



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 2, 2024 – 09:47 am GMT

PDB ID : 5DM6  
Title : Crystal structure of the 50S ribosomal subunit from *Deinococcus radiodurans*  
Authors : Kaminishi, T.; Schedlbauer, A.; Ochoa-Lizarralde, B.; Connell, S.R.; Fucini, P.  
Deposited on : 2015-09-08  
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](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.

The types of validation reports are described at

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

---

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

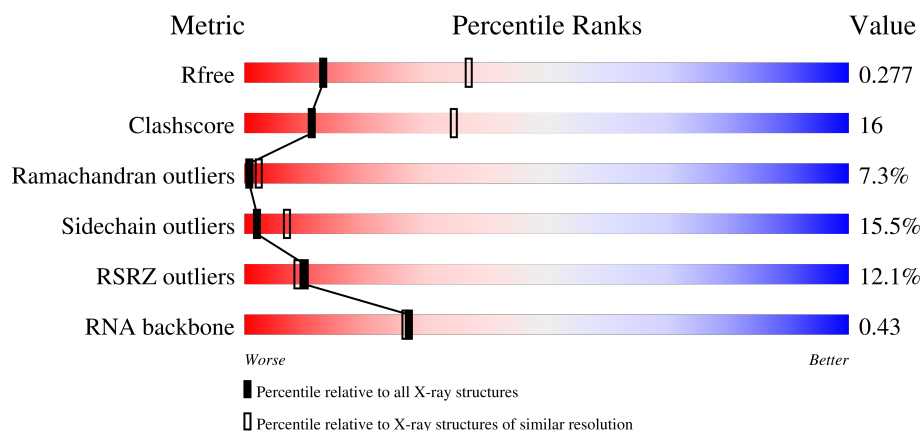
# 1 Overall quality at a glance

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))
$R_{free}$	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)
RNA backbone	3690	1039 (3.10-2.70)

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 of 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	0	224	<div> <div>26%</div> <div>54%</div> <div>38%</div> <div>8%</div> </div>
2	A	274	<div> <div>27%</div> <div>58%</div> <div>37%</div> <div>5%</div> </div>
3	B	205	<div> <div>6%</div> <div>53%</div> <div>40%</div> <div>7%</div> </div>
4	C	197	<div> <div>7%</div> <div>44%</div> <div>46%</div> <div>10%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	D	177	
6	E	171	
7	F	144	
8	G	142	
9	H	134	
10	I	141	
11	J	136	
12	K	113	
13	L	104	
14	M	109	
15	N	117	
16	O	94	
17	P	127	
18	Q	93	
19	R	110	
20	S	175	
21	T	84	
22	U	72	
23	V	66	
24	W	55	
25	Z	57	
26	1	54	
27	2	47	
28	3	65	
29	X	2881	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
30	Y	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
31	MG	X	6001	-	-	-	X
31	MG	X	6003	-	-	-	X
31	MG	X	6006	-	-	-	X
31	MG	X	6013	-	-	-	X
31	MG	X	6017	-	-	-	X
31	MG	X	6019	-	-	-	X
31	MG	X	6021	-	-	-	X
31	MG	X	6023	-	-	-	X
31	MG	X	6024	-	-	-	X
31	MG	X	6034	-	-	-	X
31	MG	X	6038	-	-	-	X
31	MG	X	6039	-	-	-	X
31	MG	X	6040	-	-	-	X
31	MG	X	6045	-	-	-	X
31	MG	X	6047	-	-	-	X
31	MG	X	6048	-	-	-	X
31	MG	X	6049	-	-	-	X
31	MG	X	6052	-	-	-	X
31	MG	X	6053	-	-	-	X
31	MG	X	6054	-	-	-	X
31	MG	X	6056	-	-	-	X
31	MG	X	6057	-	-	-	X
31	MG	X	6060	-	-	-	X
31	MG	X	6061	-	-	-	X
31	MG	X	6063	-	-	-	X
31	MG	X	6064	-	-	-	X
31	MG	X	6067	-	-	-	X
31	MG	X	6069	-	-	-	X
31	MG	X	6072	-	-	-	X
31	MG	X	6073	-	-	-	X
31	MG	X	6075	-	-	-	X
31	MG	X	6076	-	-	-	X
31	MG	X	6078	-	-	-	X
31	MG	X	6080	-	-	-	X
31	MG	X	6082	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	6085	-	-	-	X
31	MG	X	6087	-	-	-	X
31	MG	X	6088	-	-	-	X
31	MG	X	6093	-	-	-	X
31	MG	X	6098	-	-	-	X
31	MG	X	6099	-	-	-	X
31	MG	X	6100	-	-	-	X
31	MG	X	6101	-	-	-	X
31	MG	X	6105	-	-	-	X
31	MG	X	6107	-	-	-	X
31	MG	X	6108	-	-	-	X
31	MG	X	6111	-	-	-	X
31	MG	X	6112	-	-	-	X
31	MG	X	6113	-	-	-	X
31	MG	X	6114	-	-	-	X
31	MG	X	6115	-	-	-	X
31	MG	X	6116	-	-	-	X
31	MG	X	6117	-	-	-	X
31	MG	X	6118	-	-	-	X
31	MG	X	6119	-	-	-	X
31	MG	X	6120	-	-	-	X
31	MG	X	6121	-	-	-	X
31	MG	X	6122	-	-	-	X
31	MG	X	6123	-	-	-	X
31	MG	X	6124	-	-	-	X
31	MG	X	6125	-	-	-	X
31	MG	X	6126	-	-	-	X
31	MG	X	6127	-	-	-	X
31	MG	X	6128	-	-	-	X
31	MG	X	6129	-	-	-	X
31	MG	X	6131	-	-	-	X
31	MG	X	6133	-	-	-	X
31	MG	X	6134	-	-	-	X
31	MG	X	6135	-	-	-	X
31	MG	X	6137	-	-	-	X
31	MG	X	6139	-	-	-	X
31	MG	X	6140	-	-	-	X
31	MG	X	6141	-	-	-	X
31	MG	X	6142	-	-	-	X
31	MG	X	6144	-	-	-	X
31	MG	X	6146	-	-	-	X
31	MG	X	6147	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	6148	-	-	-	X
31	MG	X	6149	-	-	-	X
31	MG	X	6150	-	-	-	X
31	MG	X	6153	-	-	-	X
31	MG	X	6158	-	-	-	X
31	MG	X	6160	-	-	-	X
31	MG	X	6161	-	-	-	X
31	MG	X	6162	-	-	-	X
31	MG	X	6163	-	-	-	X
31	MG	X	6164	-	-	-	X
31	MG	X	6165	-	-	-	X
31	MG	X	6166	-	-	-	X
31	MG	X	6167	-	-	-	X
31	MG	X	6168	-	-	-	X
31	MG	X	6169	-	-	-	X
31	MG	X	6170	-	-	-	X
31	MG	X	6171	-	-	-	X
31	MG	X	6172	-	-	-	X
31	MG	X	6173	-	-	-	X
31	MG	X	6176	-	-	-	X
31	MG	X	6177	-	-	-	X
31	MG	X	6179	-	-	-	X
31	MG	X	6180	-	-	-	X
31	MG	X	6182	-	-	-	X
31	MG	X	6183	-	-	-	X
31	MG	X	6184	-	-	-	X
31	MG	X	6186	-	-	-	X
31	MG	X	6189	-	-	-	X
31	MG	X	6190	-	-	-	X
31	MG	X	6192	-	-	-	X
31	MG	Y	201	-	-	-	X
31	MG	Y	204	-	-	-	X
31	MG	Y	205	-	-	-	X

## 2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 89337 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 L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	224	Total	C	N	O	S	0	0	0
			1651	1031	302	313	5			

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	274	Total	C	N	O	S	0	0	0
			2107	1313	423	368	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	LYS	ARG	conflict	UNP Q9RXJ9
A	25	ALA	THR	conflict	UNP Q9RXJ9
A	270	LEU	ILE	conflict	UNP Q9RXJ9

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	205	Total	C	N	O	S	0	0	0
			1540	965	295	272	8			

- Molecule 4 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	197	Total	C	N	O	S	0	0	0
			1507	935	287	283	2			

- Molecule 5 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	177	Total	C	N	O	S	0	0	0
			1401	892	247	255	7			

- Molecule 6 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	171	Total	C	N	O	S	0	0	0
			1287	812	237	237	1			

- Molecule 7 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	144	Total	C	N	O	S	0	0	0
			1048	663	183	197	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	1	MET	-	expression tag	UNP Q9RSS7
F	2	ARG	-	expression tag	UNP Q9RSS7
F	3	ARG	-	expression tag	UNP Q9RSS7

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	142	Total	C	N	O	S	0	0	0
			1115	704	209	199	3			

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	141	Total	C	N	O		0	0	0
			1068	655	216	197				

- Molecule 11 is a protein called 50S ribosomal protein L16.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	136	Total	C	N	O	S	0	0	0
			1091	696	202	186	7			

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	113	Total	C	N	O	S	0	0	0
			879	541	178	158	2			

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	104	Total	C	N	O	0	0	0
			778	476	159	143			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	26	LYS	ARG	conflict	UNP Q9RSL2

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	109	Total	C	N	O	0	0	0
			867	540	171	156			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	107	GLY	-	expression tag	UNP Q9RWB4
M	108	LYS	-	expression tag	UNP Q9RWB4
M	109	ALA	-	expression tag	UNP Q9RWB4
M	110	ALA	-	expression tag	UNP Q9RWB4

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	O	94	Total	C	N	O	0	0	0
			742	465	139	138			

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	127	Total	C	N	O	S	0	0	0
			1014	639	199	174	2			

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	93	Total	C	N	O	S	0	0	0
			727	458	136	131	2			

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	110	Total	C	N	O	S	0	0	0
			826	513	160	152	1			

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	175	Total	C	N	O	S	0	0	0
			1346	849	236	255	6			

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	84	Total	C	N	O	S	0	0	0
			626	393	122	110	1			

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	72	Total	C	N	O	0	0	0
			553	341	116	96			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	67	ILE	LEU	conflict	UNP Q9RRG8

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	66	Total	C	N	O	S	0	0	0
			534	327	107	97	3			

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	57	Total	C	N	O	S	0	0	0
			453	278	93	77	5			

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1	54	Total	C	N	O	S	0	0	0
			404	256	73	74	1			

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	2	47	Total	C	N	O	S	0	0	0
			393	235	92	64	2			

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	3	65	Total	C	N	O	S	0	0	0
			509	320	104	80	5			

- Molecule 29 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	X	2780	Total	C	N	O	P	0	0	0
			59673	26617	11011	19265	2780			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1510	U	UNK	conflict	GB 11612676

- Molecule 30 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Y	122	Total	C	N	O	P	0	0	0
			2601	1161	476	842	122			

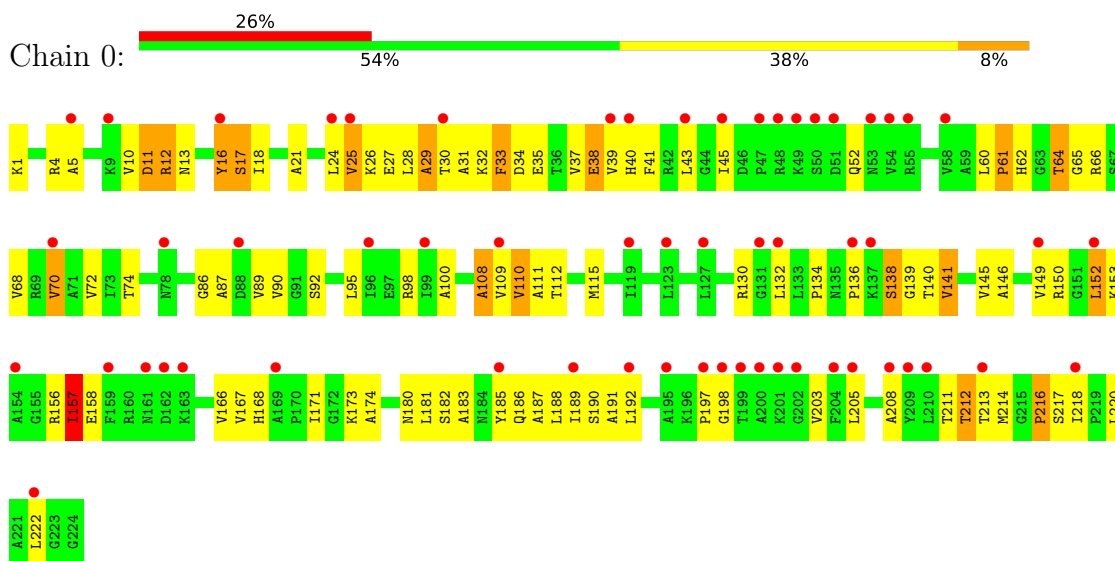
- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	M	1	Total	Mg	0	0
			1	1		
31	X	192	Total	Mg	0	0
			192	192		
31	Y	5	Total	Mg	0	0
			5	5		

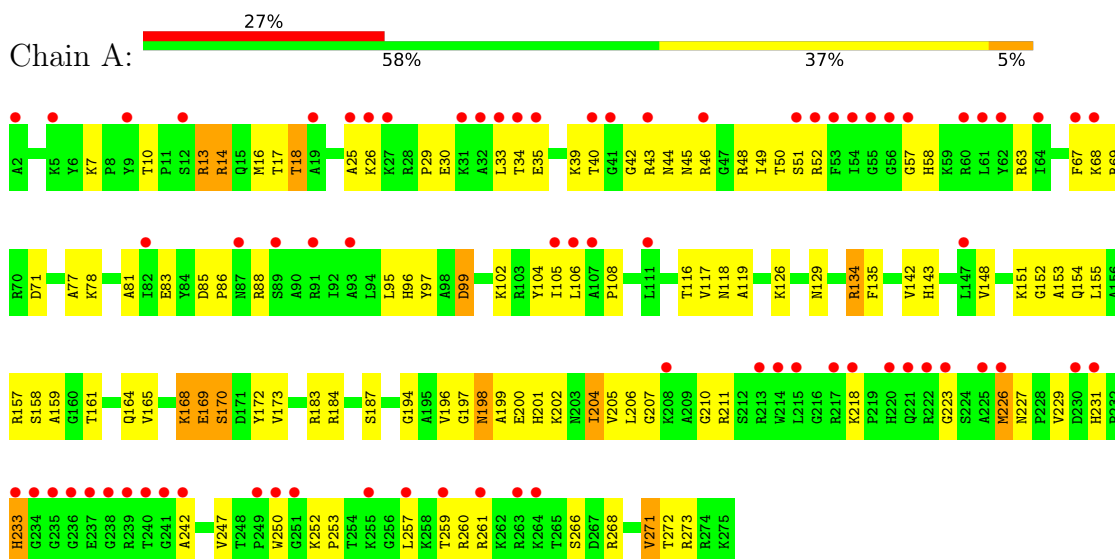
### 3 Residue-property plots

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

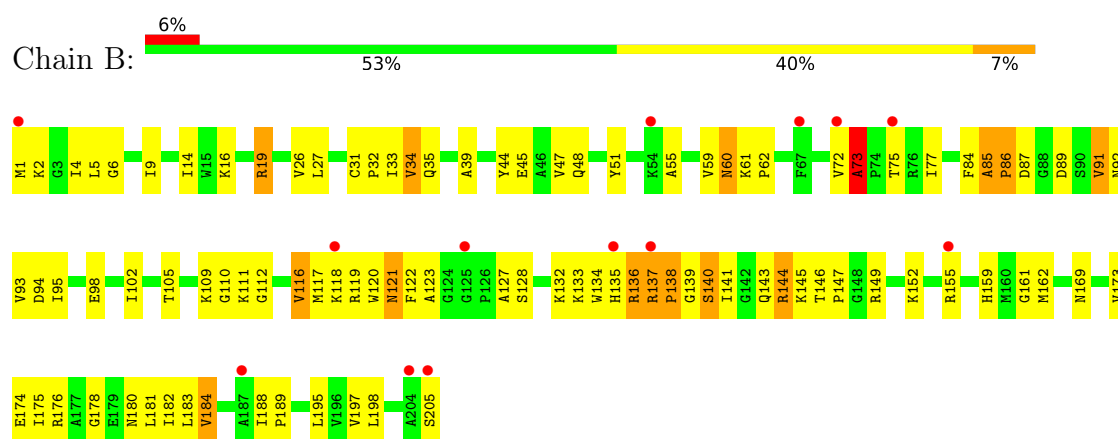
#### • Molecule 1: 50S ribosomal protein L1



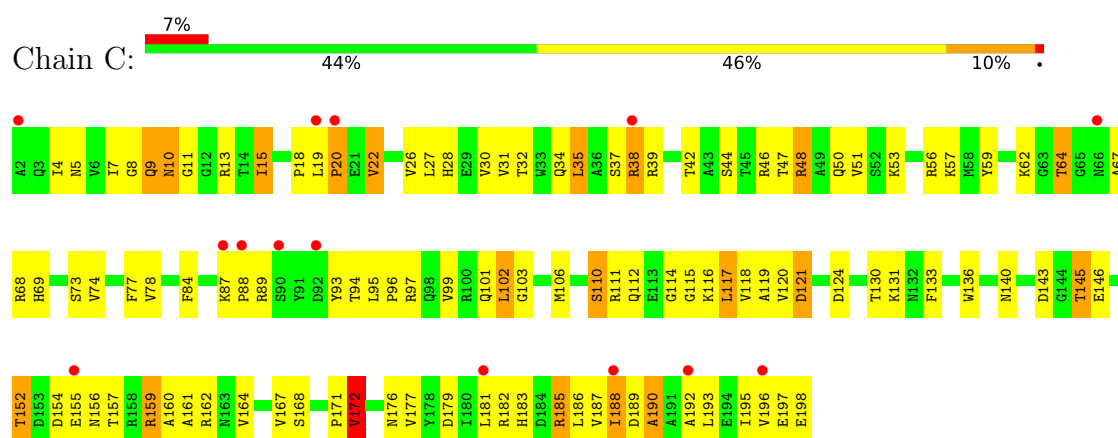
#### • Molecule 2: 50S ribosomal protein L2



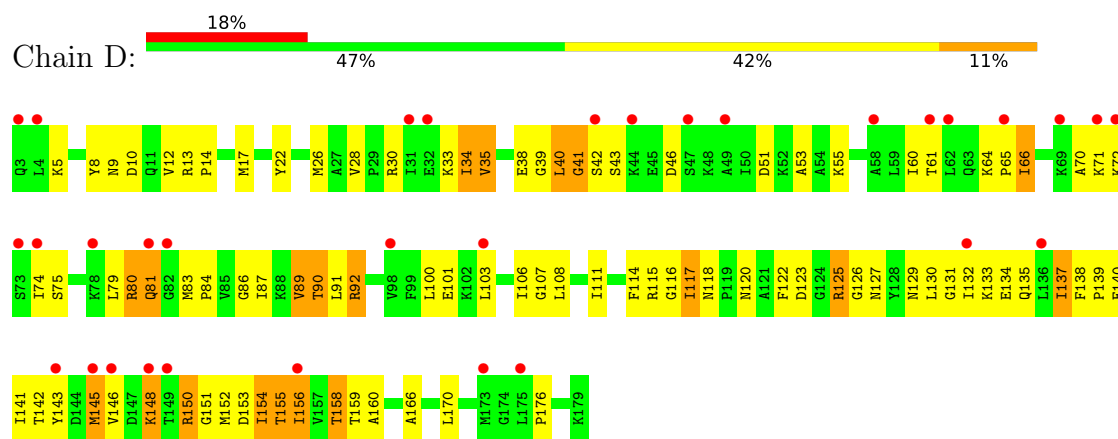
#### • Molecule 3: 50S ribosomal protein L3



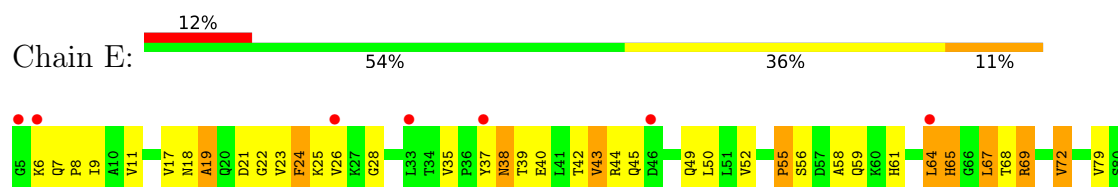
- Molecule 4: 50S ribosomal protein L4

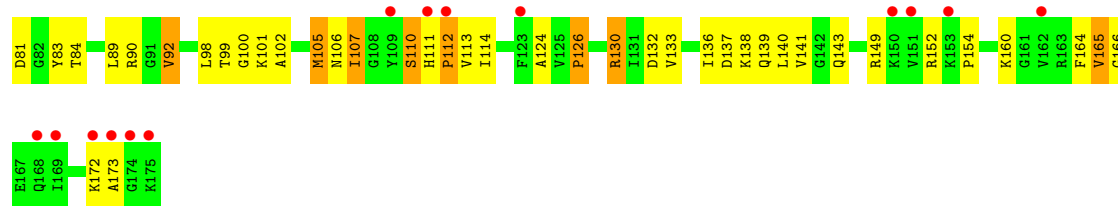


- Molecule 5: 50S ribosomal protein L5

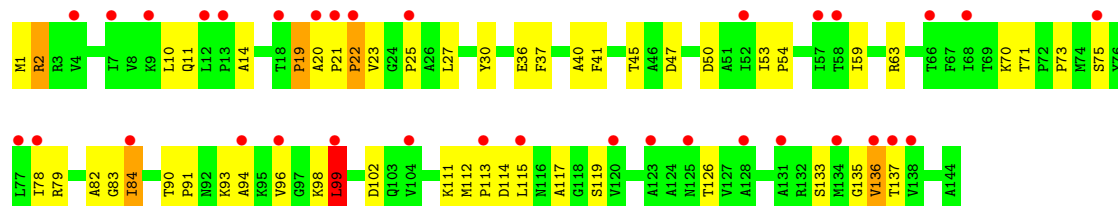


- Molecule 6: 50S ribosomal protein L6

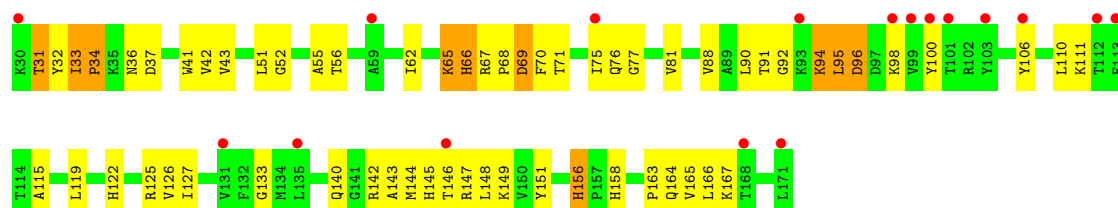




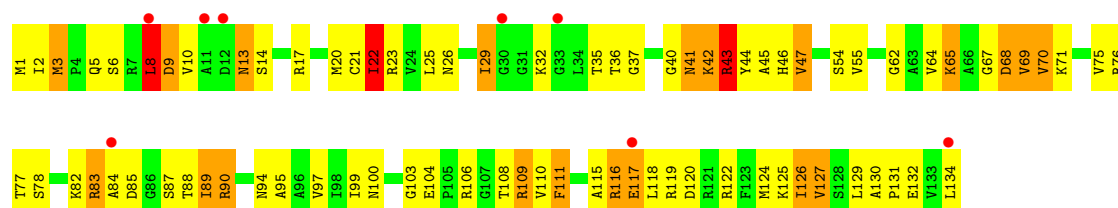
• Molecule 7: 50S ribosomal protein L11



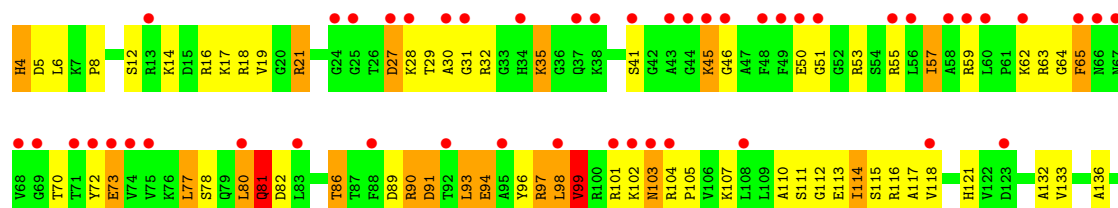
• Molecule 8: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L14

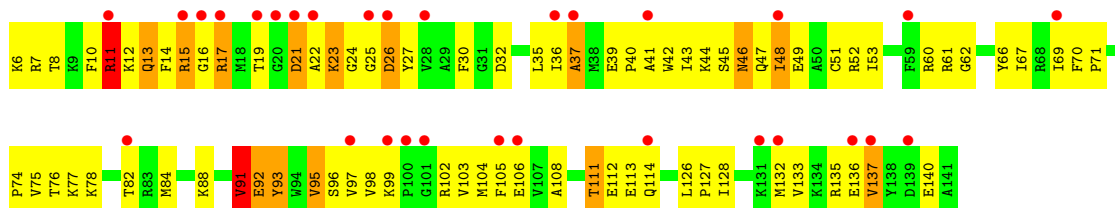


• Molecule 10: 50S ribosomal protein L15

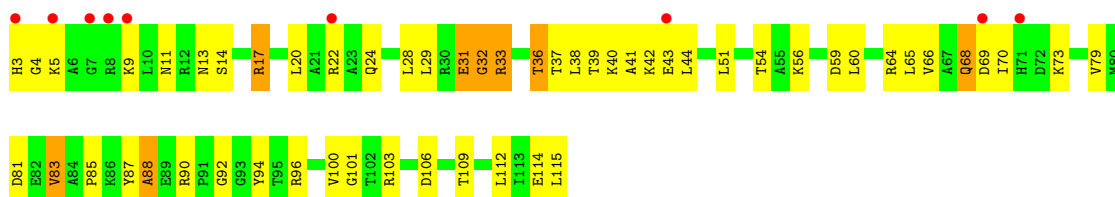




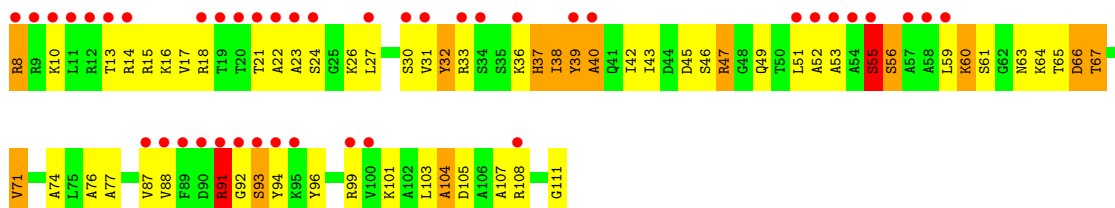
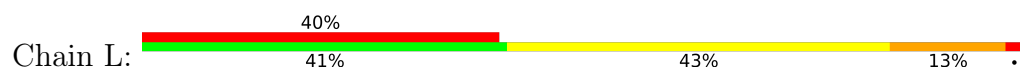
• Molecule 11: 50S ribosomal protein L16



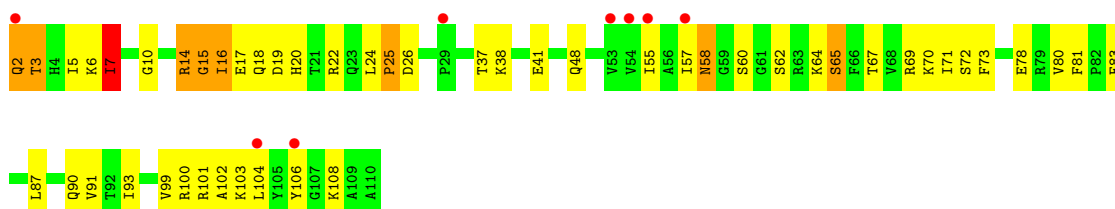
• Molecule 12: 50S ribosomal protein L17



• Molecule 13: 50S ribosomal protein L18



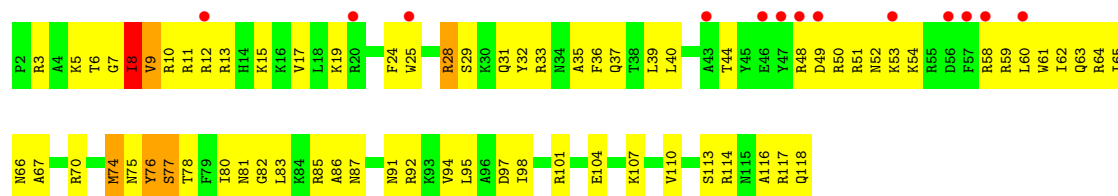
• Molecule 14: 50S ribosomal protein L19



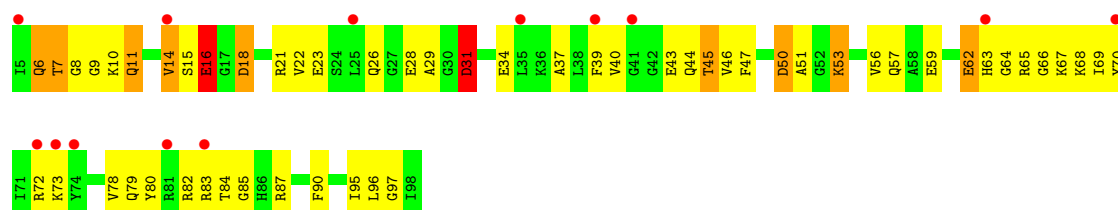
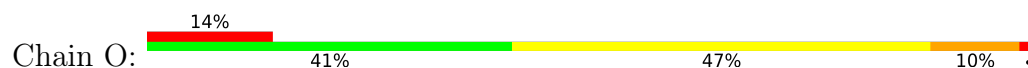
• Molecule 15: 50S ribosomal protein L20



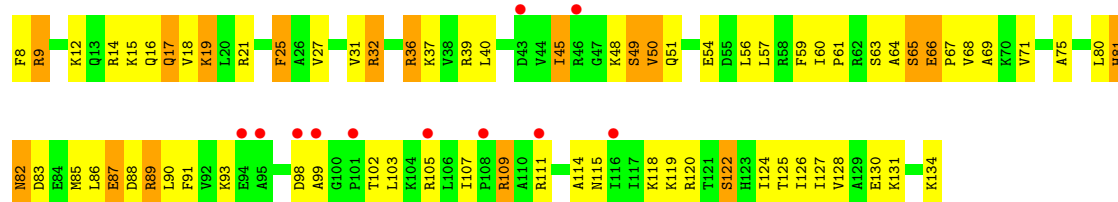
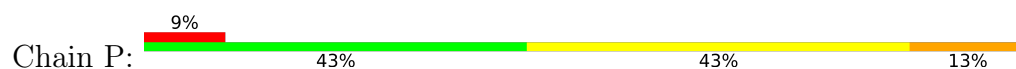




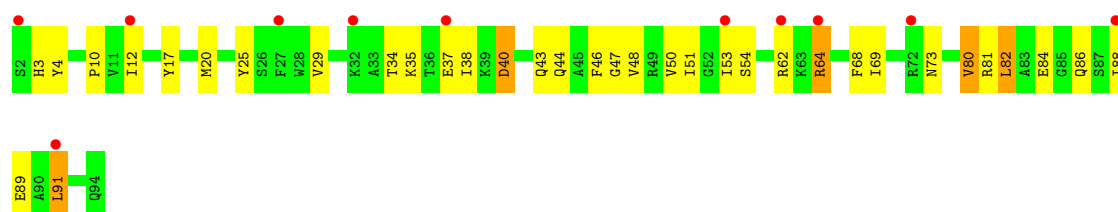
• Molecule 16: 50S ribosomal protein L21



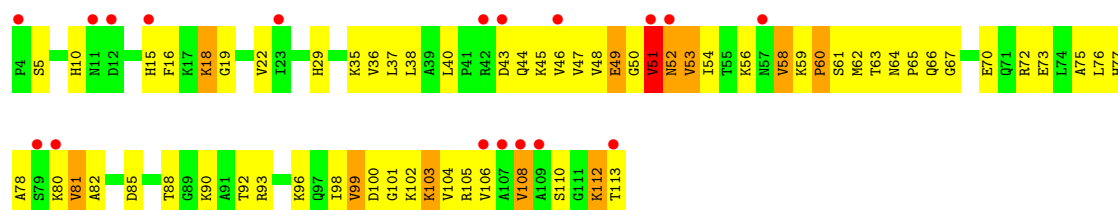
• Molecule 17: 50S ribosomal protein L22



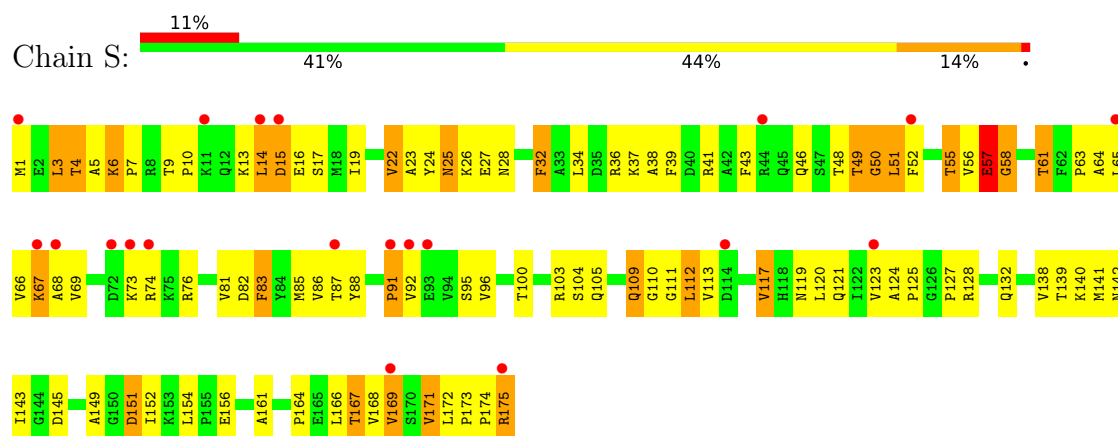
• Molecule 18: 50S ribosomal protein L23



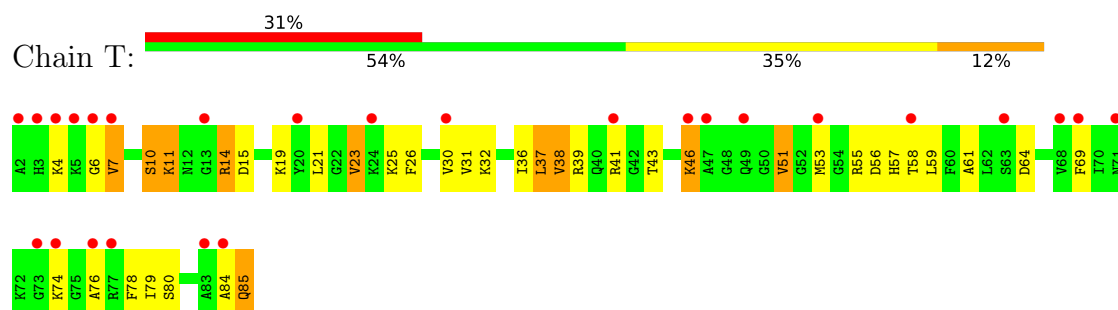
• Molecule 19: 50S ribosomal protein L24



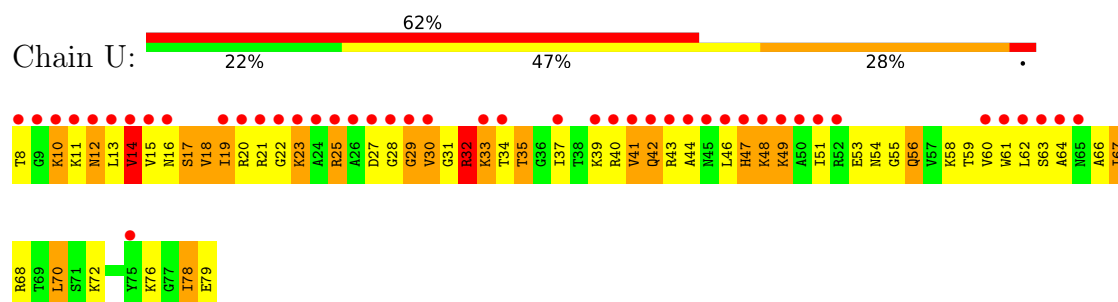
- Molecule 20: 50S ribosomal protein L25



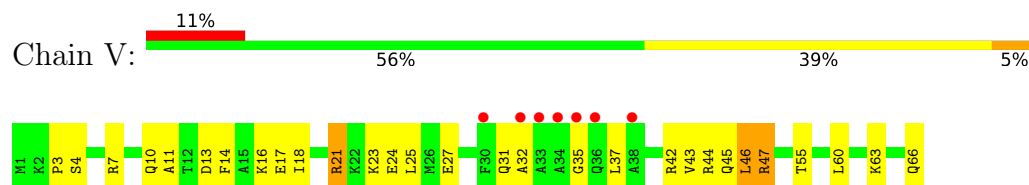
- Molecule 21: 50S ribosomal protein L27



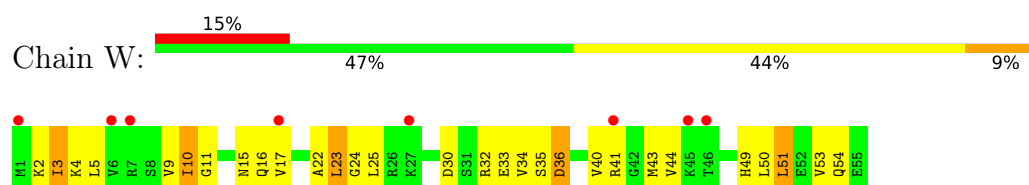
- Molecule 22: 50S ribosomal protein L28



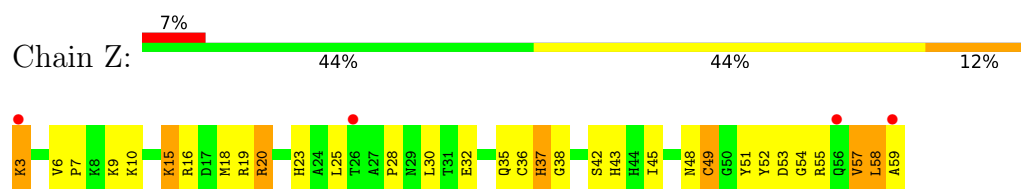
- Molecule 23: 50S ribosomal protein L29



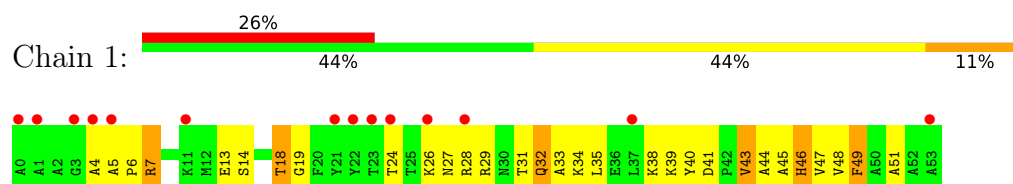
- Molecule 24: 50S ribosomal protein L30



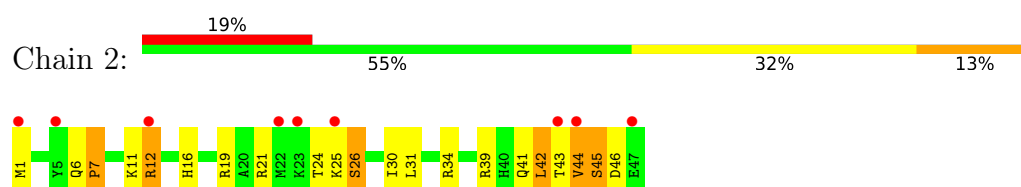
- Molecule 25: 50S ribosomal protein L32



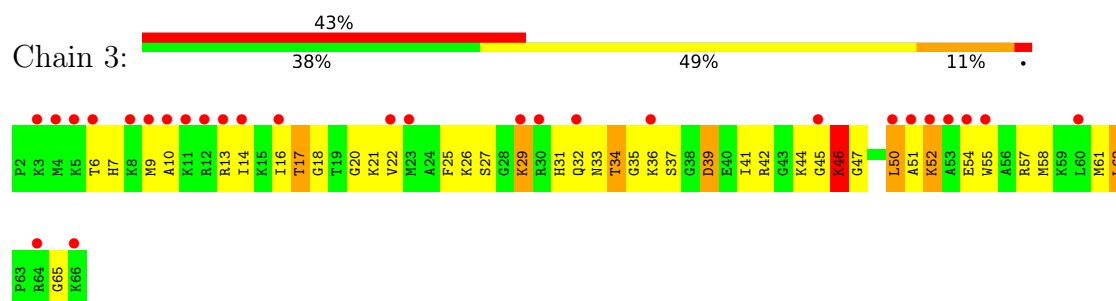
- Molecule 26: 50S ribosomal protein L33



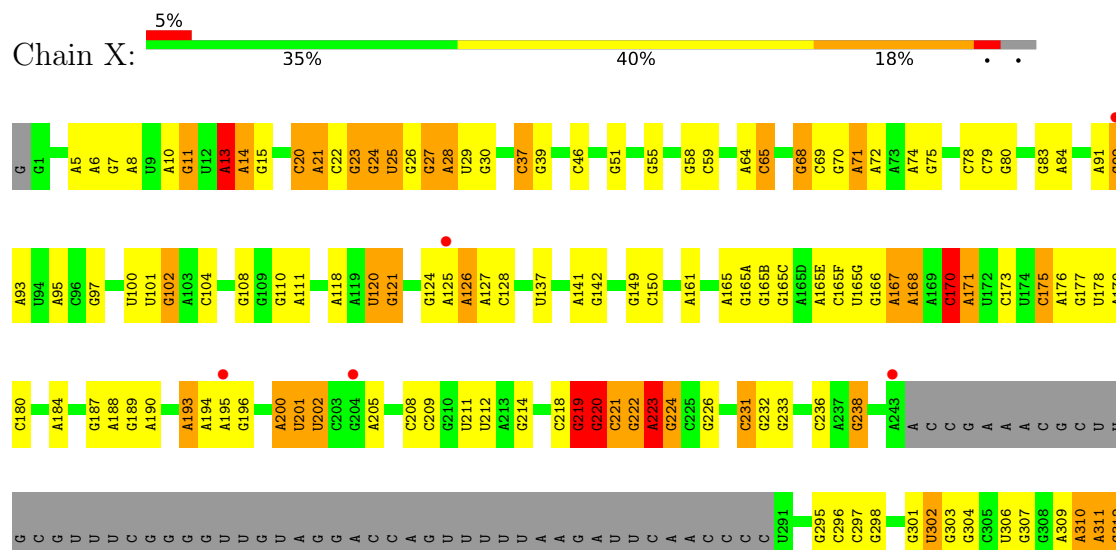
- Molecule 27: 50S ribosomal protein L34



- Molecule 28: 50S ribosomal protein L35

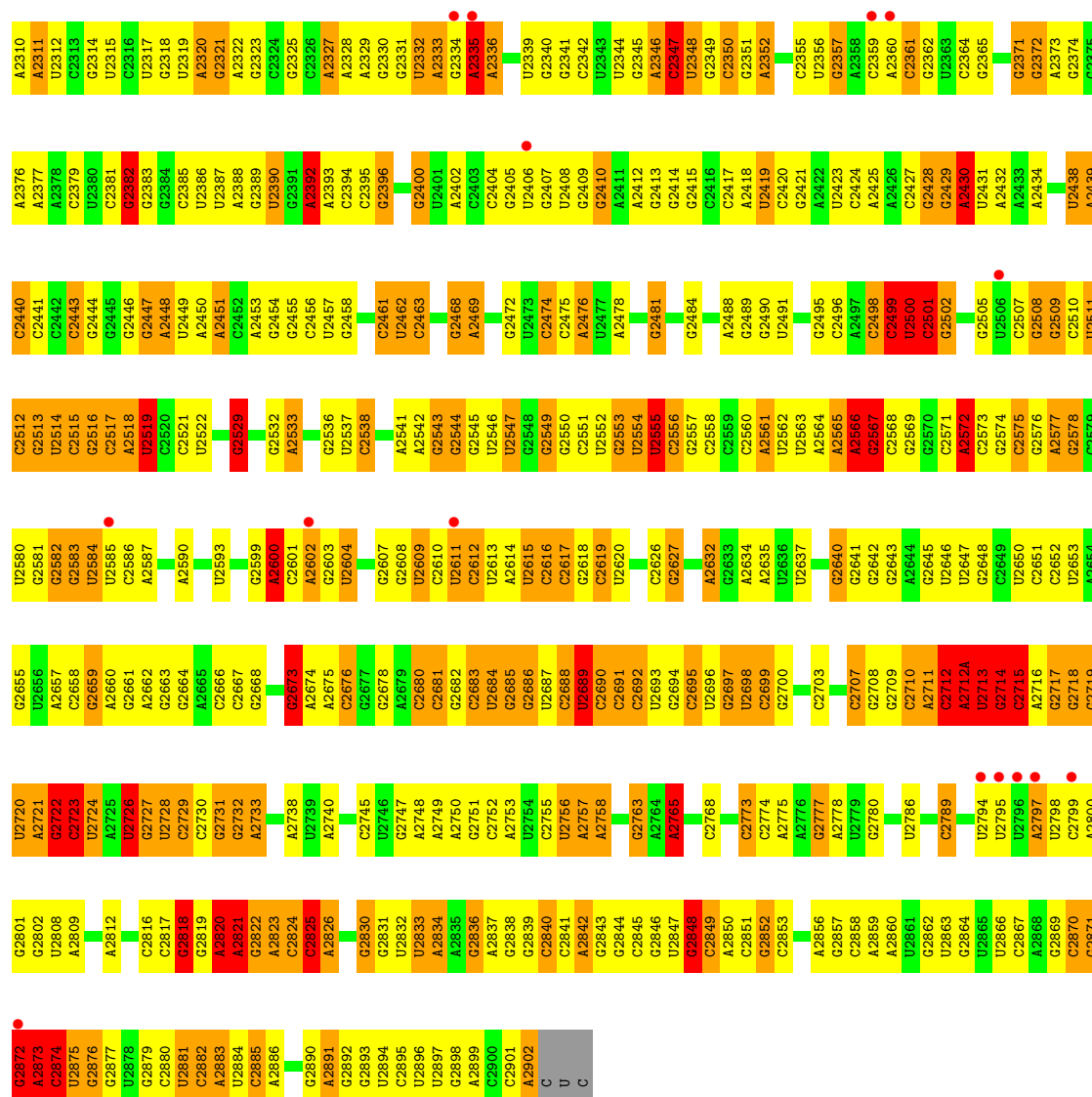


- Molecule 29: 23S ribosomal RNA

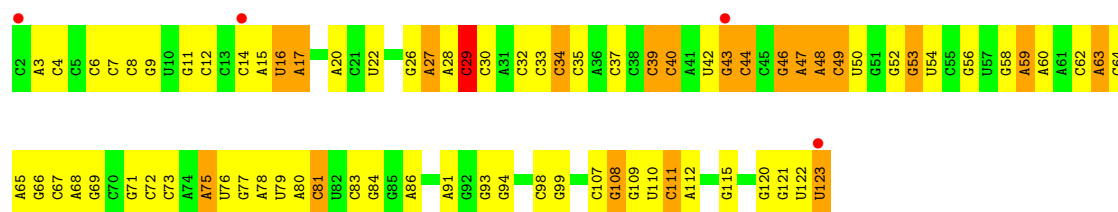


U1231	A1164	A1098	U1026	G950	G	U813	G738	A658	C592A	A526	C463	U	C313
U1233	U1165	U1101	U1027	C951	G	C814	G739	C659	U598	A526	C462	A374	U314
G1235	A1168	C1102	A1028	G954	C	C815	U740	G660	U599	G530	C465	A374	A315
G1236	A1169	A1103	A1029	A955	U	C816	G741	U661	G600	C531	A466	G382	C316
A1237	C1104	C1104	G1030	G956	A	G817	C742	C662	C601	A532	A467	G386	A317
G1238	G1172B	U1033	U1033	C957	C	A819	U744	G664	A602	G533	C468	U387	C318
C1239	G1172C	U1034	U1034	U958	C	A820	G745	G669	G603	A536	C469	G388	C319
C1240	G1173	U1035	U1035	A959	A	A821	G746	A670	C604	U537	A470	A389	U320
G1241	A1174	C1109	A960	G960	G	G822	U747	A671	U610	G538	A471	A390	C321
A1242	U1037	U1037	C961	C961	C	G823	G748	C671	U611	G539	A472	A391	A322
C1243	C1038	C1038	U962	U962	U	U824	A749	U672	G612	C540	G473	C392	G323
U1244	U1041	U1041	U963	U963	U	A825	A750	C673	G612	G474	G474	C393	A324
G1245	G1042	U1113	C964	C964	A	U826	A751	G676	A613	C544	U475	A394	A325
A1246	G1043	U1114	G969	G969	C	U827	G752	A677	A614	U545	U475	U395	G326
A1247	A1115	A1115	C970	C970	C	G828	G754	A678	A615	U546	U475	U396	G327
U1248	G1116	A1044	C971	C971	A899	A829	G754	C679	A616	U547	A480	A397	G329
U1249	G1117	U1045	G972	G972	C902	U832	A761	A680	A617	U548	A481	C398	G330
U1250	U1046	U1046	A973	A973	C903	A833	U762	G681	C618	G549	A482	U399	G331
C1251	G1047	U1048	G974	G974	C903	A834	U765	G682	G620	C550	A483	G400	A332
G1252	C1049	C1049	A980	A980	A906	A835	G765	G683	A621	U553	C485	A401	G333
A1253	U1054	U1054	C981	C981	U907	U839	A774	G684	A622	U554	C486	U403	U334
U1254	G1055	G1055	C982	C982	A908	U840	G775	G685	G623	U555	C487	C405	C335
G1255	G1056	G1056	A983	A983	A909	G841	G776	G686	G624	U556	C488	C406	C336
A1256	A1057	A1057	A984	A984	A911	G841	G777	G687	G625	U557	C489	G406	U337
U1257	U1058	U1058	G989	G989	A912	U844	A778	A690	G626	U558	C491	C407	G338
U1258	U1059	U1059	C990	C990	U913	G845	G779	A691	A627	C560	C492	C408	U339
U1259	U1060	U1060	A990	A990	U914	U846	G780	A692	G628	G561	C493	G409	A340
U1260	G1061	U1061	C991	C991	C915	U847	A781	U694	C629	U562	C494	G410	G344
U1261	G1062	G1062	C992	C992	A915	U848	A782	G695	G630	G563	C495	G411	A345
U1262	U1066	U1066	A993	A993	A918	U849	A783	G696	A631	C564	C496	A412	A346
U1263	A1067	A1067	U994	U994	G920	A850	A784	C698	A632	C565	C497	C413	C347
U1264	C1068	C1068	C995	C995	G921	G851	G785	A699	A633	U566	C498	G348	A349
U1265	A1069	A1069	A996	A996	G921	A852	C786	U568	C635	U569	C500	A422	G350
U1266	U1070	U1070	G997	G997	A925	U853	U787	G701	G636	U569	A501	A423	C
U1267	G1071	G1071	C998	C998	C926	C856	A788	G704	A637	G570	A502	G438	G
U1268	C1072	C1072	G1003	G1003	G927	C857	C791	A705	G638	A571	A503	A439	G
U1269	A1073	A1073	U1004	U1004	C928	C857	G792	A706	U639	A572	G504	C440	U
A1270	C1074	C1074	C1005	C1005	G929	G858	A793	C574	C640	C574	G506	U441	G
U1271	C1075	C1075	U1006	U1006	U930	G859	A794	G713	G642	A575	A507	G442	A
U1272	C1076	C1076	C1007	C1007	U931	G862	A794	G714	G643	U576	A508	A443	C
U1273	A1077	A1077	U1008	U1008	U932	A863	U797	G715	A644	G577	C509	C444	U
U1274	C1078	C1078	U1009	U1009	A933	G864	G798	A716	U645	A578	C510	C445	G
U1275	C1079	C1079	A1010	A1010	G934	G865	G799	C717	A646	G579	U511	G446	U
U1276	C1080	C1080	U1011	U1011	U935	A866	A800	A718	G647	C580	G512	A447	A
U1277	U1012	U1012	U1012	U1012	C936	G866	G801	G719	G648	C581	G513	U448	C
U1278	G1083	G1083	G1013	G1013	C937	C871	A802	G720	G649	G582	A514	A449	U
U1279	A1088	A1088	A1014	A1014	G940	A872	U803	G726	C650	G583	A515	G450	G
U1280	U1089	U1089	U1015	U1015	A941	A873	G805	A904	G651	C594	C516	C451	G
U1281	G1090	G1090	U1019	U1019	G942	G874	C806	G651A	G651A	C517	C517	C452	C
U1282	U1091	U1091	C1020	C1020	U943	G875	C906	G729	C651B	A586	G518	C453	A
U1283	G1094	G1094	A1021	A1021	U944	U807	A730	C731	C652	C587	U519	A454	C
U1284	U1095	U1095	G1022	G1022	A945	A878	G809	C732	U653	U588	G520	U456	C
U1285	A1096	A1096	U1023	U1023	G946	G	U810	A734	U654	U589	G521	A457	U
U1286	U1097	U1097	G1025	G1025	G947	U811	U811	G733	A655	A590	A522	C458	G
U1287	U1098	U1098	U1098	U1098	C948	G	C812	A734	A656	G591	C523	U459	A
U1288	U1099	U1099	U1099	U1099	U949	G			U657	A592	C523	A460	G

U2244	U2167	U2098	G2023	G1954	G1879	G1799	C1729	A1637	U1547	G1369	U1298
A2247	G2168	G2099	G2024	U1985	U1880	C1800	C1730	C1638	G1547	C1370	U1294
C2248	A2169	G2100	C2025	U1956	G1881	C1801	A1731	A1639	G1557	G1371	C1296
U2249	A2170	U2026	U2026	C1957	G1882	C1882	U1734	A1640	U1465	G1372	C1297
G2250	A2171	G2101	G2027	C1958	G1883	A1905	U1735	A1641	C1559	A1373	C1298
G2251	U2172	G2102	U2028	U1963	A1884	C1906	U1736	G1642	G1468	G1378	G1299
G2252	A2173	U2108	A2029	A1885	G1885	A1808	G1737	G1643	U1474	A1378	U1300
G2253	C2174	U2109	A2030	C1965	G1886	G1810	G1738	C1644	U1477	G1390	A1301
G2254	A2175	G2110	G2032	U1966	A1887	G1811	G1739	G1646	A1478	U1379	U1302
G2255	A2176	C2111	U2031	C1967	U1887	G1812	G1740	G1647	G1479	U1384	G1309
G2256	C2177	U2112	G2035	G1968	U1888	U1813	U1741	G1649	G1480	U1390	U1312
G2257	G2178	U2113	C2036	A1969	U1889	G1814	G1745	A1650	G1481	C1391	U1313
G2258	C2179	A2114	G2037	A1970	G1890	G1815	G1746	G1651	G1482	C1392	C1314
G2259	A2182	G2115	G2038	A1971	A1901	A1915	C1747	A1652	G1483	A1393	G1315
C2260	G2183	G2116	U2042	G1972	C1902	C1816	G1747	G1653	U1484	A1394	U1316
U2261	U2117	A2117	C2043	G1973	G1903	G1817	A1748	A1654	U1485	A1395	G1317
C2262	U2118	U2118	A2043	G1904	G1904	U1818	U1749	U1584	G1486	G1318	G1318
C2264	A2119	A2119	C2044	C1905	A1819	U1819	G1750	A1655	G1487	G1320	G1319
G2265	G2120	G2120	G2045	U1977	G1906	U1820	U1751	C1656	G1405	G1406	G1320
A2266	G2121	G2121	G2046	A1978	G1907	A1921	G1752	C1657	U1412	U1412	G1321
A2267	U2189	U2122	U2047	C1979	C1908	G1822	A1753	C1658	G1413	G1413	G1322
A2268	G2190	G2123	A2048	G1980	C1909	G1823	A1754	U1659	G1414	A1415	C1327
A2269	G2191	G2124	G2049	G1981	G1910	G1824	U1755	C1660	G1494	G1416	G1328
U2270	U2194	G2125	C2050	G1985	U1911	U1825	A1756	G1661	U1497	G1418	U1329
G2271	U2195	A2126	A2051	G1986	A1912	G1826	G1757	U1662	G1498	G1422	C1330
U2272	C2196	C2128	G2052	C1990	A1913	U1827	G1758	A1663	U1499	A1423	C1331
A2273	U2197	G2129	U2053	G1991	C1914	G1828	C1759	A1664	A1500	G1424	C1332
G2274	G2198	U2130	C2054	G1992	U1915	A1829	C1760	A1665	C1501	A1427	A1336
G2275	A2198	U2131	G2055	U1993	A1916	G1832	G1761	G1666	G1502	C1428	G1337
G2276	G2203	G2132	A2056	C1994	U1917	C1833	A1762	C1667	G1503	G1429	G1338
G2277	A2204	G2133	A2057	U1995	A1918	U1834	G1763	A1668	G1504	C1430	U1341
A2278	G2205	A2134	G2058	C1996	A1919	G1835	U1770	A1669	U1505	C1437	G1342
G2279	A2210	A2135	A2059	U1997	C1920	G1835	C1771	U1673	G1506	U1507	G1343
G2280	A2211	G2136	G2061	A1998	G1921	C1838	A1772	G1674	G1507	G1435	U1344
G2281	U2212	C2137	A2062	C1999	A1928	G1839	U1773	G1675	G1508	U1440	C1345
U2282	U2213	U2138	C2063	G2000	G1840	U1841	U1775	A1676	A1509	C1440A	G1346
G2283	U2217	G2139	C2064	A2001	G1842	U1777	G1776	A1677	G1510	U1444	A1353
A2287	U2218	C2140	C2065	A1927	U1843	C1843	U1778	C1679	G1511	G1445	G1355
A2288	U2219	C2141	G2066	A1928	A1848	U1849	A1780	C1684	G1525	G1450	G1356
G2289	G2220	U2143	U2068	G1930	G1850	C1850	C1781	C1685	G1526	C1451	U1357
U2290	G2221	U2144	C2006	U1931	U1851	G1851	C1782	C1686	U1532	U1452	G1358
G2291	G2222	U2145	G2007	A1936	C1852	A1783	A1785	G1687	C1533	A1453	A1359
C2292	G2223	U2146	G2070	A1937	A1853	A1853	U1786	U1688	U1534	G1360	G1360
G2293	G2224	G2147	A2071	A1938	U1940	A1954	A1786	G1694	U1535	G1455	G1361
G2294	A2225	G2148	G2072	A1939	C1941	A1954	A1787	C1695	G1529	U1458	A1365
G2295	U2226	G2149	U2075	U1940	G1858	G1858	U1787	G1696	U1537	U1459	A1366
U2296	U2227	U2150	U2076	C1942	U1943	G1862	C1788	G1697	G1538	U1460	G1367
A2299	G2230	C2152	A2077	U1944	U1944	G1863	U1789	A1698	U1539	G1461	G1368
C2302	G2233	G2153	A2080	U1945	G1945	U1863	C1790	G1699	U1540	U1458	U1369
G2303	G2234	U2081	U2081	G1945	U1863	U1863	U1791	A1700	U1541	U1459	U1370
G2304	U2081	U2081	U2081	U1945	U1863	U1863	U1791	A1700	U1541	U1459	U1370
U2305	G2238	U2155	A2090	G1949	G1874	U1874	A1794	A1701	U1542	U1459	U1370
U2306	G2239	G2157	U2091	G1950	G1875	C1875	C1795	U1701	U1543	U1459	U1370
G2307	G2240	A2158	U2092	U1951	A1876	U1876	C1796	U1702	U1544	U1459	U1370
G2308	G2241	G2159	U2093	U1952	A1877	U1877	C1797	U1703	U1545	U1459	U1370
A2309	U2242	C2164	G2094	A1953	G1878	U1878	U1798	C1728	U1546	U1459	U1370



• Molecule 30: 5S ribosomal RNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.90Å 410.76Å 696.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.96 – 2.90 58.96 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (58.96-2.90) 81.6 (58.96-2.90)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.61 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.235 , 0.270 0.243 , 0.277	Depositor DCC
$R_{free}$ test set	24732 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.9	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 46.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	89337	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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

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	O	0.30	0/1674	0.49	0/2257
2	A	0.39	0/2149	0.59	0/2890
3	B	0.69	1/1568 (0.1%)	0.86	1/2105 (0.0%)
4	C	0.51	0/1530	0.73	1/2070 (0.0%)
5	D	0.36	0/1420	0.56	0/1903
6	E	0.39	0/1309	0.55	0/1771
7	F	0.33	0/1067	0.52	1/1446 (0.1%)
8	G	0.47	0/1139	0.67	0/1539
9	H	0.76	0/1007	0.91	2/1352 (0.1%)
10	I	0.52	0/1082	0.76	1/1448 (0.1%)
11	J	0.65	0/1114	0.78	0/1486
12	K	0.83	0/887	1.04	0/1188
13	L	0.52	0/784	0.73	0/1045
14	M	0.77	0/880	0.83	0/1179
15	N	0.64	0/994	0.80	1/1323 (0.1%)
16	O	0.53	0/751	0.73	0/1000
17	P	0.69	0/1027	0.83	0/1373
18	Q	0.45	0/738	0.59	0/988
19	R	0.54	0/836	0.72	0/1121
20	S	0.41	0/1371	0.67	0/1862
21	T	0.54	0/634	0.69	0/838
22	U	0.61	0/557	0.88	1/741 (0.1%)
23	V	0.41	0/538	0.57	0/714
24	W	0.51	0/426	0.68	0/568
25	Z	0.71	0/465	0.90	0/622
26	1	0.49	0/411	0.73	0/554
27	2	0.48	0/397	0.65	0/521
28	3	0.54	0/516	0.70	0/673
29	X	0.78	37/66826 (0.1%)	1.44	971/104247 (0.9%)
30	Y	0.64	0/2907	1.20	8/4529 (0.2%)
All	All	0.72	38/97004 (0.0%)	1.29	987/145353 (0.7%)



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
3	B	0	3
4	C	0	1
8	G	0	1
25	Z	0	2
All	All	0	7

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	761	A	C6-N1	8.06	1.41	1.35
29	X	1999	C	N3-C4	-7.01	1.29	1.33
29	X	1638	C	N1-C6	-6.80	1.33	1.37
29	X	1661	G	C6-N1	-6.69	1.34	1.39
29	X	1661	G	C5-C4	-6.50	1.33	1.38

The worst 5 of 987 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	761	A	N1-C6-N6	22.08	131.85	118.60
29	X	761	A	C5-N7-C8	-17.56	95.12	103.90
29	X	2713	U	O5'-P-OP2	-17.29	89.95	110.70
29	X	761	A	C4-C5-N7	16.33	118.87	110.70
29	X	761	A	C5-C6-N6	-14.62	112.00	123.70

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	178	GLY	Peptide
3	B	73	ALA	Peptide
3	B	85	ALA	Peptide
4	C	187	VAL	Peptide
8	G	37	ASP	Peptide

## 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	0	1651	0	1693	59	0
2	A	2107	0	2190	82	0
3	B	1540	0	1600	75	0
4	C	1507	0	1525	80	0
5	D	1401	0	1481	64	0
6	E	1287	0	1336	49	0
7	F	1048	0	1088	23	0
8	G	1115	0	1144	47	0
9	H	997	0	1046	67	0
10	I	1068	0	1103	60	0
11	J	1091	0	1125	64	0
12	K	879	0	930	43	0
13	L	778	0	820	38	0
14	M	867	0	890	43	0
15	N	978	0	1020	72	0
16	O	742	0	756	37	0
17	P	1014	0	1096	60	0
18	Q	727	0	753	25	0
19	R	826	0	881	54	0
20	S	1346	0	1372	65	0
21	T	626	0	655	33	0
22	U	553	0	604	59	0
23	V	534	0	558	16	0
24	W	424	0	470	20	0
25	Z	453	0	455	38	0
26	1	404	0	416	21	0
27	2	393	0	420	19	0
28	3	509	0	565	40	0
29	X	59673	0	30060	1282	0
30	Y	2601	0	1327	57	0
31	M	1	0	0	0	0
31	X	192	0	0	0	0
31	Y	5	0	0	0	0
All	All	89337	0	59379	2369	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 16.

The worst 5 of 2369 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)
12:K:103:ARG:HD2	29:X:1287:A:H5'	1.33	1.04
9:H:41:ASN:ND2	29:X:2674:A:O2'	1.91	1.04
15:N:48:ARG:HD2	29:X:1156:A:H61	1.20	1.03
8:G:31:THR:HG21	15:N:61:TRP:HE1	1.26	1.00
29:X:500:G:H22	29:X:503:A:H5''	1.26	0.97

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	0	222/224 (99%)	135 (61%)	65 (29%)	22 (10%)	0	1
2	A	272/274 (99%)	238 (88%)	25 (9%)	9 (3%)	3	13
3	B	203/205 (99%)	168 (83%)	24 (12%)	11 (5%)	1	5
4	C	195/197 (99%)	151 (77%)	30 (15%)	14 (7%)	1	2
5	D	175/177 (99%)	124 (71%)	39 (22%)	12 (7%)	1	2
6	E	169/171 (99%)	130 (77%)	22 (13%)	17 (10%)	0	1
7	F	142/144 (99%)	99 (70%)	34 (24%)	9 (6%)	1	3
8	G	140/142 (99%)	121 (86%)	13 (9%)	6 (4%)	2	8
9	H	132/134 (98%)	103 (78%)	19 (14%)	10 (8%)	1	2
10	I	139/141 (99%)	104 (75%)	23 (16%)	12 (9%)	0	1
11	J	134/136 (98%)	102 (76%)	20 (15%)	12 (9%)	0	1
12	K	111/113 (98%)	95 (86%)	11 (10%)	5 (4%)	2	8
13	L	102/104 (98%)	65 (64%)	21 (21%)	16 (16%)	0	0
14	M	107/109 (98%)	93 (87%)	7 (6%)	7 (6%)	1	3

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	N	115/117 (98%)	104 (90%)	8 (7%)	3 (3%)	4	17
16	O	92/94 (98%)	75 (82%)	11 (12%)	6 (6%)	1	3
17	P	125/127 (98%)	99 (79%)	16 (13%)	10 (8%)	1	2
18	Q	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
19	R	108/110 (98%)	84 (78%)	14 (13%)	10 (9%)	0	1
20	S	173/175 (99%)	123 (71%)	32 (18%)	18 (10%)	0	1
21	T	82/84 (98%)	68 (83%)	11 (13%)	3 (4%)	2	11
22	U	70/72 (97%)	38 (54%)	16 (23%)	16 (23%)	0	0
23	V	64/66 (97%)	55 (86%)	5 (8%)	4 (6%)	1	3
24	W	53/55 (96%)	48 (91%)	3 (6%)	2 (4%)	2	11
25	Z	55/57 (96%)	41 (74%)	11 (20%)	3 (6%)	1	5
26	1	52/54 (96%)	33 (64%)	13 (25%)	6 (12%)	0	1
27	2	45/47 (96%)	40 (89%)	3 (7%)	2 (4%)	2	8
28	3	63/65 (97%)	47 (75%)	12 (19%)	4 (6%)	1	3
All	All	3431/3487 (98%)	2670 (78%)	512 (15%)	249 (7%)	1	2

5 of 249 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	28	LEU
1	0	30	THR
1	0	45	ILE
1	0	157	ILE
1	0	216	PRO

### 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	0	167/167 (100%)	150 (90%)	17 (10%)	6	19
2	A	214/214 (100%)	190 (89%)	24 (11%)	5	16

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	155/155 (100%)	139 (90%)	16 (10%)	6	19
4	C	157/157 (100%)	137 (87%)	20 (13%)	3	11
5	D	153/153 (100%)	131 (86%)	22 (14%)	2	8
6	E	136/136 (100%)	114 (84%)	22 (16%)	2	6
7	F	107/107 (100%)	97 (91%)	10 (9%)	7	23
8	G	118/118 (100%)	108 (92%)	10 (8%)	8	27
9	H	103/103 (100%)	76 (74%)	27 (26%)	0	1
10	I	108/108 (100%)	85 (79%)	23 (21%)	1	2
11	J	110/110 (100%)	89 (81%)	21 (19%)	1	4
12	K	90/90 (100%)	78 (87%)	12 (13%)	3	10
13	L	74/74 (100%)	52 (70%)	22 (30%)	0	1
14	M	92/92 (100%)	79 (86%)	13 (14%)	3	9
15	N	96/96 (100%)	86 (90%)	10 (10%)	5	18
16	O	75/75 (100%)	57 (76%)	18 (24%)	0	1
17	P	109/109 (100%)	92 (84%)	17 (16%)	2	7
18	Q	75/75 (100%)	69 (92%)	6 (8%)	10	30
19	R	91/91 (100%)	76 (84%)	15 (16%)	2	6
20	S	149/149 (100%)	117 (78%)	32 (22%)	1	2
21	T	62/62 (100%)	48 (77%)	14 (23%)	1	2
22	U	57/57 (100%)	42 (74%)	15 (26%)	0	1
23	V	54/54 (100%)	48 (89%)	6 (11%)	5	16
24	W	48/48 (100%)	43 (90%)	5 (10%)	5	18
25	Z	51/51 (100%)	43 (84%)	8 (16%)	2	7
26	1	38/38 (100%)	30 (79%)	8 (21%)	1	2
27	2	40/40 (100%)	33 (82%)	7 (18%)	1	5
28	3	51/51 (100%)	40 (78%)	11 (22%)	1	2
All	All	2780/2780 (100%)	2349 (84%)	431 (16%)	2	7

5 of 431 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	L	37	HIS
16	O	84	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
25	Z	20	ARG
13	L	60	LYS
15	N	9	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
9	H	41	ASN
14	M	58	ASN
19	R	77	HIS
18	Q	86	GLN
19	R	69	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	X	2776/2881 (96%)	655 (23%)	41 (1%)
30	Y	121/122 (99%)	35 (28%)	1 (0%)
All	All	2897/3003 (96%)	690 (23%)	42 (1%)

5 of 690 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	X	13	A
29	X	14	A
29	X	22	C
29	X	28	A
29	X	46	C

5 of 42 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	X	2022	U
29	X	2468	G
29	X	2035	G
29	X	2347	C
29	X	2714	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 198 ligands modelled in this entry, 198 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	0	224/224 (100%)	1.45	58 (25%) 2 2	238, 259, 280, 290	0
2	A	274/274 (100%)	1.30	73 (26%) 2 2	93, 135, 154, 161	0
3	B	205/205 (100%)	0.61	13 (6%) 27 23	60, 89, 107, 124	0
4	C	197/197 (100%)	0.68	14 (7%) 23 20	77, 125, 145, 159	0
5	D	177/177 (100%)	0.98	32 (18%) 4 4	155, 174, 190, 197	0
6	E	171/171 (100%)	0.76	21 (12%) 9 8	110, 148, 175, 177	0
7	F	144/144 (100%)	1.22	34 (23%) 2 2	213, 230, 235, 237	0
8	G	142/142 (100%)	0.74	17 (11%) 10 9	79, 112, 127, 144	0
9	H	134/134 (100%)	0.45	8 (5%) 29 24	62, 79, 94, 111	0
10	I	141/141 (100%)	1.66	48 (34%) 1 1	86, 138, 155, 161	0
11	J	136/136 (100%)	1.26	30 (22%) 3 2	94, 113, 135, 141	0
12	K	113/113 (100%)	0.42	9 (7%) 20 17	61, 72, 83, 88	0
13	L	104/104 (100%)	2.12	42 (40%) 1 1	121, 136, 153, 162	0
14	M	109/109 (100%)	0.33	8 (7%) 22 19	65, 80, 98, 127	0
15	N	117/117 (100%)	0.93	13 (11%) 12 10	80, 107, 126, 133	0
16	O	94/94 (100%)	1.09	13 (13%) 8 7	89, 122, 141, 152	0
17	P	127/127 (100%)	0.77	11 (8%) 17 15	71, 85, 109, 156	0
18	Q	93/93 (100%)	0.90	11 (11%) 10 9	98, 124, 140, 144	0
19	R	110/110 (100%)	1.17	18 (16%) 5 5	110, 121, 146, 157	0
20	S	175/175 (100%)	0.88	20 (11%) 11 10	124, 151, 164, 168	0
21	T	84/84 (100%)	1.61	26 (30%) 1 1	102, 117, 133, 146	0
22	U	72/72 (100%)	3.31	45 (62%) 0 0	117, 148, 161, 164	0
23	V	66/66 (100%)	0.66	7 (10%) 13 11	129, 141, 159, 163	0
24	W	55/55 (100%)	0.82	8 (14%) 7 6	95, 110, 126, 139	0

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Z	57/57 (100%)	0.45	4 (7%) 24 20	74, 82, 104, 112	0
26	1	54/54 (100%)	1.39	14 (25%) 2 2	125, 136, 152, 168	0
27	2	47/47 (100%)	1.33	9 (19%) 4 3	91, 108, 116, 117	0
28	3	65/65 (100%)	2.12	28 (43%) 1 1	107, 118, 127, 129	0
29	X	2780/2881 (96%)	0.17	136 (4%) 36 30	51, 111, 221, 347	0
30	Y	122/122 (100%)	0.33	4 (3%) 49 43	96, 136, 161, 172	0
All	All	6389/6490 (98%)	0.66	774 (12%) 10 9	51, 119, 242, 347	0

The worst 5 of 774 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	X	2137	C	20.9
29	X	2138	U	17.0
22	U	8	THR	11.5
22	U	27	ASP	11.2
29	X	2144	U	10.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 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, 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
31	MG	X	6163	1/1	0.08	0.41	156,156,156,156	0
31	MG	X	6146	1/1	0.14	1.21	129,129,129,129	0
31	MG	X	6093	1/1	0.18	0.59	106,106,106,106	0
31	MG	X	6192	1/1	0.23	0.49	138,138,138,138	0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	6110	1/1	0.35	0.39	130,130,130,130	0
31	MG	X	6054	1/1	0.35	0.44	92,92,92,92	0
31	MG	X	6170	1/1	0.36	0.59	127,127,127,127	0
31	MG	X	6020	1/1	0.36	0.37	79,79,79,79	0
31	MG	X	6177	1/1	0.38	0.49	113,113,113,113	0
31	MG	X	6076	1/1	0.38	0.49	102,102,102,102	0
31	MG	X	6052	1/1	0.39	0.67	97,97,97,97	0
31	MG	X	6127	1/1	0.40	0.59	122,122,122,122	0
31	MG	X	6108	1/1	0.40	0.66	120,120,120,120	0
31	MG	X	6019	1/1	0.40	0.55	77,77,77,77	0
31	MG	X	6186	1/1	0.42	0.58	134,134,134,134	0
31	MG	X	6018	1/1	0.42	0.38	74,74,74,74	0
31	MG	Y	202	1/1	0.42	0.35	125,125,125,125	0
31	MG	X	6105	1/1	0.43	0.86	118,118,118,118	0
31	MG	X	6141	1/1	0.43	0.51	122,122,122,122	0
31	MG	X	6012	1/1	0.43	0.39	82,82,82,82	0
31	MG	X	6157	1/1	0.43	0.31	111,111,111,111	0
31	MG	X	6048	1/1	0.43	0.57	102,102,102,102	0
31	MG	X	6070	1/1	0.45	0.37	107,107,107,107	0
31	MG	X	6123	1/1	0.45	0.48	130,130,130,130	0
31	MG	X	6109	1/1	0.45	0.27	101,101,101,101	0
31	MG	X	6148	1/1	0.47	0.42	130,130,130,130	0
31	MG	X	6153	1/1	0.47	0.57	113,113,113,113	0
31	MG	X	6037	1/1	0.47	0.34	86,86,86,86	0
31	MG	X	6084	1/1	0.48	0.28	93,93,93,93	0
31	MG	X	6089	1/1	0.48	0.37	90,90,90,90	0
31	MG	X	6072	1/1	0.49	0.55	102,102,102,102	0
31	MG	X	6090	1/1	0.49	0.35	117,117,117,117	0
31	MG	X	6058	1/1	0.50	0.39	97,97,97,97	0
31	MG	X	6024	1/1	0.50	0.54	87,87,87,87	0
31	MG	X	6023	1/1	0.50	0.51	97,97,97,97	0
31	MG	X	6046	1/1	0.50	0.30	91,91,91,91	0
31	MG	X	6057	1/1	0.50	0.69	93,93,93,93	0
31	MG	X	6125	1/1	0.51	0.44	123,123,123,123	0
31	MG	X	6051	1/1	0.52	0.31	69,69,69,69	0
31	MG	X	6111	1/1	0.52	0.61	98,98,98,98	0
31	MG	X	6038	1/1	0.53	0.57	85,85,85,85	0
31	MG	X	6190	1/1	0.53	0.63	129,129,129,129	0
31	MG	X	6033	1/1	0.54	0.39	98,98,98,98	0
31	MG	X	6175	1/1	0.54	0.38	121,121,121,121	0
31	MG	X	6164	1/1	0.54	0.59	124,124,124,124	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	6182	1/1	0.54	0.55	120,120,120,120	0
31	MG	X	6139	1/1	0.55	0.43	126,126,126,126	0
31	MG	X	6172	1/1	0.55	0.55	124,124,124,124	0
31	MG	X	6137	1/1	0.55	0.42	135,135,135,135	0
31	MG	X	6113	1/1	0.56	0.55	115,115,115,115	0
31	MG	X	6007	1/1	0.56	0.27	70,70,70,70	0
31	MG	X	6181	1/1	0.56	0.31	121,121,121,121	0
31	MG	X	6025	1/1	0.56	0.31	83,83,83,83	0
31	MG	X	6160	1/1	0.57	0.56	104,104,104,104	0
31	MG	X	6006	1/1	0.57	0.58	69,69,69,69	0
31	MG	X	6003	1/1	0.57	0.47	70,70,70,70	0
31	MG	X	6166	1/1	0.57	0.48	106,106,106,106	0
31	MG	X	6078	1/1	0.57	0.49	93,93,93,93	0
31	MG	X	6102	1/1	0.57	0.24	89,89,89,89	0
31	MG	X	6011	1/1	0.57	0.37	89,89,89,89	0
31	MG	X	6167	1/1	0.58	0.55	103,103,103,103	0
31	MG	X	6049	1/1	0.58	0.68	88,88,88,88	0
31	MG	X	6189	1/1	0.58	0.48	120,120,120,120	0
31	MG	X	6088	1/1	0.59	0.53	99,99,99,99	0
31	MG	X	6077	1/1	0.59	0.39	98,98,98,98	0
31	MG	X	6065	1/1	0.59	0.33	81,81,81,81	0
31	MG	X	6121	1/1	0.59	0.58	99,99,99,99	0
31	MG	X	6014	1/1	0.59	0.40	91,91,91,91	0
31	MG	Y	205	1/1	0.59	0.59	129,129,129,129	0
31	MG	X	6032	1/1	0.60	0.33	78,78,78,78	0
31	MG	X	6173	1/1	0.60	1.13	102,102,102,102	0
31	MG	X	6144	1/1	0.60	0.57	87,87,87,87	0
31	MG	X	6029	1/1	0.60	0.31	69,69,69,69	0
31	MG	X	6116	1/1	0.61	0.40	106,106,106,106	0
31	MG	X	6101	1/1	0.61	0.48	89,89,89,89	0
31	MG	X	6162	1/1	0.61	1.43	111,111,111,111	0
31	MG	X	6064	1/1	0.61	0.52	96,96,96,96	0
31	MG	X	6115	1/1	0.61	0.47	103,103,103,103	0
31	MG	X	6015	1/1	0.62	0.38	77,77,77,77	0
31	MG	X	6069	1/1	0.62	0.46	91,91,91,91	0
31	MG	X	6059	1/1	0.62	0.37	87,87,87,87	0
31	MG	X	6179	1/1	0.62	0.65	117,117,117,117	0
31	MG	X	6026	1/1	0.62	0.27	91,91,91,91	0
31	MG	X	6094	1/1	0.62	0.39	92,92,92,92	0
31	MG	X	6001	1/1	0.63	0.58	69,69,69,69	0
31	MG	X	6145	1/1	0.63	0.26	104,104,104,104	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	6155	1/1	0.63	0.37	115,115,115,115	0
31	MG	X	6107	1/1	0.63	0.67	113,113,113,113	0
31	MG	X	6034	1/1	0.64	0.58	90,90,90,90	0
31	MG	X	6056	1/1	0.64	0.75	85,85,85,85	0
31	MG	X	6129	1/1	0.64	0.55	104,104,104,104	0
31	MG	X	6075	1/1	0.64	0.69	103,103,103,103	0
31	MG	X	6149	1/1	0.64	0.45	94,94,94,94	0
31	MG	X	6047	1/1	0.64	0.42	74,74,74,74	0
31	MG	X	6044	1/1	0.64	0.34	73,73,73,73	0
31	MG	X	6140	1/1	0.65	0.80	97,97,97,97	0
31	MG	X	6112	1/1	0.65	0.61	84,84,84,84	0
31	MG	X	6079	1/1	0.66	0.25	102,102,102,102	0
31	MG	X	6039	1/1	0.66	0.57	104,104,104,104	0
31	MG	X	6119	1/1	0.66	1.22	128,128,128,128	0
31	MG	X	6017	1/1	0.66	0.40	83,83,83,83	0
31	MG	X	6103	1/1	0.66	0.34	117,117,117,117	0
31	MG	X	6040	1/1	0.67	0.57	80,80,80,80	0
31	MG	X	6073	1/1	0.67	0.57	85,85,85,85	0
31	MG	X	6063	1/1	0.67	1.21	87,87,87,87	0
31	MG	X	6050	1/1	0.67	0.35	84,84,84,84	0
31	MG	X	6022	1/1	0.68	0.26	77,77,77,77	0
31	MG	X	6117	1/1	0.68	0.46	90,90,90,90	0
31	MG	X	6183	1/1	0.68	0.45	105,105,105,105	0
31	MG	X	6098	1/1	0.68	0.57	97,97,97,97	0
31	MG	X	6085	1/1	0.68	0.41	101,101,101,101	0
31	MG	X	6004	1/1	0.68	0.33	76,76,76,76	0
31	MG	X	6060	1/1	0.68	0.58	80,80,80,80	0
31	MG	X	6009	1/1	0.68	0.37	69,69,69,69	0
31	MG	X	6013	1/1	0.68	0.55	76,76,76,76	0
31	MG	X	6082	1/1	0.69	0.72	83,83,83,83	0
31	MG	X	6168	1/1	0.69	0.42	107,107,107,107	0
31	MG	X	6180	1/1	0.69	0.91	101,101,101,101	0
31	MG	X	6067	1/1	0.69	0.50	79,79,79,79	0
31	MG	X	6133	1/1	0.70	0.59	111,111,111,111	0
31	MG	X	6135	1/1	0.70	0.50	91,91,91,91	0
31	MG	X	6171	1/1	0.70	0.57	111,111,111,111	0
31	MG	X	6134	1/1	0.71	0.57	112,112,112,112	0
31	MG	Y	201	1/1	0.71	0.56	112,112,112,112	0
31	MG	X	6021	1/1	0.71	0.45	75,75,75,75	0
31	MG	X	6185	1/1	0.71	0.39	109,109,109,109	0
31	MG	X	6161	1/1	0.72	0.54	95,95,95,95	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	6120	1/1	0.72	0.98	102,102,102,102	0
31	MG	X	6031	1/1	0.72	0.36	69,69,69,69	0
31	MG	X	6128	1/1	0.72	0.79	97,97,97,97	0
31	MG	X	6080	1/1	0.72	0.61	108,108,108,108	0
31	MG	X	6124	1/1	0.72	0.80	107,107,107,107	0
31	MG	Y	204	1/1	0.72	0.44	109,109,109,109	0
31	MG	X	6176	1/1	0.72	0.46	107,107,107,107	0
31	MG	X	6174	1/1	0.73	0.35	87,87,87,87	0
31	MG	X	6042	1/1	0.73	0.34	83,83,83,83	0
31	MG	X	6100	1/1	0.74	0.52	97,97,97,97	0
31	MG	X	6099	1/1	0.74	0.59	89,89,89,89	0
31	MG	X	6156	1/1	0.74	0.40	105,105,105,105	0
31	MG	X	6114	1/1	0.74	0.41	91,91,91,91	0
31	MG	X	6158	1/1	0.74	0.97	114,114,114,114	0
31	MG	X	6184	1/1	0.75	0.65	102,102,102,102	0
31	MG	X	6147	1/1	0.75	0.45	82,82,82,82	0
31	MG	X	6061	1/1	0.76	0.40	83,83,83,83	0
31	MG	X	6151	1/1	0.76	0.26	98,98,98,98	0
31	MG	X	6142	1/1	0.77	0.52	89,89,89,89	0
31	MG	X	6045	1/1	0.77	0.76	89,89,89,89	0
31	MG	X	6126	1/1	0.77	0.79	94,94,94,94	0
31	MG	X	6053	1/1	0.77	0.68	91,91,91,91	0
31	MG	X	6122	1/1	0.78	0.70	100,100,100,100	0
31	MG	X	6118	1/1	0.79	0.66	90,90,90,90	0
31	MG	X	6169	1/1	0.79	0.44	101,101,101,101	0
31	MG	X	6016	1/1	0.79	0.21	77,77,77,77	0
31	MG	X	6150	1/1	0.79	0.48	111,111,111,111	0
31	MG	X	6131	1/1	0.79	0.72	101,101,101,101	0
31	MG	X	6165	1/1	0.80	0.77	99,99,99,99	0
31	MG	X	6087	1/1	0.80	0.47	98,98,98,98	0
31	MG	X	6138	1/1	0.80	0.65	94,94,94,94	0
31	MG	X	6027	1/1	0.80	0.68	86,86,86,86	0
31	MG	X	6159	1/1	0.82	0.42	111,111,111,111	0
31	MG	X	6068	1/1	0.82	0.86	90,90,90,90	0
31	MG	X	6136	1/1	0.84	0.63	122,122,122,122	0
31	MG	X	6132	1/1	0.84	0.50	94,94,94,94	0
31	MG	X	6062	1/1	0.84	0.42	85,85,85,85	0
31	MG	X	6143	1/1	0.85	0.82	100,100,100,100	0
31	MG	X	6091	1/1	0.85	0.75	88,88,88,88	0
31	MG	X	6035	1/1	0.85	0.34	86,86,86,86	0
31	MG	X	6028	1/1	0.85	0.24	88,88,88,88	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	6152	1/1	0.86	0.60	112,112,112,112	0
31	MG	X	6066	1/1	0.86	0.85	84,84,84,84	0
31	MG	X	6081	1/1	0.86	0.35	78,78,78,78	0
31	MG	Y	203	1/1	0.86	0.72	102,102,102,102	0
31	MG	X	6036	1/1	0.86	0.76	82,82,82,82	0
31	MG	X	6083	1/1	0.86	0.48	91,91,91,91	0
31	MG	X	6030	1/1	0.87	0.94	83,83,83,83	0
31	MG	X	6041	1/1	0.87	0.21	83,83,83,83	0
31	MG	X	6055	1/1	0.87	0.64	90,90,90,90	0
31	MG	X	6002	1/1	0.87	0.21	78,78,78,78	0
31	MG	X	6074	1/1	0.87	0.58	80,80,80,80	0
31	MG	X	6008	1/1	0.88	0.32	81,81,81,81	0
31	MG	X	6092	1/1	0.88	0.08	93,93,93,93	0
31	MG	X	6010	1/1	0.89	0.61	69,69,69,69	0
31	MG	X	6095	1/1	0.89	0.64	79,79,79,79	0
31	MG	X	6154	1/1	0.89	0.91	113,113,113,113	0
31	MG	X	6043	1/1	0.89	0.69	69,69,69,69	0
31	MG	X	6187	1/1	0.89	0.37	92,92,92,92	0
31	MG	X	6188	1/1	0.89	0.37	98,98,98,98	0
31	MG	X	6106	1/1	0.89	0.75	80,80,80,80	0
31	MG	X	6130	1/1	0.90	0.55	108,108,108,108	0
31	MG	X	6096	1/1	0.90	0.68	89,89,89,89	0
31	MG	X	6071	1/1	0.90	0.26	81,81,81,81	0
31	MG	X	6104	1/1	0.91	0.49	86,86,86,86	0
31	MG	M	201	1/1	0.91	0.56	69,69,69,69	0
31	MG	X	6191	1/1	0.91	0.78	101,101,101,101	0
31	MG	X	6097	1/1	0.92	0.65	93,93,93,93	0
31	MG	X	6086	1/1	0.92	0.67	87,87,87,87	0
31	MG	X	6178	1/1	0.93	0.43	103,103,103,103	0
31	MG	X	6005	1/1	0.96	0.70	69,69,69,69	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.