



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 25, 2020 – 07:12 PM BST

PDB ID : 3CCL
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation U2535C. Density for Anisomycin is visible but not included in model.
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-26
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
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) : 2.13

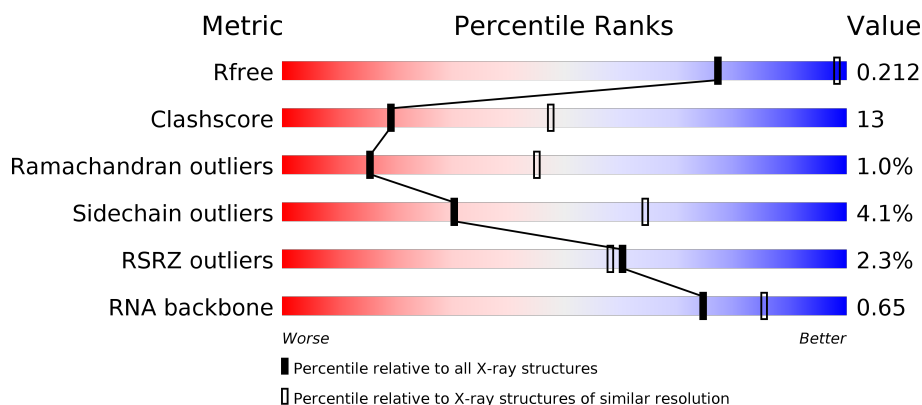
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



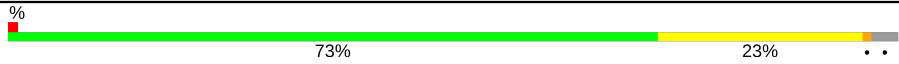

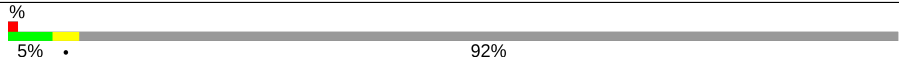
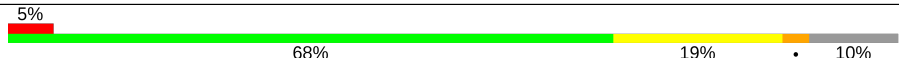

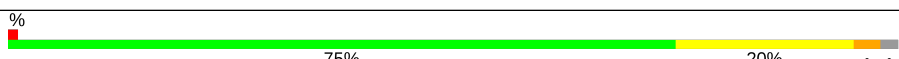
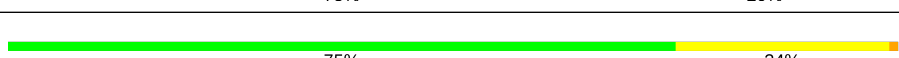
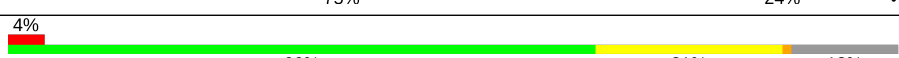
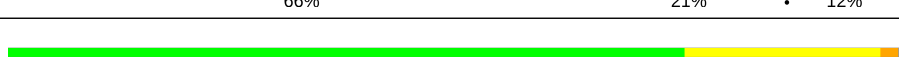

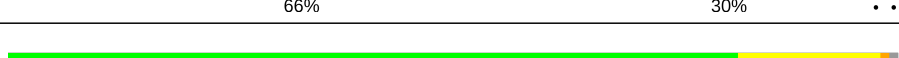







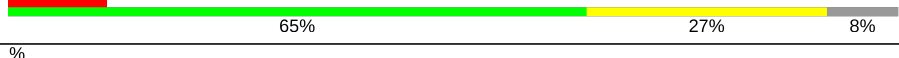
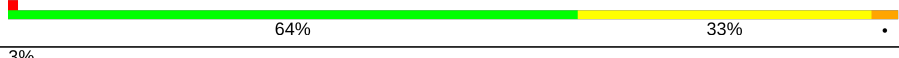

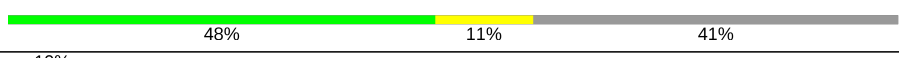
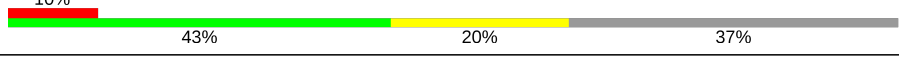


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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>2%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>• •</div> </div> </div>
2	B	338	<div> <div>66%</div> <div>31%</div> <div>•</div> </div>
3	C	246	<div> <div>72%</div> <div>24%</div> <div>•</div> </div>
4	D	177	<div> <div>16%</div> <div>45%</div> <div>32%</div> <div>21%</div> <div>•</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
34	SR	0	8982	-	-	-	X
34	SR	0	8994	-	-	-	X
34	SR	0	8997	-	-	-	X
34	SR	0	9006	-	-	-	X
34	SR	B	8987	-	-	-	X
35	NA	0	8505	-	-	-	X
35	NA	0	8518	-	-	-	X
35	NA	0	8546	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8562	-	-	-	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	10874	19052	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	87	Total	Mg	0	0
			87	87		
32	9	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	10	Total 10	Cl 10	0	0
33	J	3	Total 3	Cl 3	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	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	3	Total 3	Sr 3	0	0
34	R	1	Total 1	Sr 1	0	0
34	9	3	Total 3	Sr 3	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	67	Total 67	Na 67	0	0
35	J	1	Total 1	Na 1	0	0
35	Q	1	Total 1	Na 1	0	0
35	C	1	Total 1	Na 1	0	0
35	R	1	Total 1	Na 1	0	0
35	9	2	Total 2	Na 2	0	0
35	S	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	O	1	Total 1	Cd 1	0	0
36	Z	1	Total 1	Cd 1	0	0
36	1	1	Total 1	Cd 1	0	0
36	3	1	Total 1	Cd 1	0	0
36	U	1	Total 1	Cd 1	0	0

- Molecule 37 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	2	Total 2	K 2	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	A	116	Total 116	O 116	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	B	141	Total 141	O 141	0	0
38	C	170	Total 170	O 170	0	0
38	D	44	Total 44	O 44	0	0
38	E	45	Total 45	O 45	0	0
38	F	27	Total 27	O 27	0	0
38	G	19	Total 19	O 19	0	0
38	H	63	Total 63	O 63	0	0
38	I	8	Total 8	O 8	0	0
38	J	53	Total 53	O 53	0	0
38	K	56	Total 56	O 56	0	0
38	L	85	Total 85	O 85	0	0
38	M	123	Total 123	O 123	0	0
38	N	55	Total 55	O 55	0	0
38	O	43	Total 43	O 43	0	0
38	P	67	Total 67	O 67	0	0
38	Q	50	Total 50	O 50	0	0
38	R	85	Total 85	O 85	0	0
38	S	33	Total 33	O 33	0	0
38	T	34	Total 34	O 34	0	0
38	U	27	Total 27	O 27	0	0
38	V	13	Total 13	O 13	0	0

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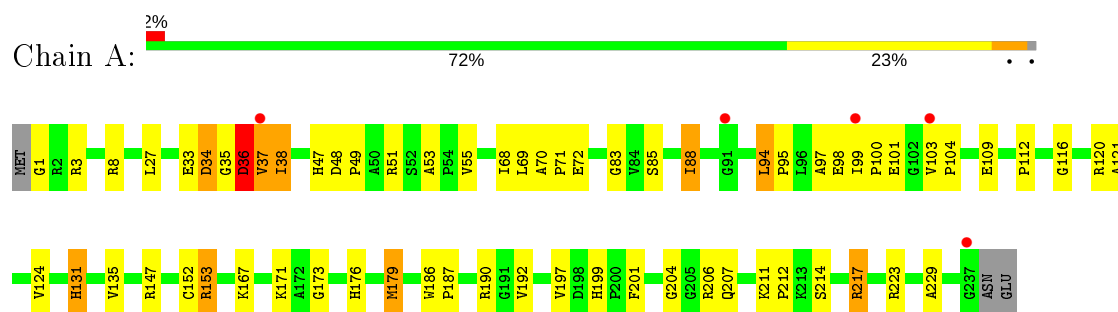
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	W	69	Total 69	O 69	0	0
38	X	25	Total 25	O 25	0	0
38	Y	95	Total 95	O 95	0	0
38	Z	26	Total 26	O 26	0	0
38	1	63	Total 63	O 63	0	0
38	2	50	Total 50	O 50	0	0
38	3	62	Total 62	O 62	0	0
38	0	5929	Total 5929	O 5929	0	0
38	9	147	Total 147	O 147	0	0

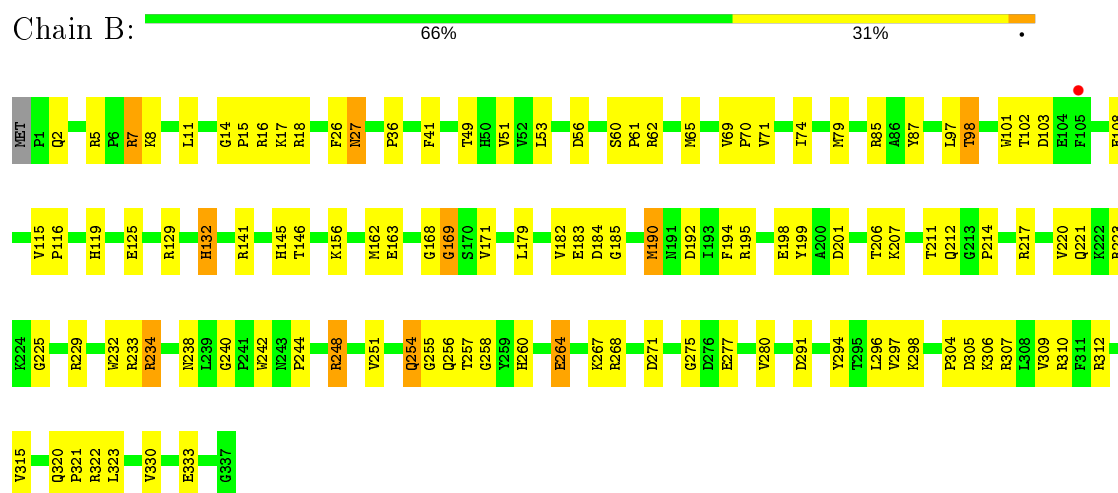
3 Residue-property plots [i](#)

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 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.

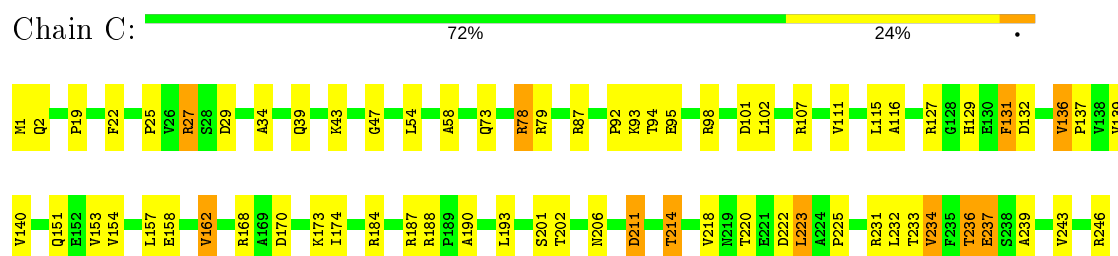
- Molecule 1: 50S ribosomal protein L2P



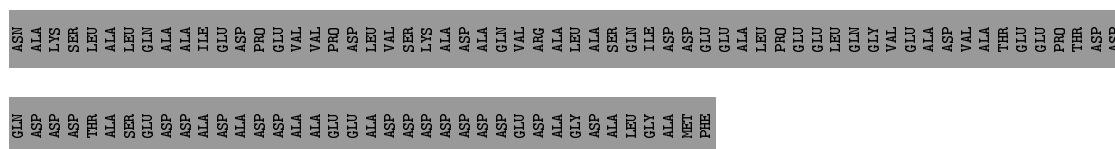
- Molecule 2: 50S ribosomal protein L3P



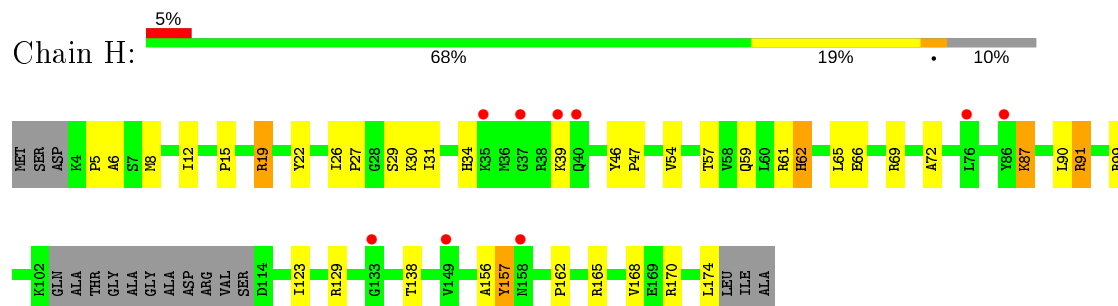
- Molecule 3: 50S ribosomal protein L4P



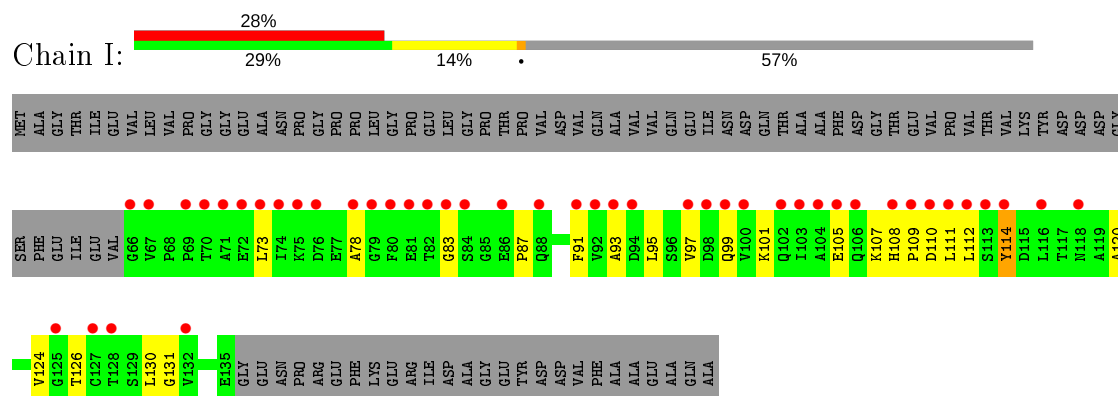
- Molecule 4: 50S ribosomal protein L5P



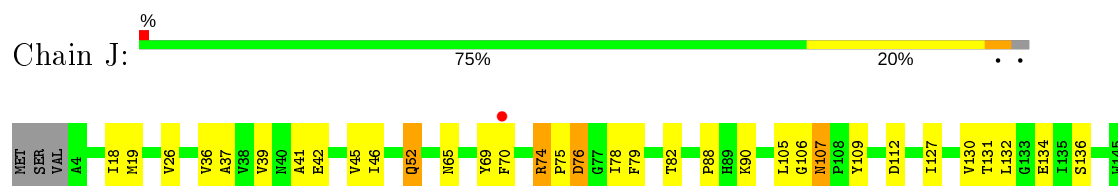
- Molecule 8: 50S ribosomal protein L10e



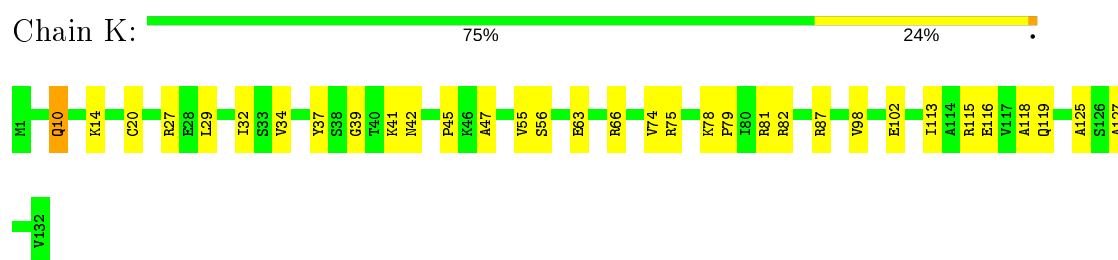
- Molecule 9: 50S ribosomal protein L11P



- Molecule 10: 50S ribosomal protein L13P

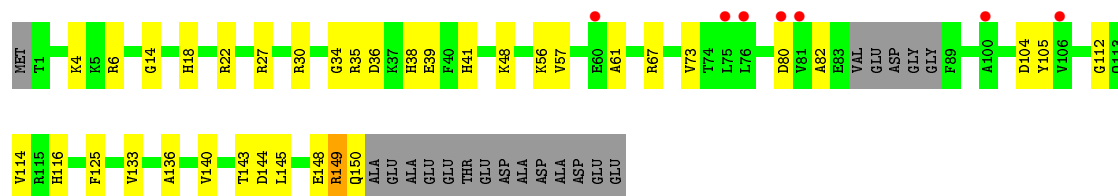


- Molecule 11: 50S ribosomal protein L14P



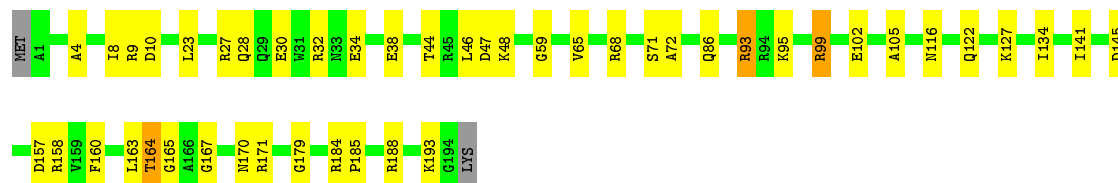
- Molecule 12: 50S ribosomal protein L15P





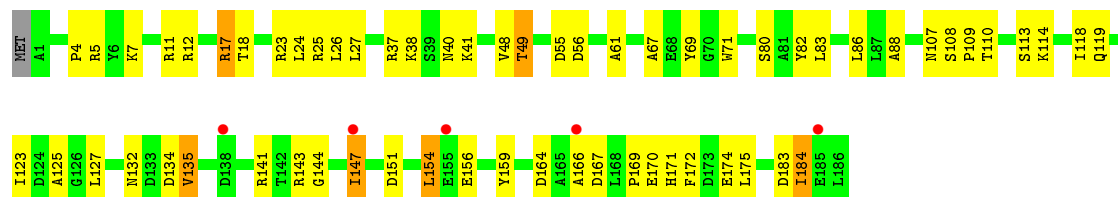
- Molecule 13: 50S ribosomal protein L15e

Chain M: 76% 22%



- Molecule 14: 50S ribosomal protein L18P

Chain N: 3% 66% 30%



- Molecule 15: 50S ribosomal protein L18e

Chain O: 82% 16%



- Molecule 16: 50S ribosomal protein L19e

Chain P: 77% 17%




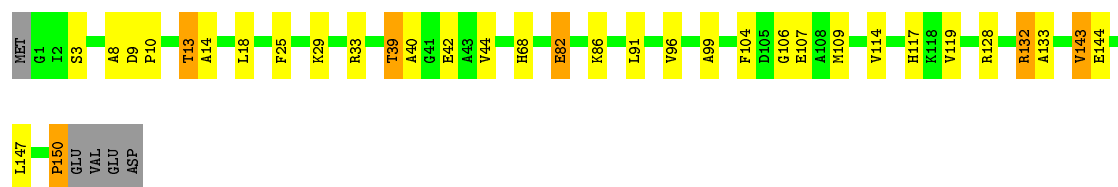
- Molecule 17: 50S ribosomal protein L21e

Chain Q: 78% 20%




- Molecule 18: 50S ribosomal protein L22P

Chain R:  75% 18%



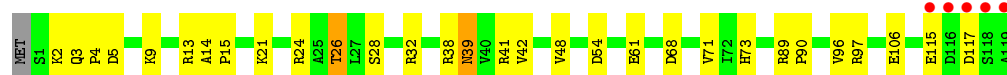
- Molecule 19: 50S ribosomal protein L23P

Chain S:  78% 18% 5%



- Molecule 20: 50S ribosomal protein L24P

Chain T:  4% 74% 23%



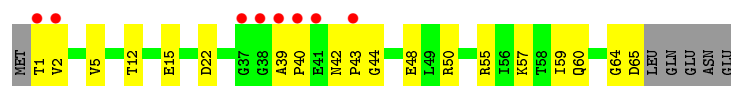
- Molecule 21: 50S ribosomal protein L24e

Chain U:  61% 18% 21%



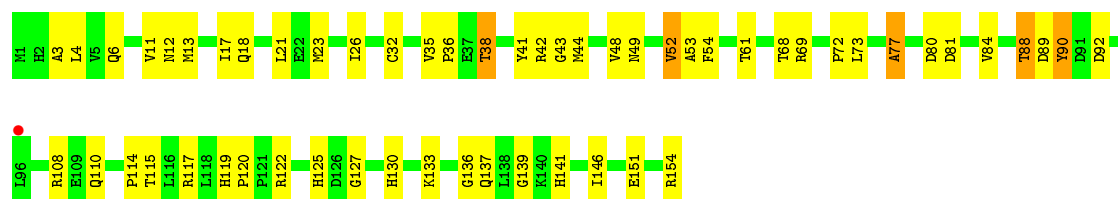
- Molecule 22: 50S ribosomal protein L29P

Chain V:  11% 65% 27% 8%

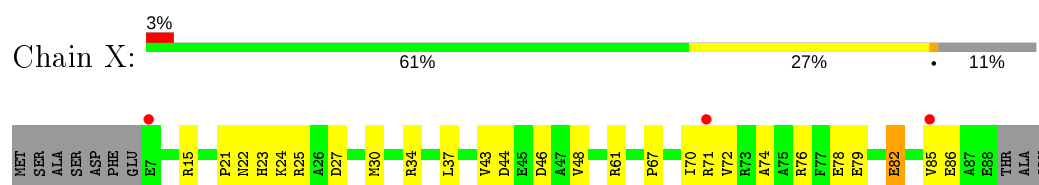


- Molecule 23: 50S ribosomal protein L30P

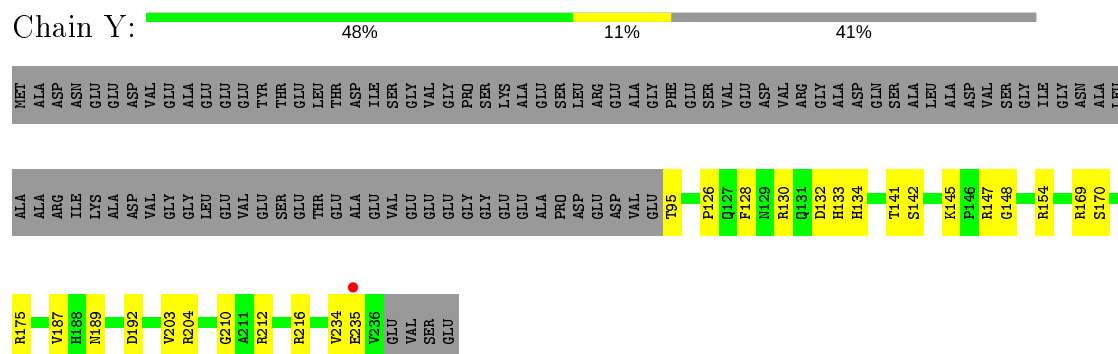
Chain W:  64% 33%



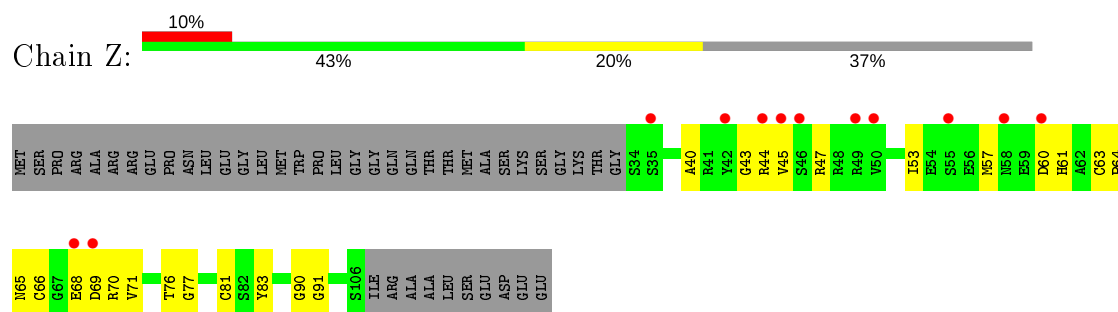
- Molecule 24: 50S ribosomal protein L31e



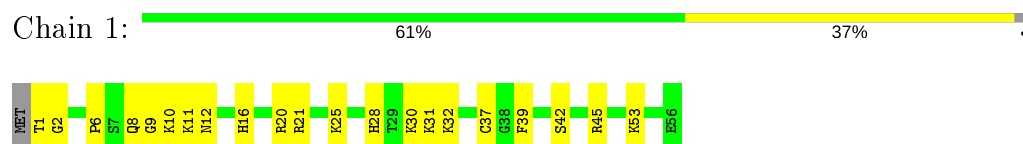
- Molecule 25: 50S ribosomal protein L32e



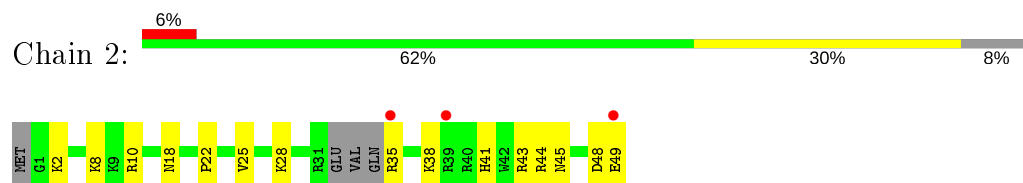
- Molecule 26: 50S ribosomal protein L37Ae



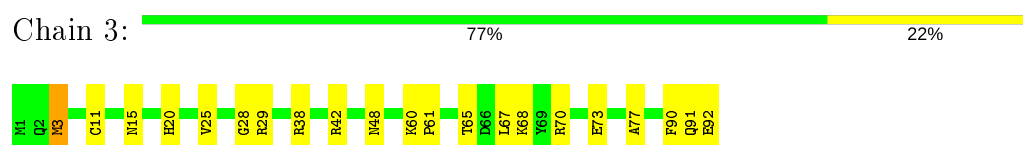
- Molecule 27: 50S ribosomal protein L37e



- Molecule 28: 50S ribosomal protein L39e

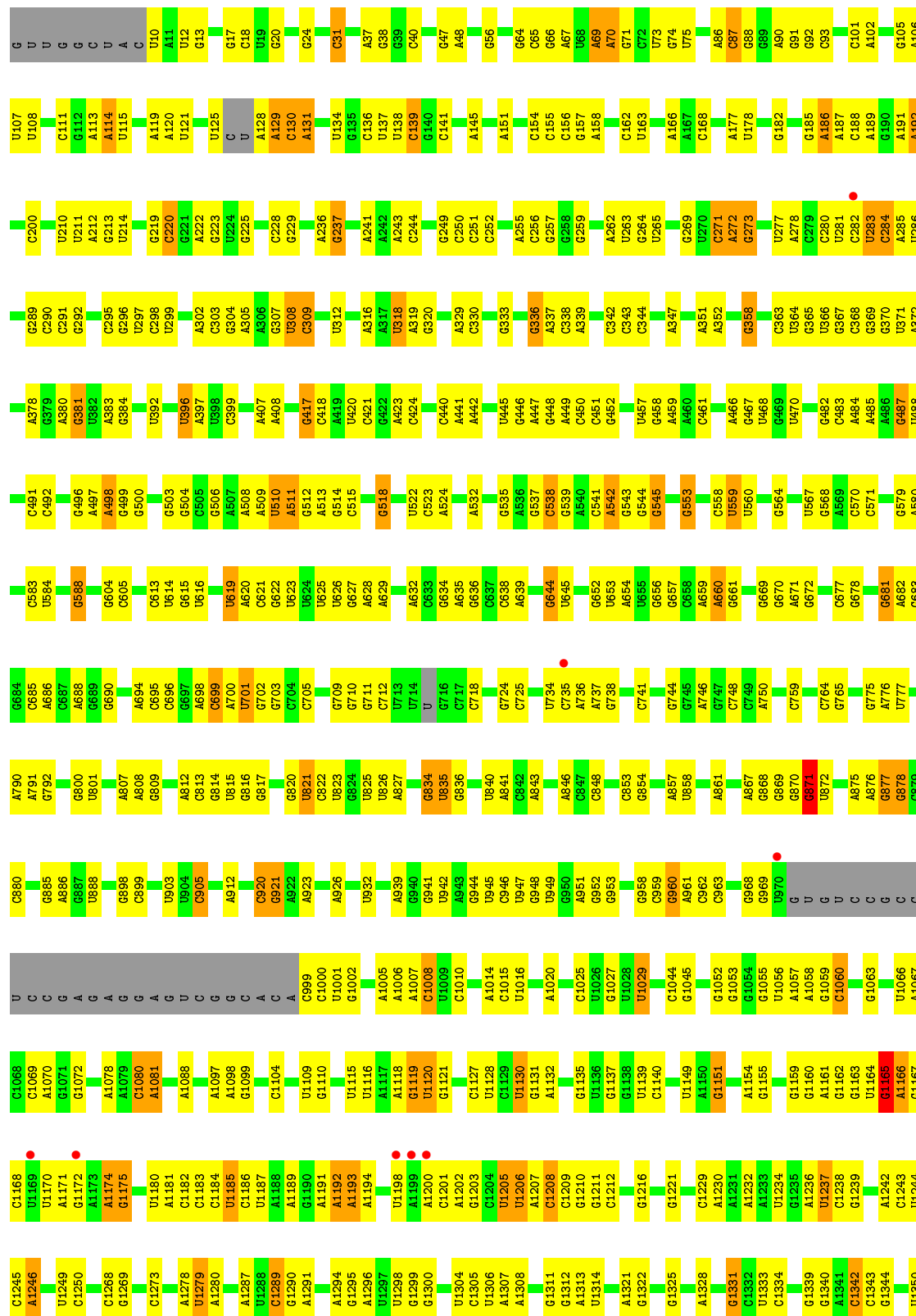


- Molecule 29: 50S ribosomal protein L44E

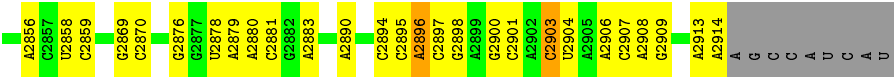


● Molecule 30: 23S RIBOSOMAL RNA

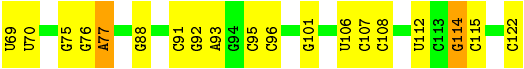
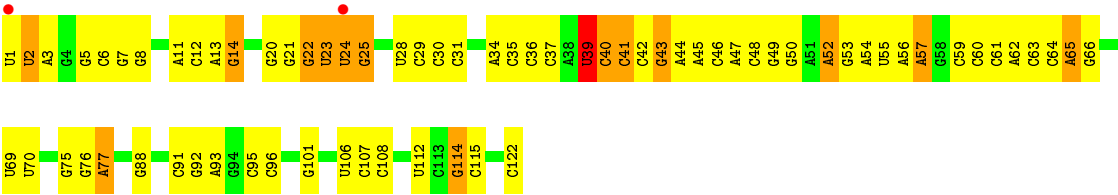
Chain 0: 



G2870	U2671	C2672	U2673	C2676	G2679	A2680	A2681	C2682	A2689	U2690	A2691	U2692	A2693	A2694	C2695	G2696	A2697	G2698	G2709	U2710	U2711	G2712	G2713	G2716	U2717	C2718	A2719	U2720	G2721	G2722	G2723	U2726	A2727	G2734	U2735	U2736	C2737	C2747	U2748	U2749	G2750	G2754	G2755	U2756	A2757	G2758	C2759	C2762	G2763									
A2577	G2578	U2586	U2587	U2588	U2589	U2590	C2591	C2592	C2593	C2594	U2595	A2596	U2597	U2598	U2599	A2600	A2601	G2602	G2603	A2604	U2607	C2608	G2613	U2614	U2615	G2616	U2617	U2621	G2630	G2634	A2635	C2636	A2637	G2638	C2644	U2645	U2646	A2649	U2652	A2653	U2654	U2655	U2656	A2657	U2658	A	U	G2667	G2668	G2669								
A2483	U2484	A2488	G2489	A2490	C2491	U2492	C2493	C2498	U2499	C2502	A2503	U2504	U2505	A2506	C2507	U2508	U2509	C2510	A2511	U2512	U2513	A2521	G2522	U2523	U2524	G2525	U2526	U2527	U2528	U2529	C2533	C2536	G2537	U2541	C2542	G2543	G2544	C2547	C2548	C2552	A2553	C2559	U2563	G2564	C2565	A2566	C2570											
G2385	U2386	U2387	C2388	U2389	A2401	A2402	C2403	G2404	A2408	G2412	A2413	A2414	A2415	G2416	U2419	G2420	G2421	U2422	G2426	A2433	A2434	U2435	U2436	A2437	G2438	C2443	U2444	U2445	G2446	G2453	A2456	U2461	G2462	A2465	G2466	A2467	A2468	A2469	C2472	C2476	C2477	U2478	A2479	G2480	G2482													
C2309	C2313	G2314	C2315	G2316	C2317	U2320	A2321	C2326	C2329	U2330	C2331	A2332	G2333	U2334	C2335	G2336	G2337	G2338	A	C	A	G	A2344	A2345	C2346	C2347	C2348	A2353	A2354	G2355	A2356	G2359	C2360	A2361	G2362	A2363	A2364	A2367	A2368	A2369	A2372	U2373	G2374	A2375	C2376	G2379	A2380	C2381										
C	C	G	U	C	G	U	G	U	C	C	G2237	A2238	C2239	U2240	C2241	U2242	C2243	C2248	G2249	G2250	G2251	A2252	G2253	A2254	A2255	C2256	G2257	A2258	G2263	A2264	U2265	A2266	C2269	G2270	G2271	C2272	G2273	A2274	G2275	U2276	U2277	C2281	U2282	U2290	A2291	G2299	A2300	A2301	A2302									
U	A	G	G	A	A	U	C	U	A	C	A	G	A	G	U	A	C	C	G	G	C	G	C	G	U	U	A	G	C	A	C	C	C	C	C	C	C	A	A	A	A	U	U	A	C	C												
G1856	A1857	A1858	G1863	U1863	U1871	C1872	G1873	G1877	G1878	U1879	U1883	A1884	A1885	A1886	U1889	U1903	A1904	U1905	A1909	A1919	C1920	A1921	A1922	G1925	G1926	A1927	C1940	A1941	A1942	C1943	G1947	G1948	G1949	G1950	U1951	U	A	C	U	U	C	C	C	C	C													
G1752	A1759	U1760	C1761	C1762	C1763	U1766	A1767	C1768	U1769	U1770	C1772	G1773	G1774	A1778	A1779	C1787	U1788	G1692	G1697	A1603	C1604	A1605	A1606	U1702	G1795	A1796	A1797	C1798	G1805	G1806	C1714	C1818	G1819	G1820	U1825	C1826	A1829	C1830	G1834	C1835	U1838	A1839	A1840	A1845	U1846	A1847	G1848	C1853	C1854	G1855								
C1554	G1555	A1559	U1561	C1562	C1566	U1668	G1586	U1587	U1588	G1589	C1592	C1593	C1594	C1595	U1596	A1597	A1598	A1603	C1604	G1605	A1606	A1607	C1613	G1614	U1615	A1616	C1617	G1622	C1623	A1624	U1625	A1626	G1627	U1722	G1723	U1724	C1725	G1730	A1731	A1732	A1733	G1734	C1735	A1736	G1739	U1740	A1845	U1846	A1847	G1848	C1853	C1854	G1855					
G1441	A1442	U1446	U1447	C1450	C1451	U1461	U1462	C1474	C1477	U1478	A1482	C1483	A1484	A1485	A1486	A1487	U1488	C1495	U1503	A1504	U1505	U1506	C1513	G1514	G1515	C1516	G1520	C1521	A1522	G1523	U1524	G1525	A1526	C1527	A1528	G1529	U1535	G1536	A1537	C1538	U1539	C1545	G1546	C1552	U1553	C1554	C1555											
G1351	A1352	C1353	U1358	U1359	C1360	C1366	A1372	G1373	C1374	A1375	G1376	C1377	A1378	A1379	U1380	A1381	U1382	U1383	G1384	G1385	G1386	G1387	G1391	A1392	C1393	C1394	C1395	C1396	C1397	C1513	G1514	G1515	C1622	C1623	A1624	U1625	A1626	G1627	U1722	G1723	U1724	C1725	G1730	A1731	A1732	A1733	G1734	C1735	A1736	G1739	U1740	A1845	U1846	A1847	G1848	C1853	C1854	G1855



● Molecule 31: 5S RIBOSOMAL RNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	213.16Å 300.03Å 576.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 2.90 85.91 – 2.41	Depositor EDS
% Data completeness (in resolution range)	92.2 (49.98-2.90) 92.3 (85.91-2.41)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.171 , 0.220 0.165 , 0.212	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 81.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99122	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.32	0/1786	0.64	0/2408
2	B	0.32	0/2690	0.64	0/3652
3	C	0.36	0/1885	0.63	0/2552
4	D	0.32	0/1111	0.56	0/1498
5	E	0.33	0/1382	0.56	0/1880
6	F	0.34	0/901	0.58	0/1224
7	G	0.31	0/241	0.49	0/324
8	H	0.33	0/1302	0.63	0/1743
9	I	0.29	0/526	0.51	0/716
10	J	0.36	0/1136	0.60	0/1530
11	K	0.35	0/1004	0.67	0/1351
12	L	0.33	0/1130	0.63	0/1509
13	M	0.35	0/1582	0.61	0/2116
14	N	0.30	0/1474	0.62	0/1999
15	O	0.34	0/874	0.59	0/1181
16	P	0.32	0/1147	0.51	0/1528
17	Q	0.33	0/749	0.65	0/1005
18	R	1.26	7/1172 (0.6%)	1.10	6/1578 (0.4%)
19	S	0.32	0/648	0.55	0/875
20	T	0.33	0/958	0.64	0/1289
21	U	0.33	0/417	0.59	0/562
22	V	0.33	0/502	0.52	0/675
23	W	0.34	0/1219	0.63	0/1655
24	X	0.35	0/664	0.60	0/895
25	Y	0.36	0/1146	0.62	0/1536
26	Z	0.37	0/584	0.60	0/781
27	1	0.39	0/438	0.59	0/578
28	2	0.34	0/401	0.60	0/529
29	3	0.36	0/771	0.55	0/1024
30	0	0.37	0/65957	0.68	13/102867 (0.0%)
31	9	0.32	0/2904	0.68	1/4526 (0.0%)
All	All	0.38	7/98701 (0.0%)	0.67	20/147586 (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	28
31	9	0	1
All	All	1	30

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	27.29	2.86	1.50
18	R	150	PRO	CA-C	-18.25	1.16	1.52
18	R	150	PRO	CG-CD	13.93	1.96	1.50
18	R	150	PRO	C-O	11.88	1.47	1.23
18	R	150	PRO	N-CA	11.37	1.66	1.47

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.47	55.83	112.00
18	R	150	PRO	N-CA-C	-19.40	61.65	112.10
18	R	150	PRO	CA-N-CD	12.30	128.92	111.70
18	R	150	PRO	N-CA-CB	10.97	116.46	103.30
18	R	150	PRO	CA-C-O	-8.51	99.79	120.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	131	A	Sidechain
30	0	220	C	Sidechain
30	0	333	G	Sidechain
30	0	48	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	63	0
2	B	2625	0	2533	89	0
3	C	1860	0	1813	59	0
4	D	1094	0	1085	45	0
5	E	1357	0	1266	29	0
6	F	890	0	843	26	0
7	G	240	0	231	8	0
8	H	1282	0	1292	33	0
9	I	519	0	500	23	0
10	J	1120	0	1098	32	0
11	K	994	0	1027	32	0
12	L	1118	0	1076	29	0
13	M	1558	0	1573	42	0
14	N	1445	0	1401	51	0
15	O	865	0	873	18	0
16	P	1136	0	1123	24	0
17	Q	735	0	729	21	0
18	R	1149	0	1122	37	0
19	S	641	0	605	10	0
20	T	950	0	924	21	0
21	U	410	0	364	8	0
22	V	499	0	511	17	0
23	W	1196	0	1137	56	0
24	X	654	0	653	18	0
25	Y	1130	0	1133	23	0
26	Z	573	0	532	15	0
27	1	431	0	426	23	0
28	2	396	0	413	15	0
29	3	755	0	728	18	0
30	0	59020	0	29811	1159	0
31	9	2599	0	1325	100	0
32	0	87	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Y	1	0	0	0	0
33	0	10	0	0	4	0
33	3	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	2	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	1	0
33	O	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	93	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0
34	9	3	0	0	0	0
34	A	3	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	67	0	0	0	0
35	9	2	0	0	0	0
35	C	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	2	0	0	0	0
38	0	5929	0	0	185	0
38	1	63	0	0	4	0
38	2	50	0	0	1	0
38	3	62	0	0	3	0
38	9	147	0	0	7	0
38	A	116	0	0	5	0
38	B	141	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	C	170	0	0	13	0
38	D	44	0	0	3	0
38	E	45	0	0	2	0
38	F	27	0	0	2	0
38	G	19	0	0	1	0
38	H	63	0	0	7	0
38	I	8	0	0	3	0
38	J	53	0	0	1	0
38	K	56	0	0	5	0
38	L	85	0	0	6	0
38	M	123	0	0	2	0
38	N	55	0	0	5	0
38	O	43	0	0	3	0
38	P	67	0	0	2	0
38	Q	50	0	0	3	0
38	R	85	0	0	1	0
38	S	33	0	0	2	0
38	T	34	0	0	2	0
38	U	27	0	0	2	0
38	V	13	0	0	2	0
38	W	69	0	0	4	0
38	X	25	0	0	2	0
38	Y	95	0	0	5	0
38	Z	26	0	0	3	0
All	All	99122	0	59913	1941	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 13.

The worst 5 of 1941 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:CG	18:R:150:PRO:CD	1.96	1.43
30:0:1160:G:C5'	30:0:1161:A:H5'	1.77	1.12
30:0:871:G:C8	30:0:871:G:H5'	1.84	1.11
30:0:871:G:H8	30:0:871:G:H5'	1.09	1.10
31:9:56:A:H2'	31:9:57:A:H5''	1.31	1.10

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/240 (98%)	211 (90%)	18 (8%)	6 (3%)	5	20
2	B	335/338 (99%)	306 (91%)	25 (8%)	4 (1%)	13	40
3	C	244/246 (99%)	224 (92%)	19 (8%)	1 (0%)	34	66
4	D	134/177 (76%)	113 (84%)	16 (12%)	5 (4%)	3	13
5	E	170/178 (96%)	161 (95%)	9 (5%)	0	100	100
6	F	117/120 (98%)	106 (91%)	8 (7%)	3 (3%)	5	20
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/177 (88%)	147 (94%)	8 (5%)	1 (1%)	25	58
9	I	68/162 (42%)	54 (79%)	13 (19%)	1 (2%)	10	34
10	J	140/145 (97%)	130 (93%)	9 (6%)	1 (1%)	22	54
11	K	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	19	51
12	L	141/165 (86%)	125 (89%)	14 (10%)	2 (1%)	11	36
13	M	192/196 (98%)	182 (95%)	9 (5%)	1 (0%)	29	61
14	N	184/187 (98%)	169 (92%)	12 (6%)	3 (2%)	9	32
15	O	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
16	P	141/149 (95%)	141 (100%)	0	0	100	100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
18	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
19	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
20	T	117/120 (98%)	110 (94%)	7 (6%)	0	100	100
21	U	51/67 (76%)	45 (88%)	5 (10%)	1 (2%)	7	27
22	V	63/71 (89%)	60 (95%)	2 (3%)	1 (2%)	9	32
23	W	152/154 (99%)	146 (96%)	4 (3%)	2 (1%)	12	37
24	X	80/92 (87%)	75 (94%)	4 (5%)	1 (1%)	12	37
25	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	71/116 (61%)	62 (87%)	7 (10%)	2 (3%)	5	19
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	88 (98%)	2 (2%)	0	100	100
All	All	3705/4472 (83%)	3447 (93%)	222 (6%)	36 (1%)	15	45

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
4	D	137	PRO
6	F	101	ALA
14	N	154	LEU
14	N	183	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/182 (98%)	170 (95%)	9 (5%)	24	57
2	B	282/283 (100%)	263 (93%)	19 (7%)	16	43
3	C	193/193 (100%)	176 (91%)	17 (9%)	10	30
4	D	117/148 (79%)	110 (94%)	7 (6%)	19	49
5	E	152/156 (97%)	149 (98%)	3 (2%)	55	82
6	F	93/94 (99%)	91 (98%)	2 (2%)	52	81
7	G	27/282 (10%)	27 (100%)	0	100	100
8	H	134/145 (92%)	129 (96%)	5 (4%)	34	68
9	I	58/130 (45%)	57 (98%)	1 (2%)	60	86
10	J	118/121 (98%)	110 (93%)	8 (7%)	16	42
11	K	106/106 (100%)	104 (98%)	2 (2%)	57	84
12	L	113/127 (89%)	110 (97%)	3 (3%)	44	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	158/160 (99%)	151 (96%)	7 (4%)	28	61
14	N	149/150 (99%)	142 (95%)	7 (5%)	26	59
15	O	93/94 (99%)	92 (99%)	1 (1%)	73	92
16	P	113/117 (97%)	111 (98%)	2 (2%)	59	85
17	Q	79/80 (99%)	76 (96%)	3 (4%)	33	67
18	R	117/122 (96%)	111 (95%)	6 (5%)	24	56
19	S	71/74 (96%)	70 (99%)	1 (1%)	67	89
20	T	105/106 (99%)	97 (92%)	8 (8%)	13	36
21	U	44/53 (83%)	43 (98%)	1 (2%)	50	80
22	V	51/57 (90%)	50 (98%)	1 (2%)	55	82
23	W	130/130 (100%)	126 (97%)	4 (3%)	40	74
24	X	66/74 (89%)	62 (94%)	4 (6%)	18	48
25	Y	120/196 (61%)	116 (97%)	4 (3%)	38	72
26	Z	60/94 (64%)	60 (100%)	0	100	100
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	49	79
29	3	79/79 (100%)	78 (99%)	1 (1%)	69	90
All	All	3095/3646 (85%)	2968 (96%)	127 (4%)	30	64

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	62	HIS
11	K	10	GLN
24	X	27	ASP
8	H	87	LYS
10	J	46	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	58	GLN
16	P	66	GLN
27	1	28	HIS
13	M	77	HIS

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Mol	Chain	Res	Type
14	N	107	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	242 (8%)	27 (0%)
31	9	121/122 (99%)	15 (12%)	1 (0%)
All	All	2866/3045 (94%)	257 (8%)	28 (0%)

5 of 257 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G

5 of 28 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	1237	U
30	0	1377	C
30	0	2718	C
30	0	1246	A
30	0	1352	A

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	OMU	0	2587	30	14,22,23	0.99	1 (7%)	14,31,34	1.14	1 (7%)
30	1MA	0	628	30	15,25,26	0.79	0	15,37,40	1.43	2 (13%)
30	OMG	0	2588	30	18,26,27	1.07	2 (11%)	20,38,41	2.57	5 (25%)
30	PSU	0	2621	30	17,21,22	1.76	3 (17%)	20,30,33	5.44	5 (25%)
30	UR3	0	2619	30	14,22,23	0.73	0	15,32,35	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	OMU	0	2587	30	-	0/7/27/28	0/2/2/2
30	1MA	0	628	30	-	0/3/25/26	0/3/3/3
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	UR3	0	2619	30	-	0/5/25/26	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-5.68	1.47	1.52
30	0	2588	OMG	C6-N1	3.39	1.38	1.33
30	0	2621	PSU	C4-N3	2.80	1.37	1.33
30	0	2587	OMU	C4-N3	2.63	1.37	1.33
30	0	2621	PSU	C2-N1	2.44	1.43	1.38

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-17.38	114.61	128.43
30	0	2621	PSU	C4-N3-C2	14.15	127.09	115.14
30	0	2588	OMG	C5-C6-N1	-8.53	111.77	123.43
30	0	2621	PSU	C5-C4-N3	-8.13	114.89	125.36
30	0	2588	OMG	C6-N1-C2	5.77	125.11	115.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides 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, 95th 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 ²)	Q<0.9
1	A	237/240 (98%)	-0.39	5 (2%) 63 61	35, 59, 97, 117	0
2	B	337/338 (99%)	-0.60	1 (0%) 94 94	36, 60, 90, 100	0
3	C	246/246 (100%)	-0.58	0 100 100	30, 51, 75, 89	0
4	D	140/177 (79%)	1.08	29 (20%) 1 0	73, 108, 135, 146	0
5	E	172/178 (96%)	-0.51	1 (0%) 89 89	51, 74, 96, 104	0
6	F	119/120 (99%)	0.13	5 (4%) 36 32	55, 78, 111, 125	0
7	G	29/348 (8%)	0.48	2 (6%) 16 13	83, 103, 109, 112	0
8	H	160/177 (90%)	0.03	9 (5%) 24 20	50, 73, 106, 113	0
9	I	70/162 (43%)	3.13	45 (64%) 0 0	137, 156, 173, 174	0
10	J	142/145 (97%)	-0.57	1 (0%) 87 87	41, 58, 78, 97	0
11	K	132/132 (100%)	-0.71	0 100 100	40, 55, 79, 82	0
12	L	145/165 (87%)	0.07	7 (4%) 30 27	34, 73, 123, 136	0
13	M	194/196 (98%)	-0.71	0 100 100	35, 50, 66, 73	0
14	N	186/187 (99%)	-0.08	5 (2%) 54 50	52, 75, 123, 135	0
15	O	115/116 (99%)	-0.60	0 100 100	45, 61, 78, 84	0
16	P	143/149 (95%)	-0.64	0 100 100	46, 61, 77, 84	0
17	Q	95/96 (98%)	-0.60	0 100 100	44, 55, 71, 86	0
18	R	150/155 (96%)	-0.73	0 100 100	39, 52, 71, 86	0
19	S	81/85 (95%)	-0.51	1 (1%) 79 79	49, 65, 86, 98	0
20	T	119/120 (99%)	-0.35	5 (4%) 36 32	47, 62, 89, 123	0
21	U	53/67 (79%)	-0.62	0 100 100	48, 62, 79, 88	0
22	V	65/71 (91%)	0.69	8 (12%) 4 3	55, 80, 129, 134	0
23	W	154/154 (100%)	-0.52	1 (0%) 89 89	41, 57, 74, 88	0
24	X	82/92 (89%)	-0.19	3 (3%) 41 37	49, 67, 90, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	-0.76	1 (0%) 87 87	31, 50, 73, 94	0
26	Z	73/116 (62%)	0.73	12 (16%) 1 1	63, 87, 101, 106	0
27	1	56/57 (98%)	-0.66	0 100 100	32, 39, 45, 53	0
28	2	46/50 (92%)	-0.12	3 (6%) 18 14	41, 69, 104, 115	0
29	3	92/92 (100%)	-0.38	0 100 100	44, 68, 81, 91	0
30	0	2749/2923 (94%)	-0.67	8 (0%) 94 94	28, 53, 96, 172	0
31	9	122/122 (100%)	-0.83	2 (1%) 72 71	45, 74, 96, 153	0
All	All	6646/7517 (88%)	-0.45	154 (2%) 60 58	28, 58, 108, 174	0

The worst 5 of 154 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	74	ILE	10.1
22	V	39	ALA	8.0
22	V	1	THR	7.6
4	D	63	ILE	7.5
9	I	71	ALA	7.5

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, 95th 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 ²)	Q<0.9
30	OMG	0	2588	24/25	0.98	0.12	38,42,43,43	0
30	UR3	0	2619	21/22	0.98	0.14	43,45,48,49	0
30	OMU	0	2587	21/22	0.99	0.13	40,43,46,49	0
30	PSU	0	2621	20/21	0.99	0.14	35,38,47,48	0
30	1MA	0	628	23/24	0.99	0.15	35,38,38,39	0

6.3 Carbohydrates ⓘ

There are no monosaccharides 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, 95th 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 ²)	Q<0.9
34	SR	0	9006	1/1	0.11	1.24	200,200,200,200	0
34	SR	0	8922	1/1	0.41	0.22	170,170,170,170	0
34	SR	0	8994	1/1	0.41	0.98	200,200,200,200	0
35	NA	0	8522	1/1	0.54	0.38	83,83,83,83	0
35	NA	0	8562	1/1	0.55	0.80	74,74,74,74	0
34	SR	0	8991	1/1	0.58	0.09	197,197,197,197	0
32	MG	0	8089	1/1	0.58	0.12	57,57,57,57	0
35	NA	0	8546	1/1	0.60	1.30	112,112,112,112	0
34	SR	0	8919	1/1	0.61	0.13	192,192,192,192	0
34	SR	0	8986	1/1	0.61	0.17	200,200,200,200	0
35	NA	0	8555	1/1	0.64	0.49	51,51,51,51	0
34	SR	B	8987	1/1	0.67	0.49	200,200,200,200	0
35	NA	0	8570	1/1	0.71	0.13	60,60,60,60	0
35	NA	0	8518	1/1	0.71	0.48	94,94,94,94	0
35	NA	0	8563	1/1	0.71	0.36	94,94,94,94	0
34	SR	0	9001	1/1	0.71	0.10	173,173,173,173	0
35	NA	9	8572	1/1	0.72	0.33	111,111,111,111	0
34	SR	0	8997	1/1	0.72	0.46	200,200,200,200	0
32	MG	0	8037	1/1	0.74	0.33	90,90,90,90	0
34	SR	0	8982	1/1	0.75	1.22	200,200,200,200	0
34	SR	9	8980	1/1	0.76	0.15	200,200,200,200	0
34	SR	0	8993	1/1	0.77	0.09	182,182,182,182	0
32	MG	0	8091	1/1	0.77	0.06	62,62,62,62	0
34	SR	0	8988	1/1	0.77	0.13	173,173,173,173	0
34	SR	0	8938	1/1	0.78	0.13	192,192,192,192	0
35	NA	0	8560	1/1	0.78	0.38	83,83,83,83	0
35	NA	0	8525	1/1	0.78	0.19	78,78,78,78	0
35	NA	0	8505	1/1	0.80	1.03	49,49,49,49	0
34	SR	0	8944	1/1	0.80	0.13	182,182,182,182	0
35	NA	0	8506	1/1	0.81	0.25	68,68,68,68	0
34	SR	0	8959	1/1	0.81	0.20	174,174,174,174	0
34	SR	0	8976	1/1	0.81	0.25	200,200,200,200	0
34	SR	0	8947	1/1	0.82	0.27	200,200,200,200	0
35	NA	0	8550	1/1	0.82	0.52	61,61,61,61	0
35	NA	0	8544	1/1	0.83	0.20	75,75,75,75	0
32	MG	0	8036	1/1	0.83	0.10	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8996	1/1	0.84	1.02	200,200,200,200	0
35	NA	0	8571	1/1	0.84	0.09	77,77,77,77	0
32	MG	0	8081	1/1	0.85	0.18	74,74,74,74	0
35	NA	J	8538	1/1	0.85	0.16	60,60,60,60	0
35	NA	0	8528	1/1	0.85	0.29	58,58,58,58	0
35	NA	0	8557	1/1	0.86	0.10	52,52,52,52	0
34	SR	0	8957	1/1	0.86	0.10	196,196,196,196	0
34	SR	0	8927	1/1	0.87	0.06	151,151,151,151	0
34	SR	A	8977	1/1	0.87	0.06	161,161,161,161	0
35	NA	0	8527	1/1	0.87	0.23	71,71,71,71	0
34	SR	0	8951	1/1	0.88	0.07	142,142,142,142	0
32	MG	A	8051	1/1	0.88	0.41	72,72,72,72	0
32	MG	0	8077	1/1	0.88	0.07	49,49,49,49	0
32	MG	0	8062	1/1	0.88	0.17	50,50,50,50	0
34	SR	0	8928	1/1	0.88	0.06	135,135,135,135	0
34	SR	0	8998	1/1	0.89	0.13	175,175,175,175	0
32	MG	0	8071	1/1	0.89	0.19	71,71,71,71	0
34	SR	0	8985	1/1	0.89	0.06	143,143,143,143	0
35	NA	0	8502	1/1	0.89	0.11	65,65,65,65	0
35	NA	0	8533	1/1	0.90	0.13	67,67,67,67	0
32	MG	0	8082	1/1	0.90	0.28	69,69,69,69	0
35	NA	0	8574	1/1	0.90	0.38	55,55,55,55	0
34	SR	0	9007	1/1	0.90	1.33	200,200,200,200	0
34	SR	0	8968	1/1	0.90	0.08	165,165,165,165	0
32	MG	0	8075	1/1	0.90	0.03	46,46,46,46	0
34	SR	0	8979	1/1	0.90	0.20	198,198,198,198	0
35	NA	0	8559	1/1	0.90	0.15	76,76,76,76	0
35	NA	0	8548	1/1	0.90	0.17	55,55,55,55	0
35	NA	C	8503	1/1	0.91	0.16	44,44,44,44	0
35	NA	0	8530	1/1	0.91	0.28	55,55,55,55	0
34	SR	0	8983	1/1	0.91	0.45	195,195,195,195	0
32	MG	0	8072	1/1	0.91	0.10	53,53,53,53	0
32	MG	0	8087	1/1	0.91	0.08	47,47,47,47	0
35	NA	S	8510	1/1	0.91	0.06	49,49,49,49	0
35	NA	0	8541	1/1	0.91	0.22	69,69,69,69	0
32	MG	0	8059	1/1	0.91	0.06	59,59,59,59	0
34	SR	0	8915	1/1	0.91	0.09	131,131,131,131	0
35	NA	0	8519	1/1	0.92	0.12	50,50,50,50	0
34	SR	0	8989	1/1	0.92	0.14	185,185,185,185	0
35	NA	0	8509	1/1	0.92	0.15	69,69,69,69	0
33	CL	0	8811	1/1	0.92	0.11	68,68,68,68	0
35	NA	Q	8540	1/1	0.92	0.08	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8960	1/1	0.92	0.05	150,150,150,150	0
34	SR	0	8958	1/1	0.92	0.11	123,123,123,123	0
34	SR	0	8984	1/1	0.92	0.04	123,123,123,123	0
34	SR	0	8942	1/1	0.92	0.08	133,133,133,133	0
32	MG	0	8083	1/1	0.92	0.11	73,73,73,73	0
35	NA	0	8561	1/1	0.92	0.49	78,78,78,78	0
32	MG	0	8066	1/1	0.92	0.15	76,76,76,76	0
34	SR	0	8962	1/1	0.93	0.05	175,175,175,175	0
32	MG	0	8038	1/1	0.93	0.10	75,75,75,75	0
37	K	0	8401	1/1	0.93	0.13	74,74,74,74	0
35	NA	0	8547	1/1	0.93	0.61	54,54,54,54	0
35	NA	0	8529	1/1	0.93	0.05	45,45,45,45	0
34	SR	S	8961	1/1	0.93	0.10	122,122,122,122	0
33	CL	O	8808	1/1	0.93	0.07	81,81,81,81	0
32	MG	0	8090	1/1	0.93	0.33	62,62,62,62	0
34	SR	0	8974	1/1	0.93	0.13	149,149,149,149	0
32	MG	T	8057	1/1	0.93	0.07	65,65,65,65	0
32	MG	0	8052	1/1	0.93	0.07	52,52,52,52	0
35	NA	0	8566	1/1	0.93	0.25	60,60,60,60	0
32	MG	0	8006	1/1	0.94	0.14	30,30,30,30	0
34	SR	0	8946	1/1	0.94	0.23	122,122,122,122	0
34	SR	0	8966	1/1	0.94	0.08	111,111,111,111	0
35	NA	0	8565	1/1	0.94	0.94	68,68,68,68	0
35	NA	0	8567	1/1	0.94	0.21	80,80,80,80	0
34	SR	0	8924	1/1	0.94	0.16	135,135,135,135	0
34	SR	0	8956	1/1	0.94	0.09	155,155,155,155	0
35	NA	0	8536	1/1	0.94	0.07	65,65,65,65	0
33	CL	A	8809	1/1	0.94	0.09	74,74,74,74	0
34	SR	0	8939	1/1	0.94	0.04	160,160,160,160	0
35	NA	0	8531	1/1	0.94	0.11	44,44,44,44	0
35	NA	0	8535	1/1	0.94	0.24	53,53,53,53	0
32	MG	0	8035	1/1	0.94	0.14	68,68,68,68	0
35	NA	0	8558	1/1	0.94	0.17	50,50,50,50	0
34	SR	0	8970	1/1	0.95	0.03	128,128,128,128	0
34	SR	0	8941	1/1	0.95	0.13	116,116,116,116	0
34	SR	0	8917	1/1	0.95	0.13	111,111,111,111	0
34	SR	A	8929	1/1	0.95	0.16	137,137,137,137	0
35	NA	0	8507	1/1	0.95	0.16	42,42,42,42	0
34	SR	0	8992	1/1	0.95	0.15	137,137,137,137	0
32	MG	0	8007	1/1	0.95	0.20	38,38,38,38	0
32	MG	0	8060	1/1	0.95	0.06	61,61,61,61	0
35	NA	0	8573	1/1	0.95	0.25	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8048	1/1	0.95	0.20	26,26,26,26	0
34	SR	0	8971	1/1	0.95	0.07	180,180,180,180	0
32	MG	K	8054	1/1	0.95	0.13	50,50,50,50	0
35	NA	0	8545	1/1	0.95	0.14	41,41,41,41	0
34	SR	0	8945	1/1	0.95	0.07	112,112,112,112	0
35	NA	0	8524	1/1	0.95	0.18	58,58,58,58	0
33	CL	0	8815	1/1	0.96	0.10	78,78,78,78	0
35	NA	0	8542	1/1	0.96	0.40	66,66,66,66	0
32	MG	0	8079	1/1	0.96	0.10	55,55,55,55	0
34	SR	0	8908	1/1	0.96	0.10	110,110,110,110	0
33	CL	L	8810	1/1	0.96	0.08	61,61,61,61	0
32	MG	9	8074	1/1	0.96	0.11	77,77,77,77	0
35	NA	0	8526	1/1	0.96	0.05	57,57,57,57	0
32	MG	0	8010	1/1	0.96	0.12	35,35,35,35	0
32	MG	0	8043	1/1	0.96	0.10	49,49,49,49	0
35	NA	0	8511	1/1	0.96	0.13	59,59,59,59	0
35	NA	0	8516	1/1	0.96	0.12	42,42,42,42	0
34	SR	0	8972	1/1	0.96	0.14	141,141,141,141	0
32	MG	0	8024	1/1	0.96	0.13	55,55,55,55	0
35	NA	0	8514	1/1	0.96	0.59	48,48,48,48	0
35	NA	0	8564	1/1	0.96	0.41	81,81,81,81	0
32	MG	0	8064	1/1	0.96	0.15	37,37,37,37	0
32	MG	0	8085	1/1	0.96	0.08	73,73,73,73	0
35	NA	9	8543	1/1	0.96	0.18	49,49,49,49	0
32	MG	0	8061	1/1	0.96	0.21	30,30,30,30	0
32	MG	0	8046	1/1	0.96	0.13	41,41,41,41	0
35	NA	0	8554	1/1	0.96	0.89	78,78,78,78	0
33	CL	J	8801	1/1	0.96	0.17	79,79,79,79	0
32	MG	0	8092	1/1	0.96	0.25	67,67,67,67	0
34	SR	0	8995	1/1	0.96	0.17	140,140,140,140	0
32	MG	0	8039	1/1	0.96	0.26	77,77,77,77	0
35	NA	0	8537	1/1	0.96	0.11	41,41,41,41	0
35	NA	0	8515	1/1	0.96	0.14	37,37,37,37	0
32	MG	0	8021	1/1	0.96	0.10	30,30,30,30	0
32	MG	0	8063	1/1	0.96	0.17	71,71,71,71	0
35	NA	0	8534	1/1	0.96	0.24	42,42,42,42	0
35	NA	0	8569	1/1	0.96	0.19	54,54,54,54	0
34	SR	0	8969	1/1	0.97	0.10	160,160,160,160	0
35	NA	0	8549	1/1	0.97	0.27	58,58,58,58	0
35	NA	0	8551	1/1	0.97	0.24	59,59,59,59	0
33	CL	R	8806	1/1	0.97	0.13	52,52,52,52	0
34	SR	0	9002	1/1	0.97	0.08	184,184,184,184	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8937	1/1	0.97	0.21	115,115,115,115	0
32	MG	0	8078	1/1	0.97	0.32	61,61,61,61	0
33	CL	0	8812	1/1	0.97	0.06	54,54,54,54	0
34	SR	0	8933	1/1	0.97	0.17	150,150,150,150	0
32	MG	0	8067	1/1	0.97	0.20	34,34,34,34	0
32	MG	0	8031	1/1	0.97	0.39	72,72,72,72	0
34	SR	9	9003	1/1	0.97	0.01	170,170,170,170	0
32	MG	0	8001	1/1	0.97	0.09	33,33,33,33	0
33	CL	0	8805	1/1	0.97	0.06	67,67,67,67	0
34	SR	0	8911	1/1	0.97	0.08	85,85,85,85	0
34	SR	0	8954	1/1	0.97	0.12	112,112,112,112	0
34	SR	0	8963	1/1	0.97	0.04	134,134,134,134	0
33	CL	J	8802	1/1	0.97	0.09	76,76,76,76	0
35	NA	0	8520	1/1	0.97	0.08	53,53,53,53	0
34	SR	0	8948	1/1	0.97	0.12	102,102,102,102	0
33	CL	0	8816	1/1	0.97	0.18	85,85,85,85	0
33	CL	N	8807	1/1	0.97	0.10	71,71,71,71	0
35	NA	0	8556	1/1	0.97	0.40	49,49,49,49	0
35	NA	0	8568	1/1	0.97	0.49	50,50,50,50	0
34	SR	0	8921	1/1	0.97	0.12	92,92,92,92	0
35	NA	0	8521	1/1	0.97	0.08	65,65,65,65	0
35	NA	R	8532	1/1	0.97	0.08	46,46,46,46	0
37	K	0	8402	1/1	0.97	0.27	87,87,87,87	0
34	SR	0	8967	1/1	0.97	0.08	132,132,132,132	0
33	CL	0	8803	1/1	0.97	0.08	62,62,62,62	0
34	SR	0	8949	1/1	0.97	0.08	119,119,119,119	0
35	NA	0	8575	1/1	0.97	0.18	86,86,86,86	0
35	NA	0	8513	1/1	0.97	0.13	58,58,58,58	0
32	MG	0	8029	1/1	0.97	0.17	48,48,48,48	0
34	SR	0	8975	1/1	0.97	0.07	135,135,135,135	0
34	SR	0	8955	1/1	0.97	0.16	200,200,200,200	0
32	MG	B	8042	1/1	0.98	0.09	50,50,50,50	0
32	MG	0	8041	1/1	0.98	0.20	31,31,31,31	0
32	MG	0	8030	1/1	0.98	0.48	69,69,69,69	0
35	NA	0	8501	1/1	0.98	0.22	44,44,44,44	0
32	MG	0	8070	1/1	0.98	0.13	45,45,45,45	0
35	NA	0	8508	1/1	0.98	0.18	39,39,39,39	0
32	MG	0	8044	1/1	0.98	0.05	53,53,53,53	0
32	MG	0	8040	1/1	0.98	0.16	96,96,96,96	0
34	SR	0	8964	1/1	0.98	0.10	139,139,139,139	0
34	SR	0	8953	1/1	0.98	0.08	157,157,157,157	0
34	SR	0	8923	1/1	0.98	0.10	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8965	1/1	0.98	0.05	124,124,124,124	0
34	SR	0	8981	1/1	0.98	0.16	153,153,153,153	0
34	SR	0	8918	1/1	0.98	0.14	85,85,85,85	0
32	MG	0	8076	1/1	0.98	0.07	42,42,42,42	0
32	MG	0	8026	1/1	0.98	0.07	37,37,37,37	0
34	SR	0	8936	1/1	0.98	0.10	94,94,94,94	0
32	MG	0	8012	1/1	0.98	0.16	25,25,25,25	0
32	MG	0	8032	1/1	0.98	0.05	46,46,46,46	0
33	CL	0	8814	1/1	0.98	0.10	60,60,60,60	0
32	MG	0	8020	1/1	0.98	0.13	43,43,43,43	0
32	MG	0	8016	1/1	0.98	0.18	60,60,60,60	0
32	MG	0	8093	1/1	0.98	0.08	35,35,35,35	0
34	SR	0	8973	1/1	0.98	0.07	137,137,137,137	0
32	MG	0	8056	1/1	0.98	0.11	51,51,51,51	0
32	MG	0	8088	1/1	0.98	0.14	42,42,42,42	0
32	MG	Y	8086	1/1	0.98	0.05	46,46,46,46	0
32	MG	0	8033	1/1	0.98	0.09	49,49,49,49	0
32	MG	0	8049	1/1	0.98	0.38	68,68,68,68	0
32	MG	0	8055	1/1	0.98	0.20	46,46,46,46	0
34	SR	0	8931	1/1	0.98	0.09	117,117,117,117	0
34	SR	B	8950	1/1	0.98	0.17	132,132,132,132	0
32	MG	0	8053	1/1	0.98	0.04	59,59,59,59	0
34	SR	0	9004	1/1	0.98	0.64	200,200,200,200	0
34	SR	0	8901	1/1	0.98	0.10	85,85,85,85	0
33	CL	0	8822	1/1	0.98	0.55	106,106,106,106	0
33	CL	M	8818	1/1	0.98	0.10	47,47,47,47	0
35	NA	0	8523	1/1	0.98	0.12	45,45,45,45	0
34	SR	0	8920	1/1	0.98	0.05	134,134,134,134	0
34	SR	F	9005	1/1	0.98	0.07	134,134,134,134	0
32	MG	0	8050	1/1	0.98	0.12	37,37,37,37	0
34	SR	0	8909	1/1	0.98	0.14	85,85,85,85	0
34	SR	0	8926	1/1	0.98	0.10	127,127,127,127	0
32	MG	0	8068	1/1	0.99	0.09	54,54,54,54	0
35	NA	0	8512	1/1	0.99	0.42	56,56,56,56	0
33	CL	0	8817	1/1	0.99	0.10	65,65,65,65	0
34	SR	0	8904	1/1	0.99	0.19	66,66,66,66	0
33	CL	J	8821	1/1	0.99	0.13	71,71,71,71	0
34	SR	0	8990	1/1	0.99	0.10	137,137,137,137	0
32	MG	0	8069	1/1	0.99	0.16	72,72,72,72	0
32	MG	0	8008	1/1	0.99	0.15	27,27,27,27	0
32	MG	0	8019	1/1	0.99	0.18	27,27,27,27	0
36	CD	Z	8703	1/1	0.99	0.09	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8034	1/1	0.99	0.07	45,45,45,45	0
32	MG	0	8058	1/1	0.99	0.07	23,23,23,23	0
36	CD	1	8702	1/1	0.99	0.10	65,65,65,65	0
34	SR	0	8935	1/1	0.99	0.10	80,80,80,80	0
32	MG	0	8002	1/1	0.99	0.07	32,32,32,32	0
32	MG	0	8017	1/1	0.99	0.22	25,25,25,25	0
34	SR	0	8916	1/1	0.99	0.06	113,113,113,113	0
33	CL	0	8813	1/1	0.99	0.06	61,61,61,61	0
33	CL	Y	8820	1/1	0.99	0.23	51,51,51,51	0
32	MG	0	8073	1/1	0.99	0.07	83,83,83,83	0
32	MG	0	8015	1/1	0.99	0.17	36,36,36,36	0
34	SR	3	8999	1/1	0.99	0.04	106,106,106,106	0
32	MG	0	8065	1/1	0.99	0.06	49,49,49,49	0
34	SR	0	9008	1/1	0.99	0.14	89,89,89,89	0
32	MG	0	8014	1/1	0.99	0.16	35,35,35,35	0
34	SR	A	8930	1/1	0.99	0.05	104,104,104,104	0
35	NA	0	8553	1/1	0.99	0.36	68,68,68,68	0
34	SR	R	8912	1/1	0.99	0.16	86,86,86,86	0
32	MG	0	8018	1/1	0.99	0.19	46,46,46,46	0
32	MG	0	8025	1/1	0.99	0.11	35,35,35,35	0
32	MG	0	8022	1/1	0.99	0.11	32,32,32,32	0
32	MG	0	8028	1/1	0.99	0.16	27,27,27,27	0
34	SR	0	9000	1/1	0.99	0.12	177,177,177,177	0
35	NA	0	8504	1/1	0.99	0.16	37,37,37,37	0
35	NA	0	8517	1/1	0.99	0.21	36,36,36,36	0
34	SR	1	8952	1/1	0.99	0.13	91,91,91,91	0
34	SR	0	8940	1/1	0.99	0.08	93,93,93,93	0
32	MG	0	8009	1/1	0.99	0.20	29,29,29,29	0
34	SR	0	8910	1/1	0.99	0.04	101,101,101,101	0
34	SR	0	8903	1/1	0.99	0.18	58,58,58,58	0
34	SR	0	8905	1/1	0.99	0.28	68,68,68,68	0
32	MG	0	8084	1/1	0.99	0.15	37,37,37,37	0
34	SR	0	8943	1/1	0.99	0.07	117,117,117,117	0
32	MG	0	8080	1/1	0.99	0.36	69,69,69,69	0
32	MG	0	8023	1/1	0.99	0.14	32,32,32,32	0
32	MG	0	8045	1/1	0.99	0.11	35,35,35,35	0
32	MG	0	8013	1/1	0.99	0.03	30,30,30,30	0
33	CL	B	8819	1/1	0.99	0.10	54,54,54,54	0
35	NA	M	8539	1/1	0.99	0.10	34,34,34,34	0
36	CD	U	8701	1/1	0.99	0.11	72,72,72,72	0
34	SR	0	8934	1/1	0.99	0.11	130,130,130,130	0
32	MG	0	8005	1/1	0.99	0.17	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	9	8978	1/1	0.99	0.08	133,133,133,133	0
32	MG	0	8027	1/1	0.99	0.09	49,49,49,49	0
33	CL	3	8804	1/1	0.99	0.06	67,67,67,67	0
32	MG	0	8047	1/1	0.99	0.28	65,65,65,65	0
36	CD	3	8704	1/1	1.00	0.07	81,81,81,81	0
34	SR	0	8907	1/1	1.00	0.14	56,56,56,56	0
32	MG	0	8004	1/1	1.00	0.17	30,30,30,30	0
32	MG	0	8011	1/1	1.00	0.16	33,33,33,33	0
35	NA	0	8552	1/1	1.00	0.28	72,72,72,72	0
36	CD	O	8705	1/1	1.00	0.07	94,94,94,94	0
32	MG	0	8003	1/1	1.00	0.18	34,34,34,34	0
34	SR	3	8932	1/1	1.00	0.12	79,79,79,79	0
34	SR	0	8914	1/1	1.00	0.27	110,110,110,110	0
34	SR	0	8902	1/1	1.00	0.11	66,66,66,66	0
34	SR	1	8913	1/1	1.00	0.09	96,96,96,96	0
34	SR	0	8925	1/1	1.00	0.12	91,91,91,91	0
34	SR	0	8906	1/1	1.00	0.21	60,60,60,60	0

6.5 Other polymers ⓘ

There are no such residues in this entry.