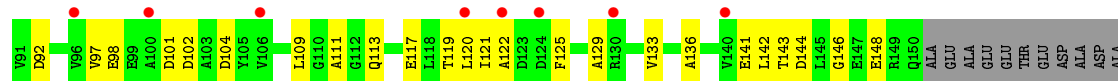
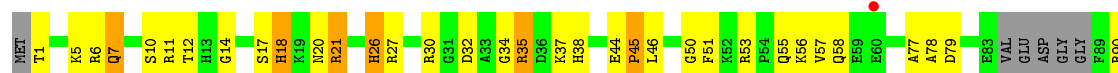




- Molecule 11: 50S ribosomal protein L14P

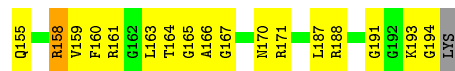
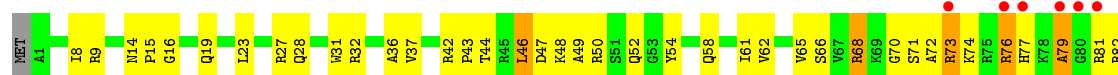


- Molecule 12: 50S ribosomal protein L15P

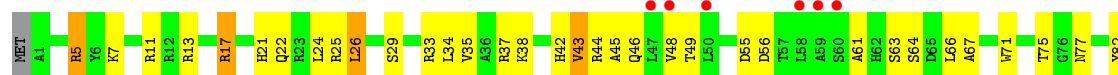


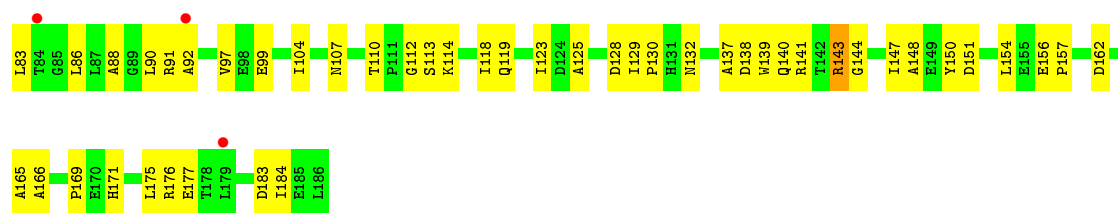
ASP  
GLU  
GLU

- Molecule 13: 50S ribosomal protein L15e

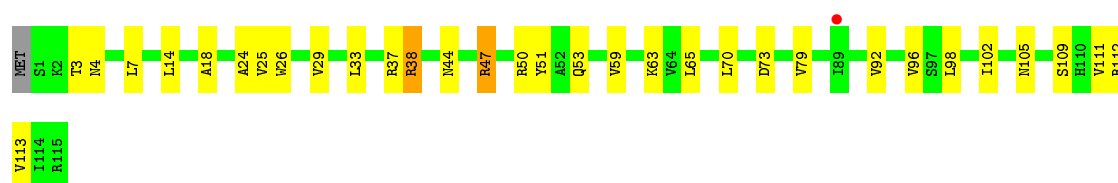


- Molecule 14: 50S ribosomal protein L18P

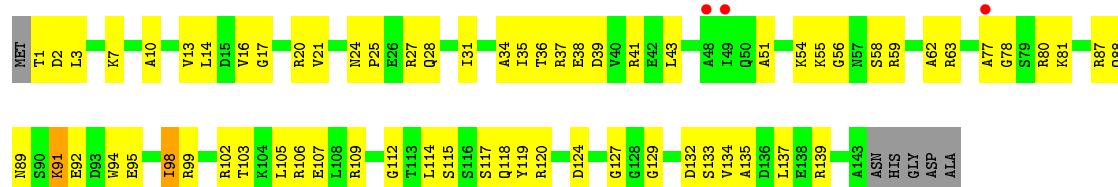




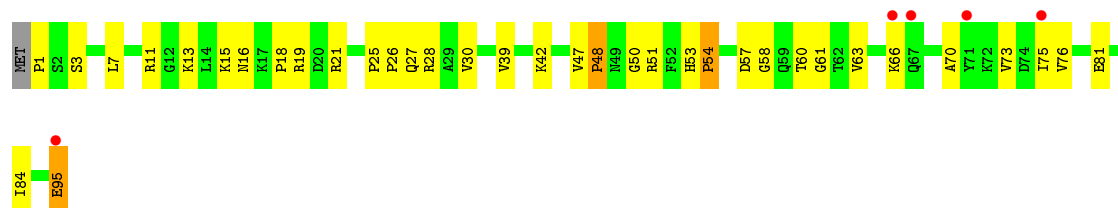
• Molecule 15: 50S ribosomal protein L18e



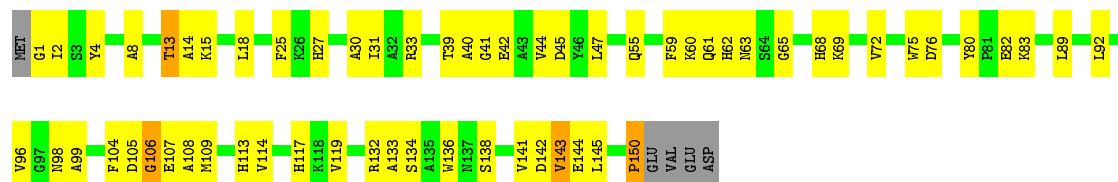
• Molecule 16: 50S ribosomal protein L19e



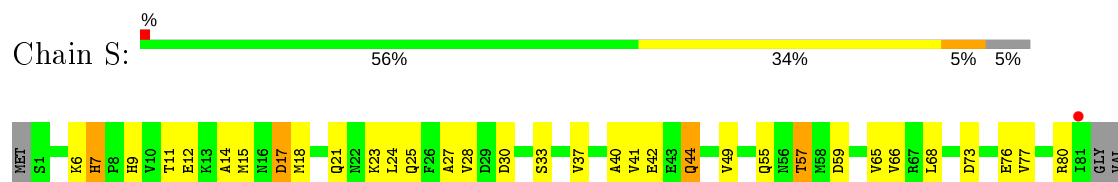
• Molecule 17: 50S ribosomal protein L21e



• Molecule 18: 50S ribosomal protein L22P

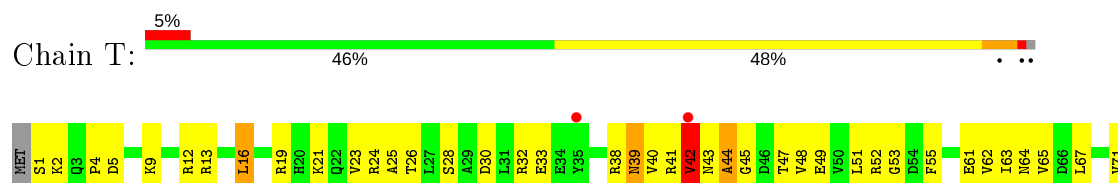


• Molecule 19: 50S ribosomal protein L23P

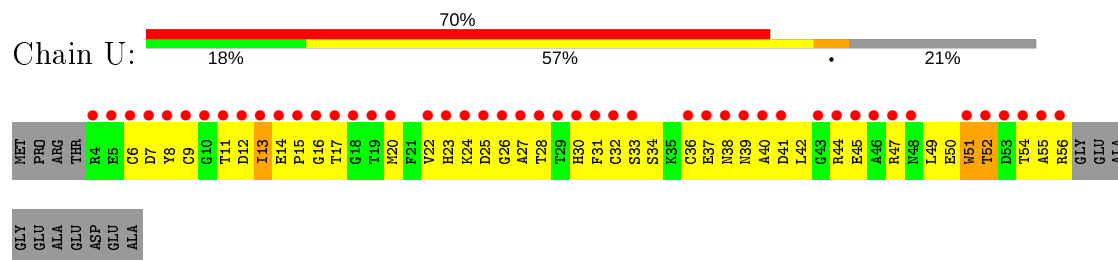


PHE

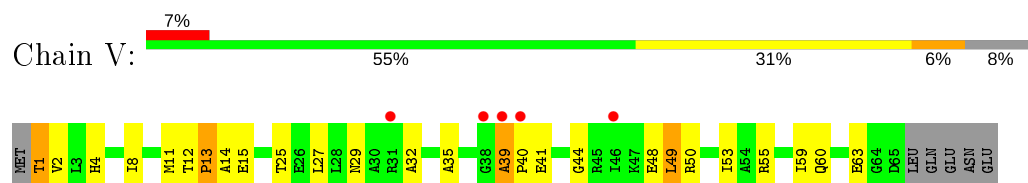
- Molecule 20: 50S ribosomal protein L24P



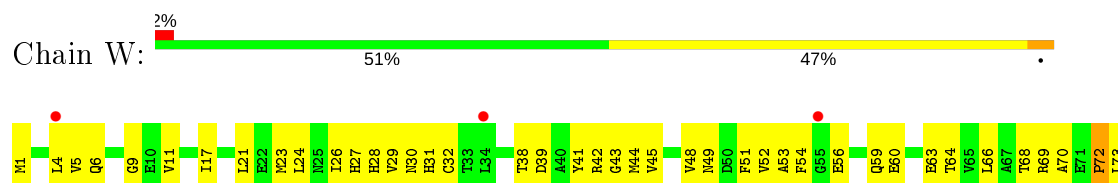
- Molecule 21: 50S ribosomal protein L24e



- Molecule 22: 50S ribosomal protein L29P

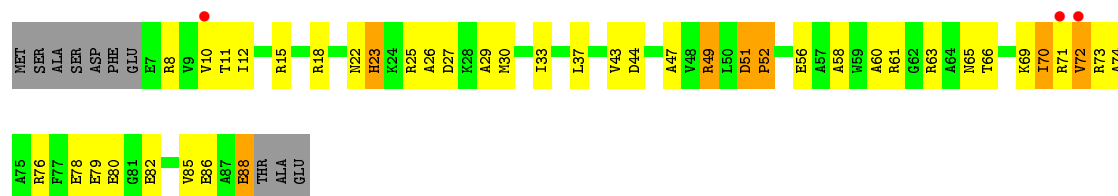


- Molecule 23: 50S ribosomal protein L30P



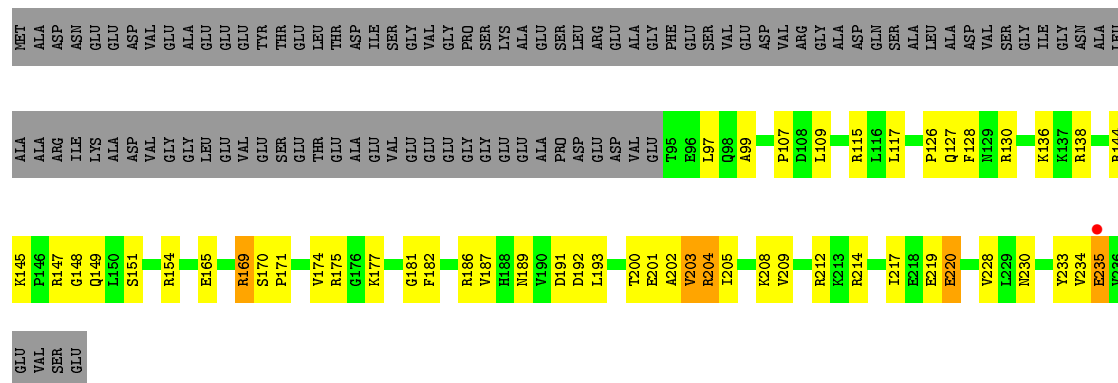
- Molecule 24: 50S ribosomal protein L31e





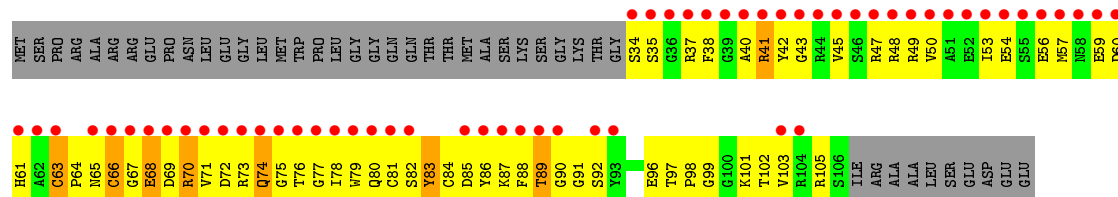
- Molecule 25: 50S ribosomal protein L32e

Chain Y: 37% 20% 41%



- Molecule 26: 50S ribosomal protein L37Ae

Chain Z: 13% 50% 43% 7% 37%



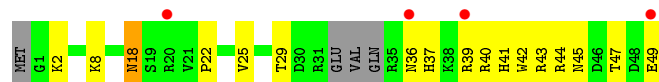
- Molecule 27: 50S ribosomal protein L37e

Chain 1: 54% 40%



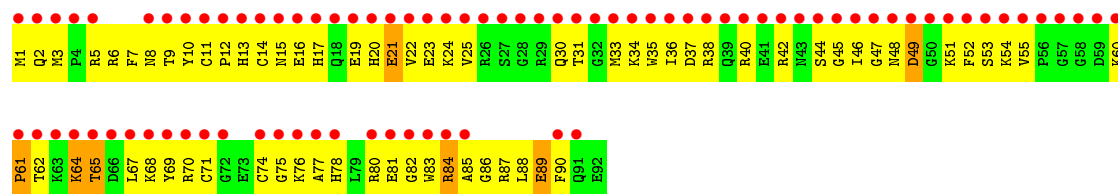
- Molecule 28: 50S ribosomal protein L39e

Chain 2: 8% 58% 32% 8%



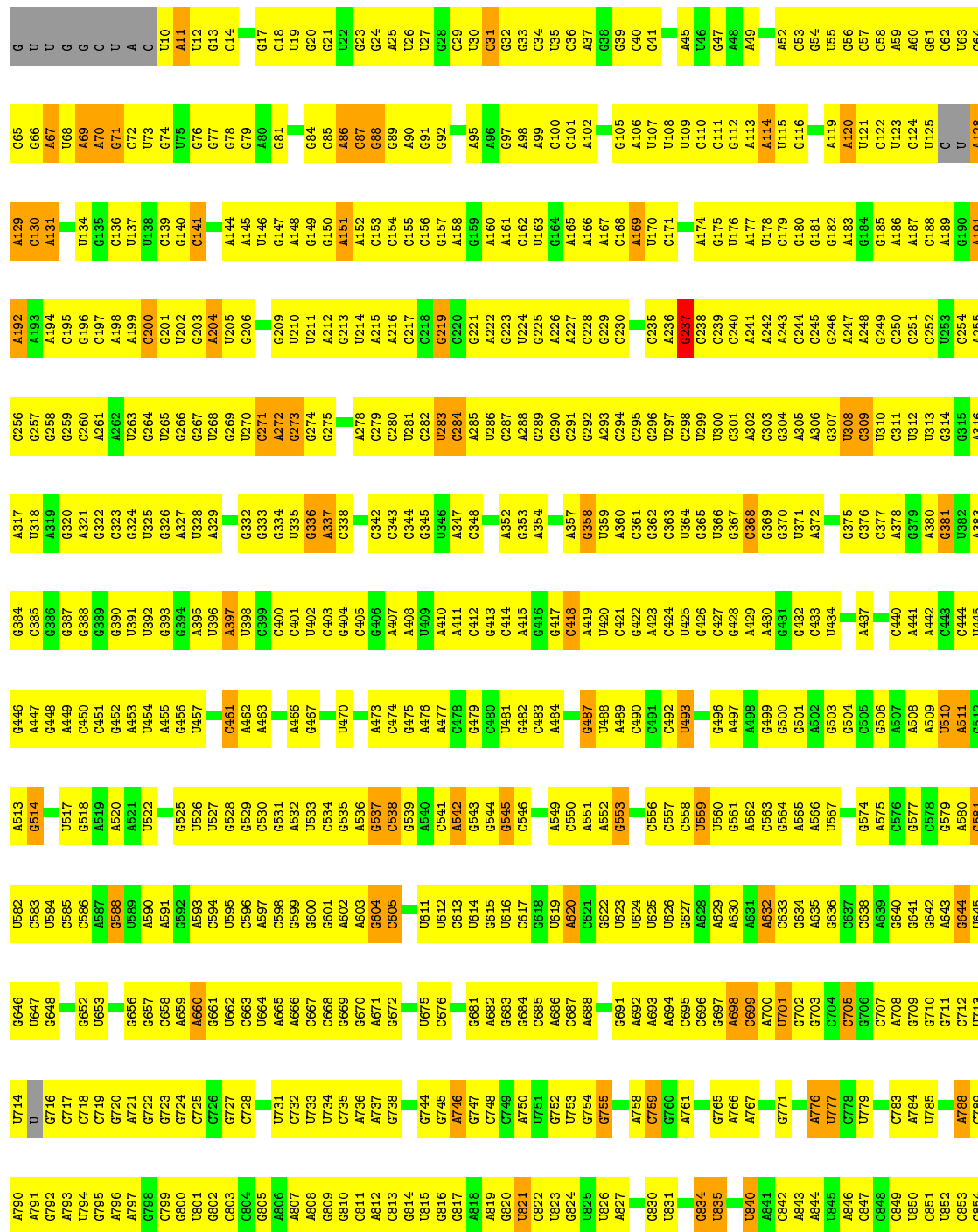
- Molecule 29: 50S ribosomal protein L44E

Chain 3: 24% 90% 68% 8%



## ● Molecule 30: 23S RIBOSOMAL RNA

Chain 0: 22% 64% 8% 6%





A2768	C2707	U2646	A2576	C2508	G2443	A2375	G2315	G2249	C	U1219	A2060	U1996	G1932	A1865
C2769	G2708	G2647	A2577	A2509	U2444	C2376	G2316	G2250	U	C2130	C2061	A1997	G1933	A1866
G2770	G2709	U2445	G2578	C2510	U2456	U2377	C2317	G2251	A	G2131	A2062	G1998	A1934	G1867
G2771	A2511	U2648	G2579	A2512	G2446	U2378	C2318	A2252	G	G2132	U2063	G1999	C1935	G1868
U2774	U2710	U2649	G2580	A2513	A2447	A2379	G2319	G2253	C	U2133	U2064	G2001	C1936	U1871
A2775	U2711	U2650	U2581	A2514	U2448	A2380	U2320	G2254	G	G2134	C2065	G2002	U1937	C1872
A2776	U2712	C2651	U2582	U2514	G2449	C2381	A2321	A2255	G	A2135	C2066	C2003	G1938	C1873
A2777	G2713	U2652	A2583	C2515	C2450	C2382	U2322	G2256	G	G2136	A2067	U2004	U1874	U1875
A2778	U2714	A2653	G2516	U2516	C2451	G2383	G2323	G2257	C	A	G2068	C2005	C1940	A1876
A2779	G2715	U2654	U2586	A2517	G2452	U2384	G2324	A2258	C	C	U2069	G2006	A1941	A1877
A2780	G2716	C2655	U2587	C2518	G2453	U2385	U2325	G2259	A	G	C2070	C2007	A1942	G1878
C2781	C2717	G2656	U2588	C2519	G2454	U2386	C2326	A2263	C	U	C2071	U2008	G1943	G1879
G2782	U2718	G2657	U2589	A2521	A2455	U2387	A2327	U2265	C	G	G2072	G2009	G1944	U1879
A2783	A2719	G2658	U2590	G2522	A2456	C2388	U2328	U2266	A	U	G2073	G2010	G1945	U1883
A2784	G2720	U2659	C2591	U2523	U2457	U2389	C2329	A2267	C	C	A2074	A2010	G1946	G1884
A2785	U2721	G2660	U2592	G2524	U2458	U2390	U2330	G2267	G	U	G2075	U2012	G1947	A1885
C2786	G2722	U2661	C2593	G2525	G2459	U2391	A2332	C2268	C	G	U2076	G2013	G1948	A1886
G2787	G2723	G2662	C2594	G2526	A2460	G2392	A2333	C2269	A	C	A2081	G2014	G1950	U1887
C2787	U2724	U2663	U2595	U2527	U2461	G2397	G2334	G2270	A	C	G2082	A2015	G1951	C1888
A2788	G2725	A2664	A2596	U2528	G2462	A2398	C2335	G2271	C	G	A2083	U2016	U	C1889
U2789	U2726	U	U2597	G2529	A2463	G2399	G2336	G2272	A	U	G2087	U2017	A	U1890
C2790	A2727	A	U2598	U2530	C2464	A2402	G2337	G2273	G	U	C2088	A2018	A	G1891
U2791	G2728	U	A2599	U2531	A2465	C2403	G2338	G2274	C	U	A2089	A2019	C	U
A2792	C2728	G2668	A2600	A2532	G2466	U2406	A	U2276	G	U	G2090	A2020	A	C1894
A2793	G2731	U2669	A2601	G2533	A2467	G2407	C	U2277	G	C	G2093	A2022	U	G1898
G2794	U2732	G2670	G2602	U2534	A2468	G2407	A	U2278	A	A	G2094	G2023	U	C1899
C2795	U2733	U2671	A2603	G2535	A2469	A2408	G	A2280	A	G	G2095	A2024	G	A1900
U2796	G2734	C2672	U2599	U2536	A2470	C2409	U	C2281	U	A	G2096	G2025	A	G1901
A2799	U2735	U2673	G2607	G2537	G2471	G2411	A	U2282	C	C	A2095	C2026	C	U1902
A2800	U2736	U2674	G2608	A2538	U2472	G2412	A2344	G2283	C	U	A2096	U2027	C	G1903
A2801	G2737	A2675	G2609	U2539	U2473	A2413	A2345	G2284	U	A	G2097	U2028	C	U1904
A2802	C2738	C2676	G2610	G2540	A2474	A2414	A2346	G2285	A	G	C2098	G2029	U1964	U1905
C2803	A2739	A2677	A2612	U2541	C2475	A2415	G2347	G2286	C	U	A2099	A2030	C1965	U1906
G2804	G2740	A2678	G2613	G2542	C2476	G2416	G2349	G2287	C	U	A2100	G2031	U1966	U1907
A2805	A2741	G2679	U2614	G2543	G2477	A2417	G2350	G2288	C	A	A2101	U2032	U1967	G1908
A2806	G2742	U2680	U2615	G2544	U2478	G2418	G2351	U2290	G	G	G2102	G2033	A1968	G1909
U2807	C2745	A2681	G2616	C2547	A2479	U2419	G2352	A2291	U	U	A2103	U2034	A1969	A1909
U2808	A2746	C2682	G2617	C2548	G2482	G2420	A2353	G2292	C	A	G2104	G2035	G1970	A1910
G2809	C2747	G2683	G2618	C2549	A2483	G2421	A2354	G2293	C	A	C2105	C2036	G1971	C1911
G2810	G2748	A2684	U2619	U2550	U2484	U2422	G2355	G2294	C	U	C2106	G2037	U1972	A1912
A2811	U2749	C2685	U2620	C2551	G2485	G2423	A2356	G2295	G	U	U2107	A2038	A1973	C1913
A2812	G2750	C2686	U2621	C2552	A2489	U2424	A2357	U2297	G	U	G2110	A2039	G1974	C1914
A2813	C2751	U2687	A2622	A2553	A2490	A2425	U2358	C2298	A	U	G2111	G2040	C1975	U1915
A2814	C2752	A2688	U2623	U2554	G2491	G2426	G2359	G2299	C	U	G2112	G2041	A1978	C1916
G2815	U2753	U2689	A2624	C2555	U2492	G2427	C2360	A2300	U	A	A2113	G2042	G1979	G1917
A2818	G2754	A2691	G2629	C2556	C2493	A2429	A2361	A2301	G	C	G2114	G2043	G1980	U1918
C2819	U2755	U2692	G2630	C2557	G2494	A2430	A2362	A2302	C	A	U2115	C2044	U1981	C1920
A2820	U2756	U2693	G2631	C2558	U2495	C2431	G2363	A2303	G	G	U2116	C2045	A1982	A1921
C2821	A2757	A2694	G2632	C2559	C2496	C2432	A2364	G2304	A	A	U2117	C2046	C1982	A1922
G2822	G2758	C2695	A2635	U2563	A2497	A2433	G2365	A2305	C	G	U2118	G2047	C1983	G1923
C2823	C2759	G2696	C2636	U2564	C2498	U2434	G2366	U2306	G	U	C2119	G2048	A1987	A1924
G2824	G2760	A2697	A2637	G2565	U2499	U2435	A2367	A2307	C	A	U2120	G2049	A1988	G1925
C2825	A2761	G2698	U2638	C2566	G2502	U2436	A2368	U2308	C	C	U2121	U2050	C1989	G1926
A2826	G2762	A2699	G2639	G2567	C2503	A2437	A2369	C2309	C	C	G2122	G2051	A1991	A1927
G2827	U2763	U2690	U2640	C2570	A2504	G2438	A2370	G2310	C	C	A2123	A2054	U1992	C1928
G2828	C2764	G2701	G2641	G2571	A2505	C2439	G2371	A2311	C	C	G2124	A2055	U1993	A1929
A2829	G2765	A2702	G2642	G2572	G2506	U2440	U2372	G2312	G	C	G2125	G2056	A1994	G1930
U2830	A2766	G2574	A2506	G2573	A2507	U2441	U2373	G2313	C	G	G2126	U2057	G1995	A1931

C2831	C2832	C2833	C2834	C2835	C2836	C2837	C2838	C2839	A2840	A2841	A2842	A2843	C2844	C2845	C2846	C2847	C2851	A2852	C2853	A2854	C2855	C2859	C2860	C2861	C2862	C2863	C2864	C2865	C2866	C2867	C2868	C2869	C2870	C2871	C2872	C2873	C2874	A2875	C2876	C2877	C2878	A2879	C2880	C2881	C2882	C2883	C2884	A2885	C2886	C2887	C2888	C2889	A2890	A2891	C2892	C2893	C2894
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C2895	A2896	C2897	G2898	A2899	G2900	C2901	A2902	C2903	U2904	A2905	A2906	C2907	A2908	C2909	A2910	C2911	C2912	A2913	A2914	A	G	C	C	A	U
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● Molecule 31: 5S RIBOSOMAL RNA



U1	U2	A3	G4	G5	C6	G7	G8	C9	C10	A11	C12	A13	G14	G17	U18	G19	G20	G21	G22	U23	U24	G25	C26	C27	U28	C29	C30	C31	G32	U33	A34	C35	C36	C37	A38	U39	C40	C41	C42	G43	A44	A45	C46	A47	C48	G49	G50	A51	A52	G53	A54	U55	C118	A56	A57	G58	C59	C60	C61
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A62	C63	C64	A65	G66	U69	U70	G74	G75	G76	A77	G78	U79	A80	C81	U82	G83	G84	A85	G86	U87	G88	C89	G90	C91	G92	A93	G94	C95	C96	U97	C98	U99	G100	G101	G102	A103	A104	A105	U106	C107	C108	G109	G110	U111	U112	C113	G114	C115	C116	G117	C118	C119	A120	C121	C122
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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.01Å 299.25Å 573.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 85.53 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.6 (50.00-3.30) 89.1 (85.53-2.40)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.208 , 0.287 0.184 , 0.263	Depositor DCC
$R_{free}$ test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.9	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 138.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	99122	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, SR, NA, K, CD, OMU, UR3, 1MA, 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  > 5$	RMSZ	# $ Z  > 5$
1	A	0.37	0/1786	0.66	0/2408
2	B	0.38	0/2690	0.67	0/3652
3	C	0.42	0/1885	0.65	0/2552
4	D	0.35	0/1111	0.58	0/1498
5	E	0.36	0/1382	0.61	0/1880
6	F	0.36	0/901	0.60	0/1224
7	G	0.40	0/241	0.53	0/324
8	H	0.36	0/1302	0.66	0/1743
9	I	0.33	0/526	0.54	0/716
10	J	0.42	0/1136	0.63	0/1530
11	K	0.40	0/1004	0.71	0/1351
12	L	0.35	0/1130	0.64	0/1509
13	M	0.41	0/1582	0.64	0/2116
14	N	0.33	0/1474	0.62	0/1999
15	O	0.37	0/874	0.64	0/1181
16	P	0.39	0/1147	0.56	0/1528
17	Q	0.37	0/749	0.67	0/1005
18	R	1.28	7/1172 (0.6%)	1.10	6/1578 (0.4%)
19	S	0.38	0/648	0.59	0/875
20	T	0.39	0/958	0.67	0/1289
21	U	0.46	0/417	0.64	0/562
22	V	0.35	0/502	0.56	0/675
23	W	0.41	0/1219	0.68	0/1655
24	X	0.39	0/664	0.62	0/895
25	Y	0.39	0/1146	0.64	0/1536
26	Z	0.42	0/584	0.63	0/781
27	1	0.47	0/438	0.63	0/578
28	2	0.38	0/401	0.61	0/529
29	3	0.43	0/771	0.67	0/1024
30	0	0.49	0/65957	0.70	6/102867 (0.0%)
31	9	0.37	0/2904	0.68	0/4526
All	All	0.48	7/98701 (0.0%)	0.69	12/147586 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
18	R	1	0
23	W	0	1
30	0	0	19
All	All	1	20

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.13	2.85	1.50
18	R	150	PRO	CA-C	-18.46	1.16	1.52
18	R	150	PRO	CG-CD	14.04	1.97	1.50
18	R	150	PRO	C-O	11.94	1.47	1.23
18	R	150	PRO	N-CA	11.49	1.66	1.47

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.46	55.84	112.00
18	R	150	PRO	N-CA-C	-19.38	61.71	112.10
18	R	150	PRO	CA-N-CD	12.12	128.68	111.70
18	R	150	PRO	N-CA-CB	11.03	116.54	103.30
18	R	150	PRO	CA-C-O	-8.33	100.20	120.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	493	U	Sidechain
30	0	788	A	Sidechain
30	0	862	U	Sidechain
30	0	882	A	Sidechain
23	W	90	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	123	0
2	B	2625	0	2533	168	0
3	C	1860	0	1813	98	0
4	D	1094	0	1085	71	0
5	E	1357	0	1266	49	0
6	F	890	0	843	39	0
7	G	240	0	231	18	0
8	H	1282	0	1292	62	0
9	I	519	0	500	24	0
10	J	1120	0	1098	56	0
11	K	994	0	1027	54	0
12	L	1118	0	1076	54	0
13	M	1558	0	1573	120	0
14	N	1445	0	1401	74	0
15	O	865	0	873	47	0
16	P	1136	0	1123	64	0
17	Q	735	0	729	32	0
18	R	1149	0	1122	58	0
19	S	641	0	605	29	0
20	T	950	0	924	56	0
21	U	410	0	368	58	0
22	V	499	0	511	26	0
23	W	1196	0	1137	79	0
24	X	654	0	653	42	0
25	Y	1130	0	1133	69	0
26	Z	573	0	534	84	0
27	1	431	0	426	27	0
28	2	396	0	413	20	0
29	3	755	0	732	138	0
30	0	59020	0	29802	3476	0
31	9	2599	0	1325	195	0
32	0	85	0	0	0	0
32	9	2	0	0	0	0
32	A	2	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	0	8	0	0	6	0
33	3	1	0	0	4	0
33	A	1	0	0	0	0
33	B	1	0	0	1	0
33	J	4	0	0	4	0
33	L	1	0	0	0	0
33	M	1	0	0	2	0
33	N	1	0	0	2	0
33	O	1	0	0	1	0
33	Q	1	0	0	1	0
33	R	1	0	0	0	0
33	Y	1	0	0	1	0
34	0	93	0	0	0	0
34	1	2	0	0	0	0
34	2	1	0	0	0	0
34	3	2	0	0	0	0
34	9	2	0	0	0	0
34	A	2	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	J	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	63	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	1	0	0	0	0
36	M	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5813	0	0	458	0
38	1	53	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	2	48	0	0	0	0
38	3	80	0	0	12	0
38	9	144	0	0	18	0
38	A	122	0	0	13	0
38	B	158	0	0	21	0
38	C	176	0	0	16	0
38	D	51	0	0	7	0
38	E	51	0	0	3	0
38	F	27	0	0	2	0
38	G	15	0	0	1	0
38	H	73	0	0	2	0
38	I	3	0	0	0	0
38	J	55	0	0	4	0
38	K	61	0	0	5	0
38	L	99	0	0	11	0
38	M	148	0	0	15	0
38	N	56	0	0	7	0
38	O	42	0	0	3	0
38	P	56	0	0	4	0
38	Q	58	0	0	5	0
38	R	78	0	0	1	0
38	S	37	0	0	3	0
38	T	41	0	0	3	0
38	U	34	0	0	4	0
38	V	10	0	0	2	0
38	W	71	0	0	4	0
38	X	28	0	0	1	0
38	Y	102	0	0	8	0
38	Z	33	0	0	7	0
All	All	99122	0	59914	5051	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 34.

The worst 5 of 5051 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)
18:R:150:PRO:CD	18:R:150:PRO:CG	1.97	1.43
30:0:871:G:C8	30:0:871:G:H5'	1.74	1.22
31:9:29:C:H2'	31:9:30:C:H5'	1.21	1.17
14:N:37:ARG:NH1	31:9:6:C:H5''	1.59	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:56:A:H2'	31:9:57:A:H5''	1.23	1.16

There are no symmetry-related clashes.

## 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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/240 (98%)	198 (84%)	28 (12%)	9 (4%)	3	19
2	B	335/338 (99%)	287 (86%)	42 (12%)	6 (2%)	8	35
3	C	244/246 (99%)	211 (86%)	29 (12%)	4 (2%)	9	36
4	D	134/177 (76%)	109 (81%)	22 (16%)	3 (2%)	6	30
5	E	170/178 (96%)	152 (89%)	16 (9%)	2 (1%)	13	42
6	F	117/120 (98%)	102 (87%)	11 (9%)	4 (3%)	3	22
7	G	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
8	H	156/177 (88%)	139 (89%)	14 (9%)	3 (2%)	8	34
9	I	68/162 (42%)	56 (82%)	10 (15%)	2 (3%)	4	24
10	J	140/145 (97%)	125 (89%)	12 (9%)	3 (2%)	7	31
11	K	130/132 (98%)	107 (82%)	21 (16%)	2 (2%)	10	38
12	L	141/165 (86%)	112 (79%)	25 (18%)	4 (3%)	5	25
13	M	192/196 (98%)	165 (86%)	22 (12%)	5 (3%)	5	27
14	N	184/187 (98%)	156 (85%)	23 (12%)	5 (3%)	5	26
15	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
16	P	141/149 (95%)	125 (89%)	13 (9%)	3 (2%)	7	31
17	Q	93/96 (97%)	82 (88%)	7 (8%)	4 (4%)	2	16
18	R	148/155 (96%)	132 (89%)	15 (10%)	1 (1%)	22	54
19	S	79/85 (93%)	67 (85%)	11 (14%)	1 (1%)	12	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	117/120 (98%)	95 (81%)	18 (15%)	4 (3%)	3	22
21	U	51/67 (76%)	46 (90%)	3 (6%)	2 (4%)	3	18
22	V	63/71 (89%)	57 (90%)	5 (8%)	1 (2%)	9	36
23	W	152/154 (99%)	129 (85%)	21 (14%)	2 (1%)	12	40
24	X	80/92 (87%)	68 (85%)	8 (10%)	4 (5%)	2	14
25	Y	140/241 (58%)	131 (94%)	8 (6%)	1 (1%)	22	54
26	Z	71/116 (61%)	52 (73%)	13 (18%)	6 (8%)	1	5
27	1	54/57 (95%)	48 (89%)	5 (9%)	1 (2%)	8	34
28	2	42/50 (84%)	37 (88%)	4 (10%)	1 (2%)	6	28
29	3	90/92 (98%)	73 (81%)	14 (16%)	3 (3%)	4	22
All	All	3705/4472 (83%)	3193 (86%)	426 (12%)	86 (2%)	6	29

5 of 86 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLY
4	D	65	GLU
4	D	137	PRO
6	F	61	MET
6	F	101	ALA

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/182 (98%)	172 (96%)	7 (4%)	32	62
2	B	282/283 (100%)	261 (93%)	21 (7%)	13	40
3	C	193/193 (100%)	178 (92%)	15 (8%)	12	38
4	D	117/148 (79%)	109 (93%)	8 (7%)	16	44
5	E	152/156 (97%)	146 (96%)	6 (4%)	32	62
6	F	93/94 (99%)	89 (96%)	4 (4%)	29	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	27/282 (10%)	25 (93%)	2 (7%)	13	40
8	H	134/145 (92%)	125 (93%)	9 (7%)	16	45
9	I	58/130 (45%)	55 (95%)	3 (5%)	23	54
10	J	118/121 (98%)	112 (95%)	6 (5%)	24	54
11	K	106/106 (100%)	98 (92%)	8 (8%)	13	39
12	L	113/127 (89%)	105 (93%)	8 (7%)	14	42
13	M	158/160 (99%)	148 (94%)	10 (6%)	18	47
14	N	149/150 (99%)	143 (96%)	6 (4%)	31	61
15	O	93/94 (99%)	90 (97%)	3 (3%)	39	67
16	P	113/117 (97%)	111 (98%)	2 (2%)	59	78
17	Q	79/80 (99%)	75 (95%)	4 (5%)	24	54
18	R	117/122 (96%)	110 (94%)	7 (6%)	19	49
19	S	71/74 (96%)	67 (94%)	4 (6%)	21	52
20	T	105/106 (99%)	97 (92%)	8 (8%)	13	39
21	U	44/53 (83%)	42 (96%)	2 (4%)	27	58
22	V	51/57 (90%)	48 (94%)	3 (6%)	19	49
23	W	130/130 (100%)	124 (95%)	6 (5%)	27	58
24	X	66/74 (89%)	57 (86%)	9 (14%)	3	16
25	Y	120/196 (61%)	115 (96%)	5 (4%)	30	60
26	Z	60/94 (64%)	54 (90%)	6 (10%)	7	27
27	1	46/47 (98%)	45 (98%)	1 (2%)	52	74
28	2	42/46 (91%)	41 (98%)	1 (2%)	49	73
29	3	79/79 (100%)	75 (95%)	4 (5%)	24	54
All	All	3095/3646 (85%)	2917 (94%)	178 (6%)	20	50

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	132	LEU
13	M	76	ARG
25	Y	220	GLU
11	K	12	LEU
12	L	18	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
12	L	58	GLN
14	N	107	ASN
28	2	36	ASN
13	M	24	GLN
13	M	170	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	263 (9%)	14 (0%)
31	9	121/122 (99%)	18 (14%)	1 (0%)
All	All	2866/3045 (94%)	281 (9%)	15 (0%)

5 of 281 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	11	A
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	1237	U
30	0	1352	A
30	0	2526	C
30	0	871	G
30	0	2466	G

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

5 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
30	UR3	0	2619	30	14,22,23	0.74	1 (7%)	15,32,35	0.56	0
30	PSU	0	2621	30	17,21,22	1.70	3 (17%)	20,30,33	5.47	4 (20%)
30	OMG	0	2588	30	18,26,27	1.08	2 (11%)	20,38,41	2.61	4 (20%)
30	OMU	0	2587	30	14,22,23	0.92	1 (7%)	14,31,34	1.17	1 (7%)
30	1MA	0	628	30,35	15,25,26	0.77	0	15,37,40	1.41	1 (6%)

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
30	UR3	0	2619	30	-	0/5/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	OMU	0	2587	30	-	0/7/27/28	0/2/2/2
30	1MA	0	628	30,35	-	0/3/25/26	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-5.36	1.47	1.52
30	0	2588	OMG	C6-N1	3.55	1.39	1.33
30	0	2621	PSU	C4-N3	2.82	1.38	1.33
30	0	2587	OMU	C4-N3	2.27	1.37	1.33
30	0	2621	PSU	C2-N1	2.19	1.42	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-17.46	114.55	128.43
30	0	2621	PSU	C4-N3-C2	14.38	127.28	115.14
30	0	2588	OMG	C5-C6-N1	-8.75	111.46	123.43
30	0	2621	PSU	C5-C4-N3	-8.16	114.84	125.36
30	0	2588	OMG	C6-N1-C2	5.83	125.19	115.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2619	UR3	2	0
30	0	2621	PSU	2	0
30	0	2588	OMG	3	0
30	0	2587	OMU	5	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 305 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.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	237/240 (98%)	-0.28	3 (1%) 77 77	36, 78, 117, 135	0
2	B	337/338 (99%)	-0.40	3 (0%) 84 84	36, 72, 106, 116	0
3	C	246/246 (100%)	-0.46	2 (0%) 86 86	31, 60, 87, 97	0
4	D	140/177 (79%)	0.83	30 (21%) 0 1	91, 126, 152, 162	0
5	E	172/178 (96%)	-0.27	1 (0%) 89 90	62, 89, 116, 123	0
6	F	119/120 (99%)	0.12	8 (6%) 17 17	68, 96, 130, 142	0
7	G	29/348 (8%)	0.21	0 100 100	104, 117, 126, 127	0
8	H	160/177 (90%)	0.04	2 (1%) 77 77	57, 81, 125, 130	0
9	I	70/162 (43%)	1.77	29 (41%) 0 0	149, 172, 188, 190	0
10	J	142/145 (97%)	-0.28	1 (0%) 87 88	48, 67, 90, 114	0
11	K	132/132 (100%)	-0.36	2 (1%) 73 72	38, 69, 98, 107	0
12	L	145/165 (87%)	0.29	9 (6%) 20 20	50, 96, 141, 147	0
13	M	194/196 (98%)	0.00	10 (5%) 27 25	41, 61, 109, 119	0
14	N	186/187 (99%)	0.17	9 (4%) 30 28	72, 94, 145, 152	0
15	O	115/116 (99%)	-0.52	1 (0%) 84 84	57, 72, 93, 98	0
16	P	143/149 (95%)	-0.27	3 (2%) 63 62	52, 74, 92, 103	0
17	Q	95/96 (98%)	-0.09	5 (5%) 26 24	55, 71, 88, 103	0
18	R	150/155 (96%)	-0.49	0 100 100	45, 61, 87, 109	0
19	S	81/85 (95%)	-0.39	1 (1%) 79 78	61, 80, 103, 113	0
20	T	119/120 (99%)	0.02	6 (5%) 28 27	51, 74, 105, 132	0
21	U	53/67 (79%)	3.92	47 (88%) 0 0	119, 128, 137, 138	0
22	V	65/71 (91%)	0.47	5 (7%) 13 12	68, 97, 141, 146	0
23	W	154/154 (100%)	-0.13	3 (1%) 66 65	49, 66, 88, 103	0
24	X	82/92 (89%)	0.16	3 (3%) 41 38	57, 81, 104, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	142/241 (58%)	-0.49	1 (0%) 87 88	39, 59, 87, 116	0
26	Z	73/116 (62%)	5.59	58 (79%) 0 0	109, 128, 137, 141	0
27	1	56/57 (98%)	-0.45	0 100 100	34, 47, 56, 60	0
28	2	46/50 (92%)	0.06	4 (8%) 10 10	43, 84, 116, 122	0
29	3	92/92 (100%)	5.69	83 (90%) 0 0	112, 132, 141, 144	0
30	0	2749/2923 (94%)	-0.61	1 (0%) 100 100	31, 64, 118, 195	0
31	9	122/122 (100%)	-0.75	1 (0%) 86 86	53, 94, 121, 167	0
All	All	6646/7517 (88%)	-0.15	331 (4%) 28 27	31, 72, 133, 195	0

The worst 5 of 331 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	3	41	GLU	21.4
26	Z	35	SER	15.5
29	3	45	GLY	15.4
29	3	35	TRP	15.3
29	3	38	ARG	14.7

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
30	PSU	0	2621	20/21	0.96	0.20	49,51,60,60	0
30	OMG	0	2588	24/25	0.97	0.14	48,51,54,55	0
30	1MA	0	628	23/24	0.98	0.17	37,44,45,46	0
30	UR3	0	2619	21/22	0.98	0.14	56,57,60,60	0
30	OMU	0	2587	21/22	0.98	0.13	51,52,54,56	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
35	NA	L	8568	1/1	-0.00	0.63	59,59,59,59	0
34	SR	0	8979	1/1	0.43	0.69	200,200,200,200	0
34	SR	0	8982	1/1	0.54	0.78	200,200,200,200	0
35	NA	0	8553	1/1	0.55	0.22	81,81,81,81	0
35	NA	0	8560	1/1	0.56	0.43	80,80,80,80	0
34	SR	0	8991	1/1	0.57	0.09	188,188,188,188	0
33	CL	0	8822	1/1	0.60	0.91	140,140,140,140	0
35	NA	Q	8540	1/1	0.60	0.12	74,74,74,74	0
34	SR	0	9006	1/1	0.65	0.52	200,200,200,200	0
35	NA	0	8509	1/1	0.66	0.43	84,84,84,84	0
35	NA	0	8528	1/1	0.69	0.40	113,113,113,113	0
37	CD	U	8701	1/1	0.69	0.39	180,180,180,180	0
34	SR	3	8999	1/1	0.69	0.43	200,200,200,200	0
35	NA	0	8562	1/1	0.70	1.01	83,83,83,83	0
34	SR	0	8957	1/1	0.72	1.76	200,200,200,200	0
34	SR	0	8960	1/1	0.73	0.06	156,156,156,156	0
34	SR	0	9001	1/1	0.73	0.13	200,200,200,200	0
34	SR	0	8971	1/1	0.73	0.16	200,200,200,200	0
33	CL	J	8821	1/1	0.74	0.26	99,99,99,99	0
34	SR	B	8987	1/1	0.74	0.79	200,200,200,200	0
34	SR	3	8932	1/1	0.74	0.11	148,148,148,148	0
32	MG	0	8066	1/1	0.75	0.45	71,71,71,71	0
35	NA	0	8545	1/1	0.75	0.43	74,74,74,74	0
32	MG	0	8031	1/1	0.76	0.11	68,68,68,68	0
33	CL	J	8801	1/1	0.76	0.22	85,85,85,85	0
35	NA	R	8575	1/1	0.77	0.50	97,97,97,97	0
34	SR	0	9004	1/1	0.78	1.32	200,200,200,200	0
33	CL	3	8804	1/1	0.79	0.11	98,98,98,98	0
33	CL	0	8815	1/1	0.80	0.24	130,130,130,130	0
34	SR	0	8928	1/1	0.80	0.12	156,156,156,156	0
35	NA	0	8518	1/1	0.80	0.85	91,91,91,91	0
32	MG	T	8057	1/1	0.80	0.08	80,80,80,80	0
34	SR	0	8993	1/1	0.81	0.05	200,200,200,200	0
32	MG	0	8087	1/1	0.81	0.06	22,22,22,22	0
33	CL	N	8807	1/1	0.81	0.49	99,99,99,99	0
35	NA	B	8552	1/1	0.81	0.55	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8507	1/1	0.81	0.20	38,38,38,38	0
35	NA	0	8524	1/1	0.81	0.42	53,53,53,53	0
35	NA	0	8549	1/1	0.81	0.28	96,96,96,96	0
35	NA	0	8570	1/1	0.81	0.18	57,57,57,57	0
37	CD	3	8704	1/1	0.81	0.59	183,183,183,183	0
34	SR	0	8955	1/1	0.82	0.11	200,200,200,200	0
34	SR	0	8983	1/1	0.83	0.30	200,200,200,200	0
35	NA	0	8544	1/1	0.83	0.45	76,76,76,76	0
35	NA	0	8501	1/1	0.84	0.26	53,53,53,53	0
34	SR	0	8968	1/1	0.84	0.18	175,175,175,175	0
34	SR	0	8975	1/1	0.84	0.06	189,189,189,189	0
34	SR	0	8964	1/1	0.84	0.25	176,176,176,176	0
34	SR	0	8974	1/1	0.85	0.42	196,196,196,196	0
32	MG	Y	8077	1/1	0.85	0.39	58,58,58,58	0
32	MG	9	8074	1/1	0.85	0.23	97,97,97,97	0
32	MG	0	8068	1/1	0.85	0.08	44,44,44,44	0
33	CL	L	8810	1/1	0.85	0.12	91,91,91,91	0
35	NA	0	8571	1/1	0.86	0.36	99,99,99,99	0
34	SR	0	9000	1/1	0.86	0.15	200,200,200,200	0
33	CL	J	8802	1/1	0.86	0.11	86,86,86,86	0
34	SR	9	9003	1/1	0.86	0.04	200,200,200,200	0
32	MG	0	8065	1/1	0.86	0.10	66,66,66,66	0
32	MG	0	8008	1/1	0.86	0.20	26,26,26,26	0
35	NA	0	8519	1/1	0.87	0.19	51,51,51,51	0
34	SR	0	8959	1/1	0.87	0.06	190,190,190,190	0
35	NA	R	8532	1/1	0.87	0.21	68,68,68,68	0
35	NA	0	8536	1/1	0.88	0.12	64,64,64,64	0
32	MG	0	8032	1/1	0.88	0.05	47,47,47,47	0
34	SR	0	8989	1/1	0.88	0.13	174,174,174,174	0
35	NA	0	8522	1/1	0.88	0.26	130,130,130,130	0
34	SR	F	9005	1/1	0.88	0.15	170,170,170,170	0
35	NA	0	8556	1/1	0.89	0.39	94,94,94,94	0
35	NA	0	8502	1/1	0.89	0.19	66,66,66,66	0
34	SR	0	8988	1/1	0.89	0.05	200,200,200,200	0
33	CL	B	8819	1/1	0.89	1.19	83,83,83,83	0
34	SR	0	8953	1/1	0.89	0.33	179,179,179,179	0
34	SR	0	8919	1/1	0.89	0.09	185,185,185,185	0
33	CL	O	8808	1/1	0.89	0.38	114,114,114,114	0
35	NA	0	8506	1/1	0.89	0.56	91,91,91,91	0
35	NA	0	8525	1/1	0.90	0.55	113,113,113,113	0
35	NA	0	8557	1/1	0.90	0.06	70,70,70,70	0
32	MG	0	8081	1/1	0.90	0.38	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8529	1/1	0.90	0.16	61,61,61,61	0
34	SR	0	8969	1/1	0.90	1.49	200,200,200,200	0
34	SR	0	8984	1/1	0.90	0.03	124,124,124,124	0
32	MG	0	8092	1/1	0.90	0.09	53,53,53,53	0
35	NA	0	8508	1/1	0.90	0.35	118,118,118,118	0
34	SR	A	8930	1/1	0.91	0.11	131,131,131,131	0
34	SR	0	8970	1/1	0.91	0.15	158,158,158,158	0
34	SR	0	8956	1/1	0.91	0.24	200,200,200,200	0
32	MG	0	8046	1/1	0.91	0.07	44,44,44,44	0
32	MG	0	8093	1/1	0.91	0.16	48,48,48,48	0
34	SR	J	8986	1/1	0.91	0.34	200,200,200,200	0
34	SR	0	8976	1/1	0.92	0.26	195,195,195,195	0
35	NA	0	8516	1/1	0.92	0.22	27,27,27,27	0
32	MG	0	8042	1/1	0.92	0.05	75,75,75,75	0
34	SR	0	8972	1/1	0.92	0.18	138,138,138,138	0
32	MG	0	8038	1/1	0.92	0.12	94,94,94,94	0
32	MG	0	8067	1/1	0.92	0.27	47,47,47,47	0
34	SR	B	8950	1/1	0.92	0.15	123,123,123,123	0
32	MG	0	8053	1/1	0.92	0.13	88,88,88,88	0
33	CL	0	8803	1/1	0.92	0.14	82,82,82,82	0
35	NA	J	8538	1/1	0.92	0.12	84,84,84,84	0
35	NA	9	8572	1/1	0.92	0.08	71,71,71,71	0
34	SR	0	8938	1/1	0.92	0.06	200,200,200,200	0
34	SR	0	8977	1/1	0.92	0.05	200,200,200,200	0
32	MG	0	8011	1/1	0.93	0.21	33,33,33,33	0
33	CL	J	8816	1/1	0.93	2.10	99,99,99,99	0
35	NA	0	8511	1/1	0.93	0.09	53,53,53,53	0
35	NA	0	8517	1/1	0.93	0.21	69,69,69,69	0
34	SR	0	8908	1/1	0.93	0.10	99,99,99,99	0
35	NA	0	8555	1/1	0.93	0.25	80,80,80,80	0
33	CL	0	8805	1/1	0.93	0.38	105,105,105,105	0
32	MG	0	8023	1/1	0.93	0.21	38,38,38,38	0
32	MG	0	8049	1/1	0.94	0.26	82,82,82,82	0
35	NA	0	8573	1/1	0.94	0.25	89,89,89,89	0
35	NA	0	8574	1/1	0.94	1.44	92,92,92,92	0
32	MG	0	8079	1/1	0.94	0.31	57,57,57,57	0
34	SR	0	8922	1/1	0.94	0.27	181,181,181,181	0
34	SR	0	8963	1/1	0.94	0.12	117,117,117,117	0
32	MG	0	8085	1/1	0.94	0.11	67,67,67,67	0
34	SR	0	8927	1/1	0.94	0.10	171,171,171,171	0
35	NA	0	8523	1/1	0.94	0.22	51,51,51,51	0
35	NA	0	8537	1/1	0.94	0.12	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8026	1/1	0.94	0.14	37,37,37,37	0
35	NA	0	8547	1/1	0.94	0.49	115,115,115,115	0
34	SR	0	8936	1/1	0.94	0.10	114,114,114,114	0
34	SR	0	8962	1/1	0.94	0.06	168,168,168,168	0
32	MG	0	8064	1/1	0.94	0.23	51,51,51,51	0
33	CL	M	8818	1/1	0.94	0.29	58,58,58,58	0
32	MG	0	8003	1/1	0.94	0.20	27,27,27,27	0
32	MG	0	8020	1/1	0.94	0.19	50,50,50,50	0
32	MG	K	8054	1/1	0.94	0.15	42,42,42,42	0
34	SR	0	8926	1/1	0.95	0.23	131,131,131,131	0
32	MG	0	8082	1/1	0.95	0.19	62,62,62,62	0
35	NA	0	8526	1/1	0.95	0.11	67,67,67,67	0
34	SR	0	8997	1/1	0.95	0.92	200,200,200,200	0
34	SR	0	8998	1/1	0.95	0.65	200,200,200,200	0
35	NA	0	8554	1/1	0.95	0.36	124,124,124,124	0
32	MG	0	8030	1/1	0.95	0.91	75,75,75,75	0
35	NA	0	8564	1/1	0.95	0.67	87,87,87,87	0
34	SR	0	8951	1/1	0.95	0.17	183,183,183,183	0
32	MG	A	8051	1/1	0.95	0.23	95,95,95,95	0
32	MG	0	8015	1/1	0.95	0.13	30,30,30,30	0
35	NA	0	8563	1/1	0.95	0.25	66,66,66,66	0
35	NA	0	8550	1/1	0.95	0.12	129,129,129,129	0
34	SR	0	8925	1/1	0.95	0.14	98,98,98,98	0
32	MG	0	8052	1/1	0.95	0.13	63,63,63,63	0
34	SR	0	8965	1/1	0.95	0.23	160,160,160,160	0
32	MG	0	8010	1/1	0.96	0.13	46,46,46,46	0
32	MG	0	8089	1/1	0.96	0.28	56,56,56,56	0
32	MG	0	8018	1/1	0.96	0.08	34,34,34,34	0
34	SR	2	8947	1/1	0.96	0.12	195,195,195,195	0
32	MG	9	8040	1/1	0.96	0.18	101,101,101,101	0
35	NA	R	8533	1/1	0.96	0.07	94,94,94,94	0
33	CL	Q	8811	1/1	0.96	0.72	124,124,124,124	0
34	SR	0	8911	1/1	0.96	0.14	100,100,100,100	0
34	SR	0	8978	1/1	0.96	0.07	132,132,132,132	0
32	MG	0	8019	1/1	0.96	0.18	19,19,19,19	0
32	MG	0	8056	1/1	0.96	0.14	47,47,47,47	0
37	CD	Z	8703	1/1	0.96	0.43	188,188,188,188	0
32	MG	0	8043	1/1	0.96	0.22	62,62,62,62	0
35	NA	0	8515	1/1	0.96	0.09	35,35,35,35	0
32	MG	0	8091	1/1	0.96	0.30	67,67,67,67	0
32	MG	0	8061	1/1	0.96	0.31	47,47,47,47	0
34	SR	0	9002	1/1	0.96	0.14	200,200,200,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8033	1/1	0.96	0.20	69,69,69,69	0
35	NA	S	8510	1/1	0.96	0.06	41,41,41,41	0
34	SR	0	8915	1/1	0.96	0.12	123,123,123,123	0
35	NA	0	8566	1/1	0.96	0.25	86,86,86,86	0
33	CL	0	8817	1/1	0.96	0.10	84,84,84,84	0
34	SR	0	8942	1/1	0.96	0.05	123,123,123,123	0
35	NA	0	8514	1/1	0.96	0.38	74,74,74,74	0
32	MG	0	8039	1/1	0.96	0.20	94,94,94,94	0
34	SR	A	8929	1/1	0.96	0.09	139,139,139,139	0
33	CL	Y	8820	1/1	0.96	0.13	58,58,58,58	0
35	NA	0	8546	1/1	0.96	1.01	108,108,108,108	0
32	MG	0	8058	1/1	0.96	0.07	7,7,7,7	0
35	NA	0	8535	1/1	0.96	0.25	58,58,58,58	0
35	NA	M	8539	1/1	0.97	0.12	38,38,38,38	0
35	NA	0	8542	1/1	0.97	0.41	79,79,79,79	0
34	SR	0	8923	1/1	0.97	0.09	108,108,108,108	0
34	SR	0	8935	1/1	0.97	0.15	101,101,101,101	0
33	CL	0	8813	1/1	0.97	0.21	64,64,64,64	0
35	NA	0	8561	1/1	0.97	0.14	53,53,53,53	0
32	MG	0	8007	1/1	0.97	0.07	21,21,21,21	0
33	CL	0	8812	1/1	0.97	0.08	70,70,70,70	0
34	SR	0	8985	1/1	0.97	0.10	168,168,168,168	0
35	NA	0	8534	1/1	0.97	0.27	53,53,53,53	0
35	NA	0	8558	1/1	0.97	0.24	82,82,82,82	0
34	SR	0	8920	1/1	0.97	0.08	145,145,145,145	0
34	SR	0	8943	1/1	0.97	0.10	89,89,89,89	0
32	MG	0	8055	1/1	0.97	0.30	60,60,60,60	0
32	MG	0	8029	1/1	0.97	0.10	62,62,62,62	0
32	MG	A	8050	1/1	0.97	0.12	69,69,69,69	0
34	SR	0	8992	1/1	0.97	0.23	141,141,141,141	0
34	SR	0	8946	1/1	0.97	0.24	144,144,144,144	0
35	NA	9	8543	1/1	0.97	0.26	51,51,51,51	0
33	CL	A	8809	1/1	0.97	0.34	116,116,116,116	0
33	CL	0	8814	1/1	0.97	0.28	51,51,51,51	0
32	MG	0	8075	1/1	0.97	0.06	50,50,50,50	0
32	MG	0	8088	1/1	0.97	0.17	53,53,53,53	0
36	K	M	8402	1/1	0.97	0.21	96,96,96,96	0
32	MG	0	8073	1/1	0.97	0.09	89,89,89,89	0
34	SR	1	8952	1/1	0.97	0.12	92,92,92,92	0
35	NA	0	8504	1/1	0.97	0.33	41,41,41,41	0
32	MG	0	8024	1/1	0.97	0.03	39,39,39,39	0
32	MG	0	8021	1/1	0.97	0.07	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8009	1/1	0.97	0.24	24,24,24,24	0
34	SR	0	8924	1/1	0.97	0.23	131,131,131,131	0
34	SR	0	8939	1/1	0.97	0.07	155,155,155,155	0
34	SR	0	8934	1/1	0.98	0.10	138,138,138,138	0
32	MG	0	8022	1/1	0.98	0.20	25,25,25,25	0
34	SR	0	8910	1/1	0.98	0.13	118,118,118,118	0
34	SR	0	8937	1/1	0.98	0.26	126,126,126,126	0
34	SR	0	8995	1/1	0.98	0.16	123,123,123,123	0
32	MG	0	8037	1/1	0.98	0.31	92,92,92,92	0
32	MG	0	8060	1/1	0.98	0.04	58,58,58,58	0
34	SR	S	8961	1/1	0.98	0.10	130,130,130,130	0
35	NA	0	8569	1/1	0.98	0.12	71,71,71,71	0
32	MG	0	8001	1/1	0.98	0.14	42,42,42,42	0
32	MG	0	8044	1/1	0.98	0.10	59,59,59,59	0
32	MG	0	8078	1/1	0.98	0.36	72,72,72,72	0
35	NA	0	8559	1/1	0.98	0.51	96,96,96,96	0
33	CL	R	8806	1/1	0.98	0.15	66,66,66,66	0
32	MG	0	8059	1/1	0.98	0.06	55,55,55,55	0
34	SR	9	8980	1/1	0.98	0.16	191,191,191,191	0
34	SR	0	8931	1/1	0.98	0.15	120,120,120,120	0
32	MG	0	8034	1/1	0.98	0.06	50,50,50,50	0
32	MG	0	8041	1/1	0.98	0.19	25,25,25,25	0
32	MG	0	8005	1/1	0.98	0.22	24,24,24,24	0
34	SR	0	9008	1/1	0.98	0.10	94,94,94,94	0
34	SR	0	8945	1/1	0.98	0.07	119,119,119,119	0
34	SR	0	8990	1/1	0.98	0.14	113,113,113,113	0
34	SR	0	8914	1/1	0.98	0.22	133,133,133,133	0
34	SR	0	9007	1/1	0.98	1.31	200,200,200,200	0
32	MG	0	8013	1/1	0.98	0.06	19,19,19,19	0
34	SR	0	8981	1/1	0.98	0.13	198,198,198,198	0
32	MG	0	8016	1/1	0.98	0.15	41,41,41,41	0
35	NA	0	8530	1/1	0.98	0.17	53,53,53,53	0
32	MG	0	8006	1/1	0.98	0.10	44,44,44,44	0
34	SR	0	8996	1/1	0.98	0.48	200,200,200,200	0
32	MG	0	8080	1/1	0.98	0.27	65,65,65,65	0
34	SR	0	8994	1/1	0.98	0.11	200,200,200,200	0
35	NA	0	8531	1/1	0.98	0.18	54,54,54,54	0
36	K	0	8401	1/1	0.98	0.62	145,145,145,145	0
34	SR	0	8954	1/1	0.98	0.15	115,115,115,115	0
35	NA	0	8541	1/1	0.98	0.18	60,60,60,60	0
35	NA	0	8527	1/1	0.99	0.31	92,92,92,92	0
32	MG	0	8017	1/1	0.99	0.14	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8062	1/1	0.99	0.18	66,66,66,66	0
34	SR	R	8912	1/1	0.99	0.24	107,107,107,107	0
32	MG	0	8028	1/1	0.99	0.09	13,13,13,13	0
34	SR	0	8909	1/1	0.99	0.08	100,100,100,100	0
34	SR	0	8904	1/1	0.99	0.23	73,73,73,73	0
35	NA	C	8503	1/1	0.99	0.12	36,36,36,36	0
32	MG	0	8014	1/1	0.99	0.08	25,25,25,25	0
32	MG	0	8047	1/1	0.99	0.40	90,90,90,90	0
34	SR	0	8918	1/1	0.99	0.10	88,88,88,88	0
32	MG	0	8002	1/1	0.99	0.14	31,31,31,31	0
35	NA	0	8521	1/1	0.99	0.26	40,40,40,40	0
34	SR	0	8941	1/1	0.99	0.26	141,141,141,141	0
32	MG	0	8090	1/1	0.99	0.11	57,57,57,57	0
32	MG	0	8045	1/1	0.99	0.09	28,28,28,28	0
32	MG	0	8036	1/1	0.99	0.10	62,62,62,62	0
32	MG	0	8070	1/1	0.99	0.16	39,39,39,39	0
34	SR	0	8905	1/1	0.99	0.28	68,68,68,68	0
34	SR	0	8966	1/1	0.99	0.07	101,101,101,101	0
34	SR	0	8933	1/1	0.99	0.16	126,126,126,126	0
32	MG	Y	8086	1/1	0.99	0.26	52,52,52,52	0
32	MG	0	8035	1/1	0.99	0.17	76,76,76,76	0
35	NA	0	8567	1/1	0.99	0.44	83,83,83,83	0
34	SR	0	8967	1/1	0.99	0.06	163,163,163,163	0
32	MG	0	8004	1/1	0.99	0.11	19,19,19,19	0
32	MG	0	8084	1/1	0.99	0.13	37,37,37,37	0
34	SR	0	8949	1/1	0.99	0.07	128,128,128,128	0
32	MG	0	8063	1/1	0.99	0.12	60,60,60,60	0
34	SR	0	8917	1/1	0.99	0.10	111,111,111,111	0
34	SR	0	8940	1/1	0.99	0.10	93,93,93,93	0
32	MG	0	8072	1/1	0.99	0.09	45,45,45,45	0
35	NA	0	8513	1/1	0.99	0.19	67,67,67,67	0
35	NA	0	8551	1/1	0.99	0.16	75,75,75,75	0
34	SR	0	8973	1/1	0.99	0.16	142,142,142,142	0
34	SR	0	8916	1/1	0.99	0.05	110,110,110,110	0
34	SR	0	8948	1/1	0.99	0.09	110,110,110,110	0
32	MG	0	8071	1/1	0.99	0.13	78,78,78,78	0
32	MG	0	8048	1/1	0.99	0.31	26,26,26,26	0
35	NA	0	8548	1/1	0.99	0.05	44,44,44,44	0
35	NA	0	8565	1/1	0.99	0.16	85,85,85,85	0
35	NA	0	8512	1/1	0.99	0.24	40,40,40,40	0
32	MG	0	8083	1/1	0.99	0.35	58,58,58,58	0
35	NA	0	8520	1/1	0.99	0.06	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8505	1/1	0.99	0.22	37,37,37,37	0
37	CD	O	8705	1/1	0.99	0.05	105,105,105,105	0
34	SR	0	8944	1/1	0.99	0.05	168,168,168,168	0
32	MG	0	8069	1/1	0.99	0.12	73,73,73,73	0
34	SR	0	8903	1/1	0.99	0.23	63,63,63,63	0
37	CD	1	8702	1/1	0.99	0.11	78,78,78,78	0
34	SR	0	8921	1/1	0.99	0.09	88,88,88,88	0
34	SR	0	8958	1/1	1.00	0.13	126,126,126,126	0
34	SR	0	8907	1/1	1.00	0.17	60,60,60,60	0
32	MG	0	8027	1/1	1.00	0.10	44,44,44,44	0
34	SR	0	8906	1/1	1.00	0.14	66,66,66,66	0
32	MG	0	8012	1/1	1.00	0.22	26,26,26,26	0
32	MG	0	8076	1/1	1.00	0.32	76,76,76,76	0
34	SR	0	8902	1/1	1.00	0.07	72,72,72,72	0
34	SR	1	8913	1/1	1.00	0.10	108,108,108,108	0
32	MG	0	8025	1/1	1.00	0.04	23,23,23,23	0
34	SR	0	8901	1/1	1.00	0.14	73,73,73,73	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.