



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 30, 2026 – 11:17 PM UTC

PDB ID : 3CC7 / pdb\_00003cc7  
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation C2487U  
Authors : Blaha, G.; Gurel, G.  
Deposited on : 2008-02-25  
Resolution : 2.70 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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

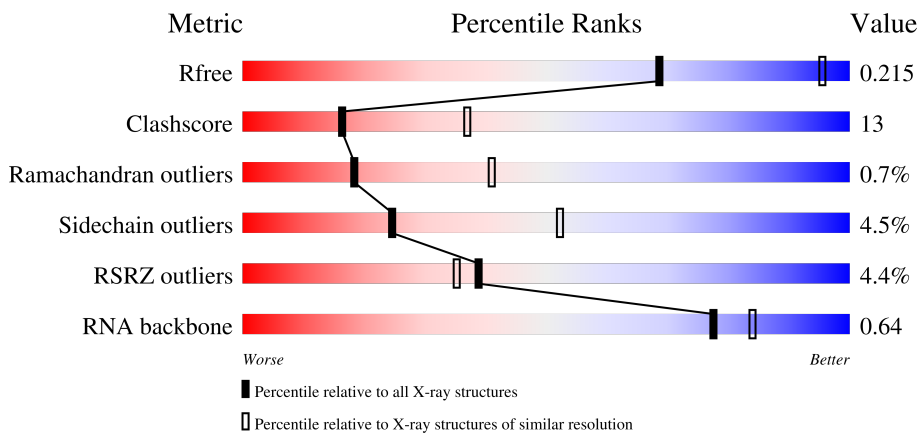
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

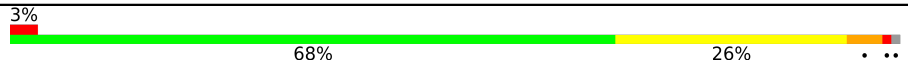
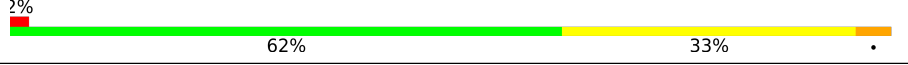
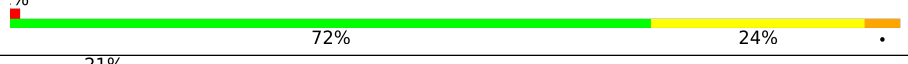
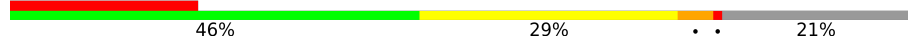
The reported resolution of this entry is 2.70 Å.

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.



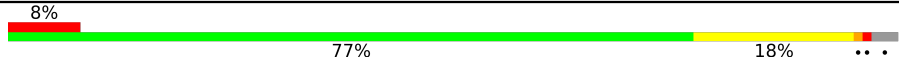
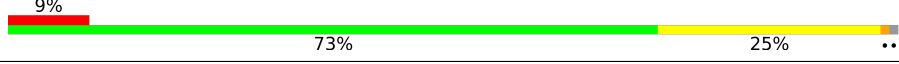
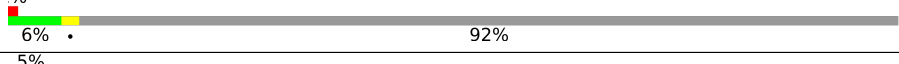


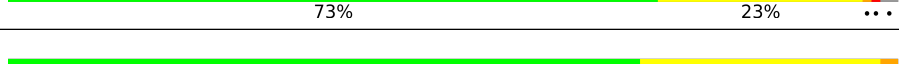
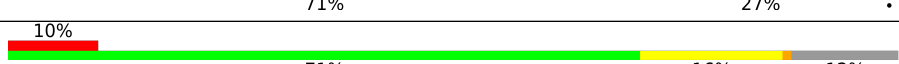
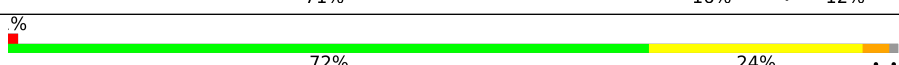
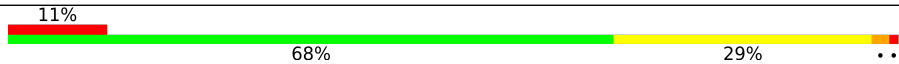


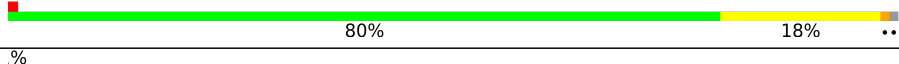
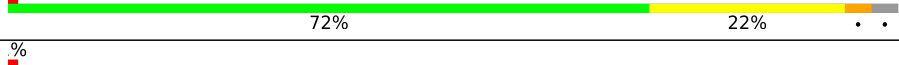

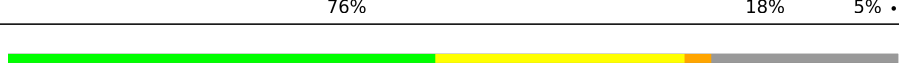



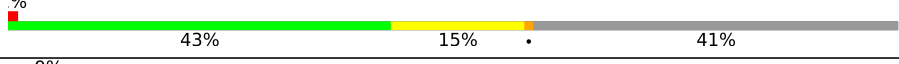
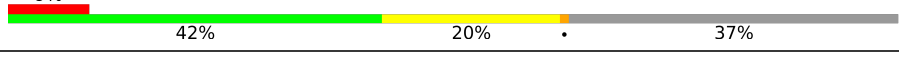





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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	A	240	
2	B	338	
3	C	246	
4	D	177	

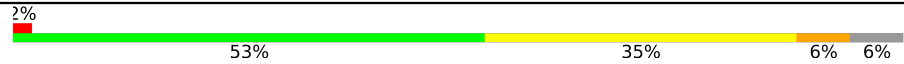

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Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1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

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Mol	Chain	Length	Quality of chain
30	0	2923	 <p>2% 53% 35% 6% 6%</p>
31	9	122	 <p>3% 38% 49% 13%</p>

## 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
			Total	C	N	O	S			
1	A	237	1753	1072	352	324	5	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 33 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total Cl 1 1	0	0
33	B	1	Total Cl 1 1	0	0
33	J	3	Total Cl 3 3	0	0
33	L	1	Total Cl 1 1	0	0
33	M	1	Total Cl 1 1	0	0
33	N	1	Total Cl 1 1	0	0
33	O	1	Total Cl 1 1	0	0
33	R	1	Total Cl 1 1	0	0
33	Y	1	Total Cl 1 1	0	0
33	3	1	Total Cl 1 1	0	0
33	0	10	Total Cl 10 10	0	0

- Molecule 34 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

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

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

- Molecule 35 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	C	1	Total	Na	0	0
			1	1		
35	J	1	Total	Na	0	0
			1	1		
35	M	1	Total	Na	0	0
			1	1		
35	Q	1	Total	Na	0	0
			1	1		
35	R	2	Total	Na	0	0
			2	2		
35	S	1	Total	Na	0	0
			1	1		
35	0	66	Total	Na	0	0
			66	66		
35	9	2	Total	Na	0	0
			2	2		

- Molecule 36 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

- Molecule 37 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	A	111	Total O 111 111	0	0
38	B	153	Total O 153 153	0	0
38	C	165	Total O 165 165	0	0
38	D	46	Total O 46 46	0	0
38	E	44	Total O 44 44	0	0
38	F	23	Total O 23 23	0	0
38	G	19	Total O 19 19	0	0
38	H	71	Total O 71 71	0	0
38	I	10	Total O 10 10	0	0
38	J	54	Total O 54 54	0	0
38	K	56	Total O 56 56	0	0
38	L	80	Total O 80 80	0	0
38	M	130	Total O 130 130	0	0
38	N	59	Total O 59 59	0	0
38	O	41	Total O 41 41	0	0
38	P	61	Total O 61 61	0	0
38	Q	51	Total O 51 51	0	0
38	R	78	Total O 78 78	0	0
38	S	33	Total O 33 33	0	0
38	T	37	Total O 37 37	0	0
38	U	25	Total O 25 25	0	0

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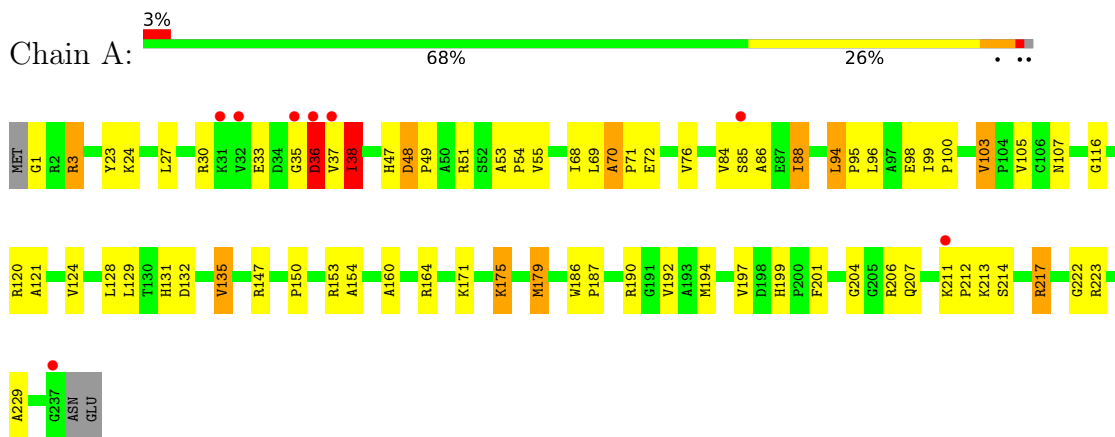
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
38	V	11	Total O 11 11	0	0
38	W	63	Total O 63 63	0	0
38	X	28	Total O 28 28	0	0
38	Y	91	Total O 91 91	0	0
38	Z	28	Total O 28 28	0	0
38	1	52	Total O 52 52	0	0
38	2	37	Total O 37 37	0	0
38	3	68	Total O 68 68	0	0
38	0	5951	Total O 5951 5951	0	0
38	9	147	Total O 147 147	0	0

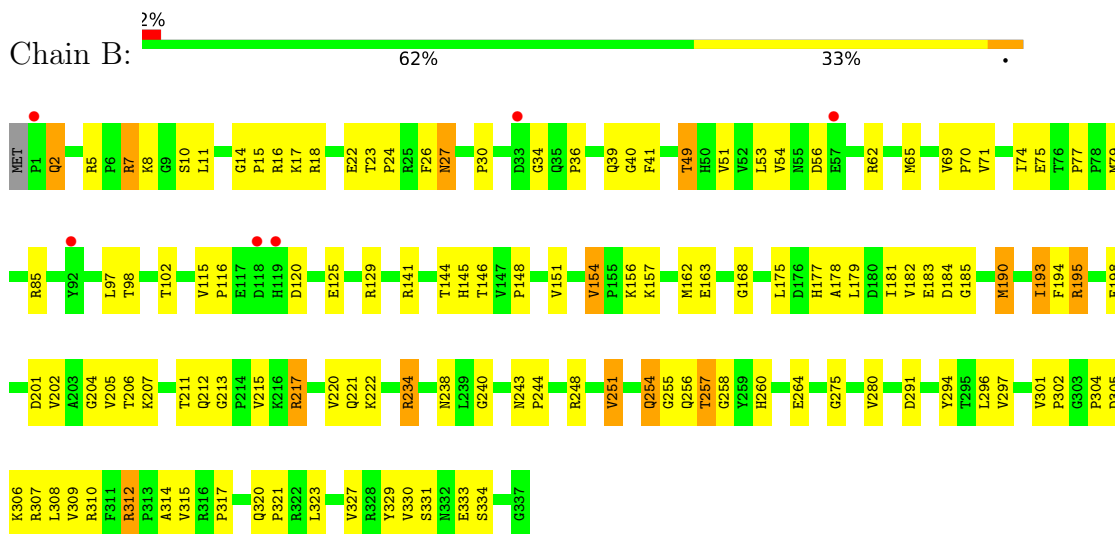
### 3 Residue-property plots [i](#)

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.

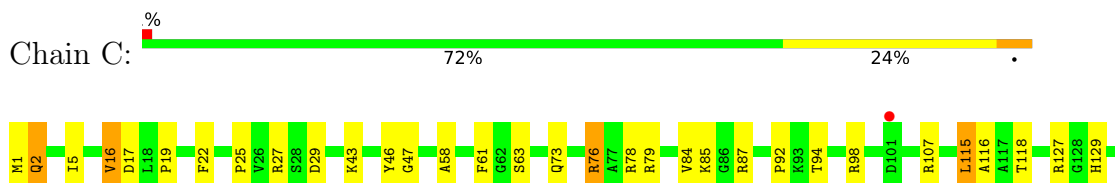
- Molecule 1: 50S ribosomal protein L2P

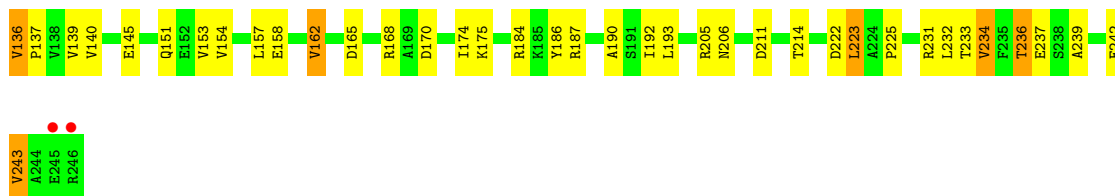


- Molecule 2: 50S ribosomal protein L3P

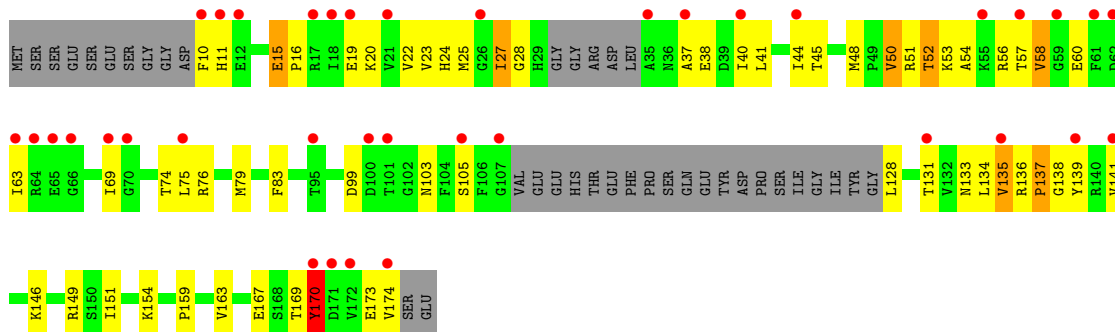


- Molecule 3: 50S ribosomal protein L4P

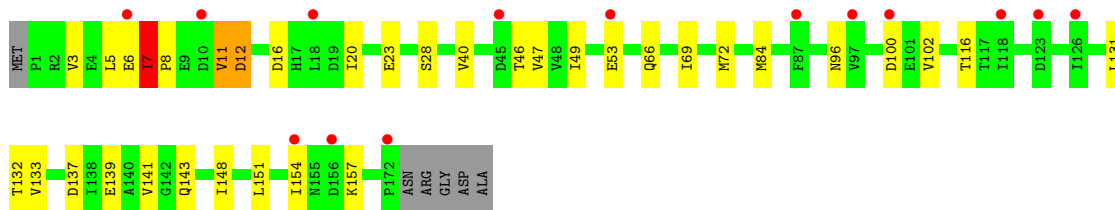
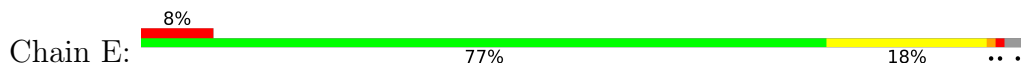




- Molecule 4: 50S ribosomal protein L5P



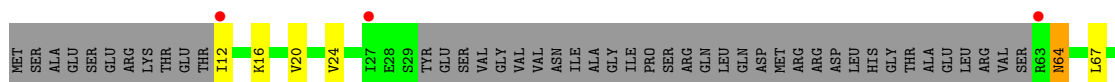
- Molecule 5: 50S ribosomal protein L6P



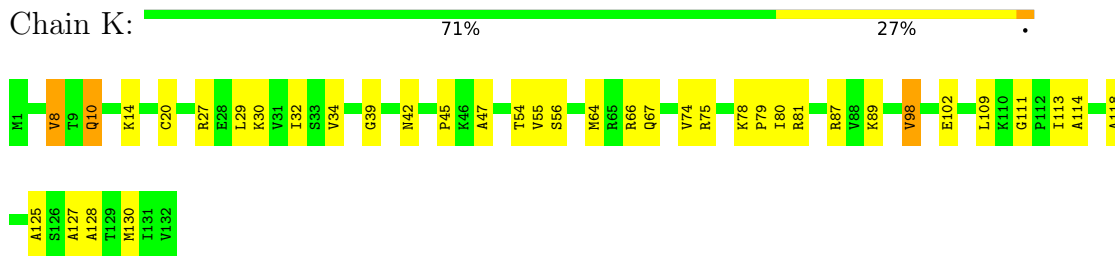
- Molecule 6: 50S ribosomal protein L7Ae



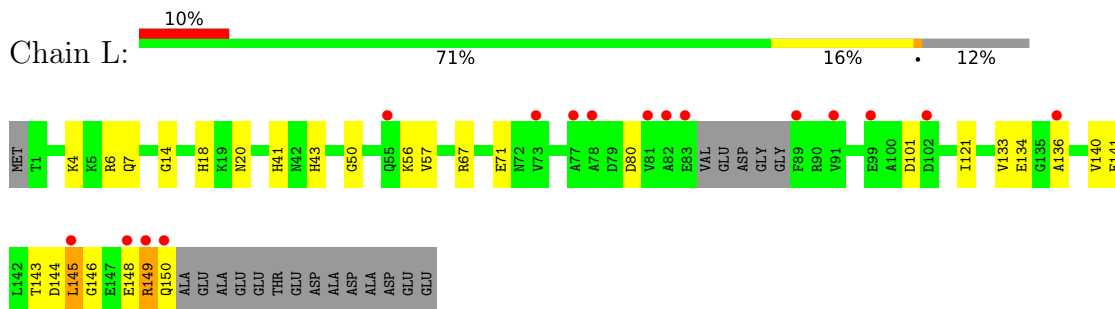
- Molecule 7: 50S ribosomal protein L10E



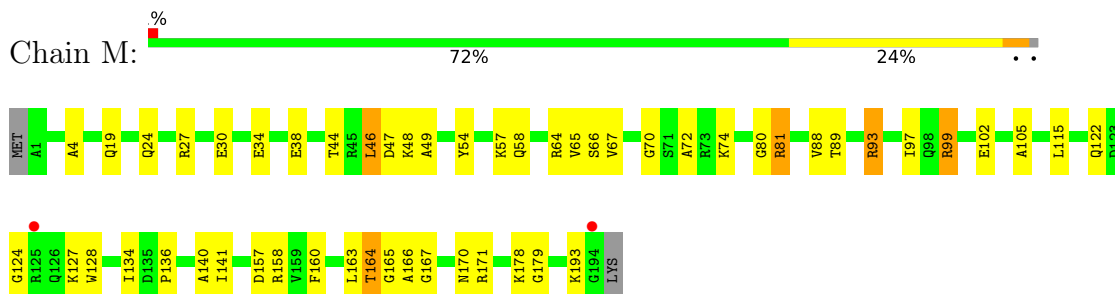




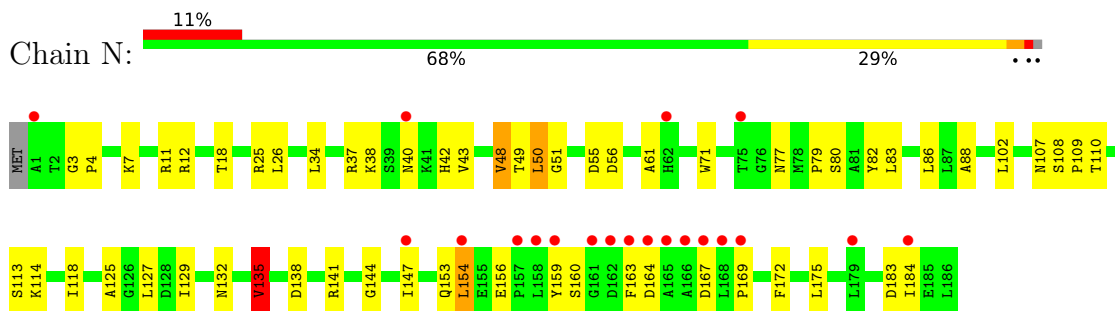
- Molecule 12: 50S ribosomal protein L15P



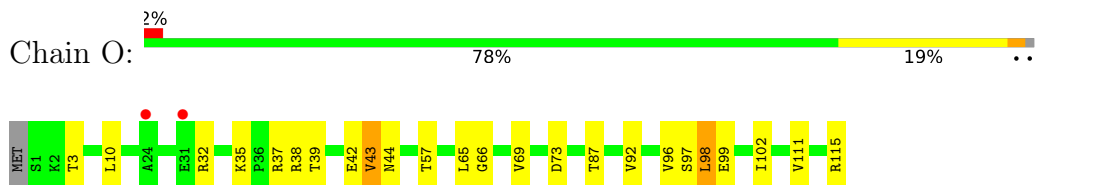
- Molecule 13: 50S ribosomal protein L15e



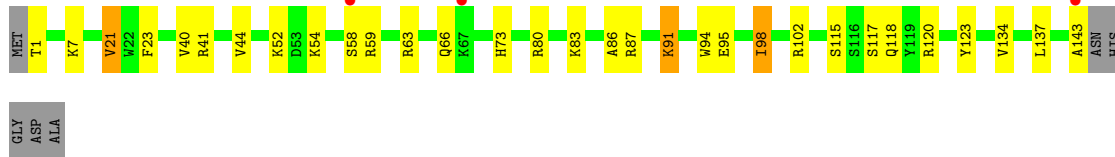
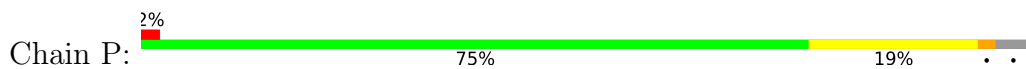
- Molecule 14: 50S ribosomal protein L18P



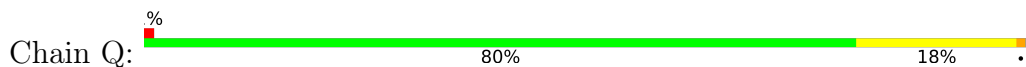
- Molecule 15: 50S ribosomal protein L18e



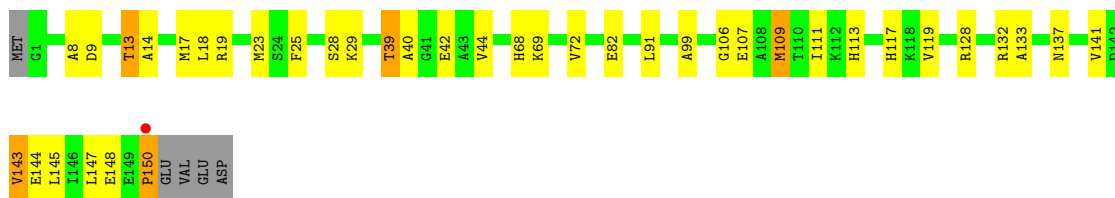
- Molecule 16: 50S ribosomal protein L19e



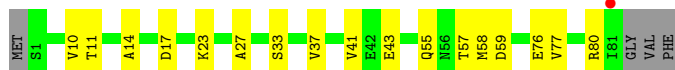
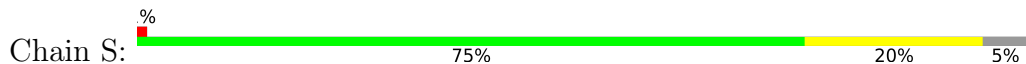
- Molecule 17: 50S ribosomal protein L21e



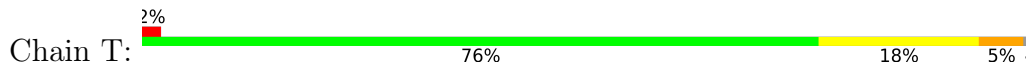
- Molecule 18: 50S ribosomal protein L22P



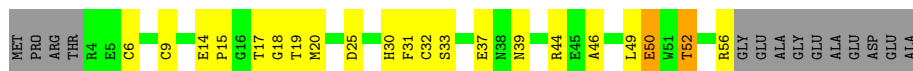
- Molecule 19: 50S ribosomal protein L23P



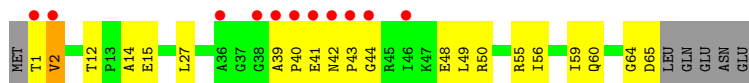
- Molecule 20: 50S ribosomal protein L24P



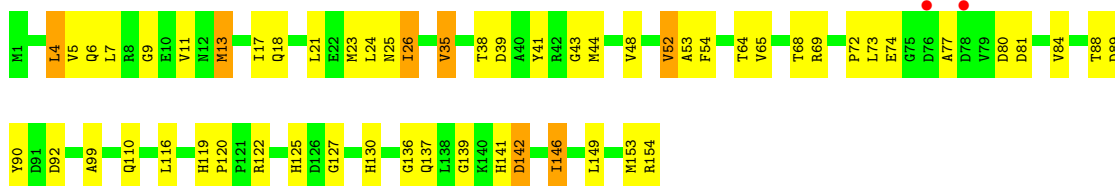
- Molecule 21: 50S ribosomal protein L24e



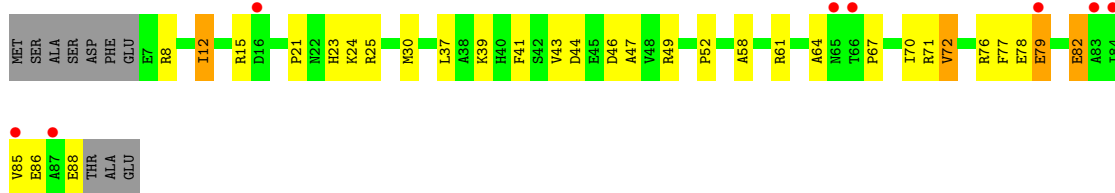
- Molecule 22: 50S ribosomal protein L29P



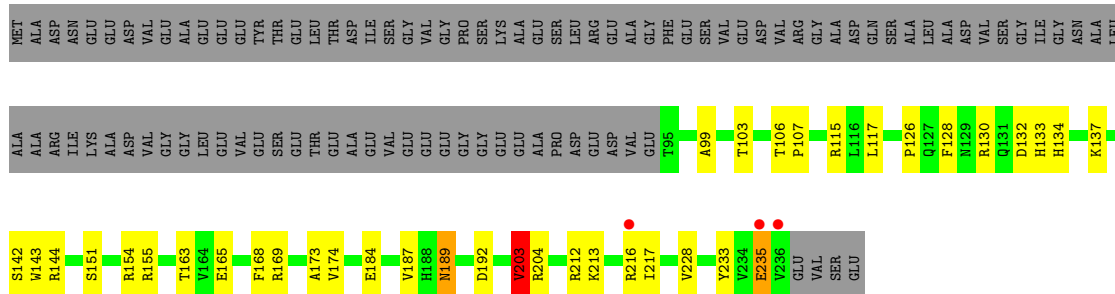
- Molecule 23: 50S ribosomal protein L30P



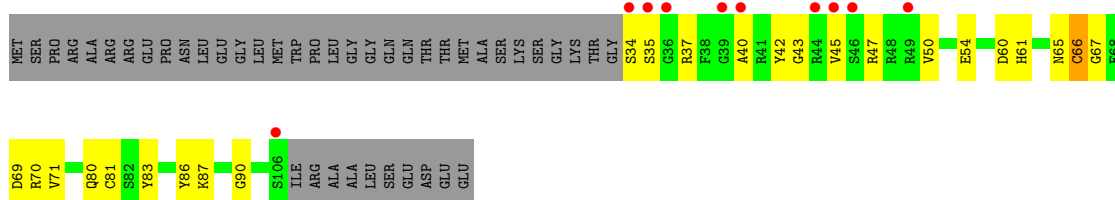
- Molecule 24: 50S ribosomal protein L31e



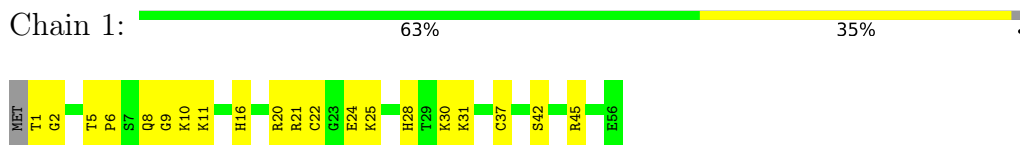
- Molecule 25: 50S ribosomal protein L32e



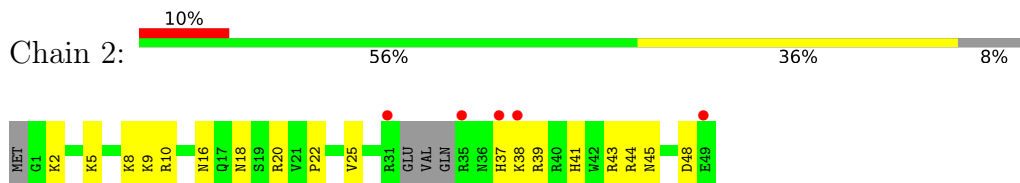
- Molecule 26: 50S ribosomal protein L37Ae



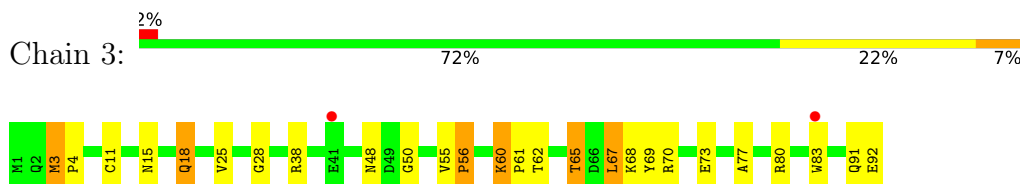
- Molecule 27: 50S ribosomal protein L37e



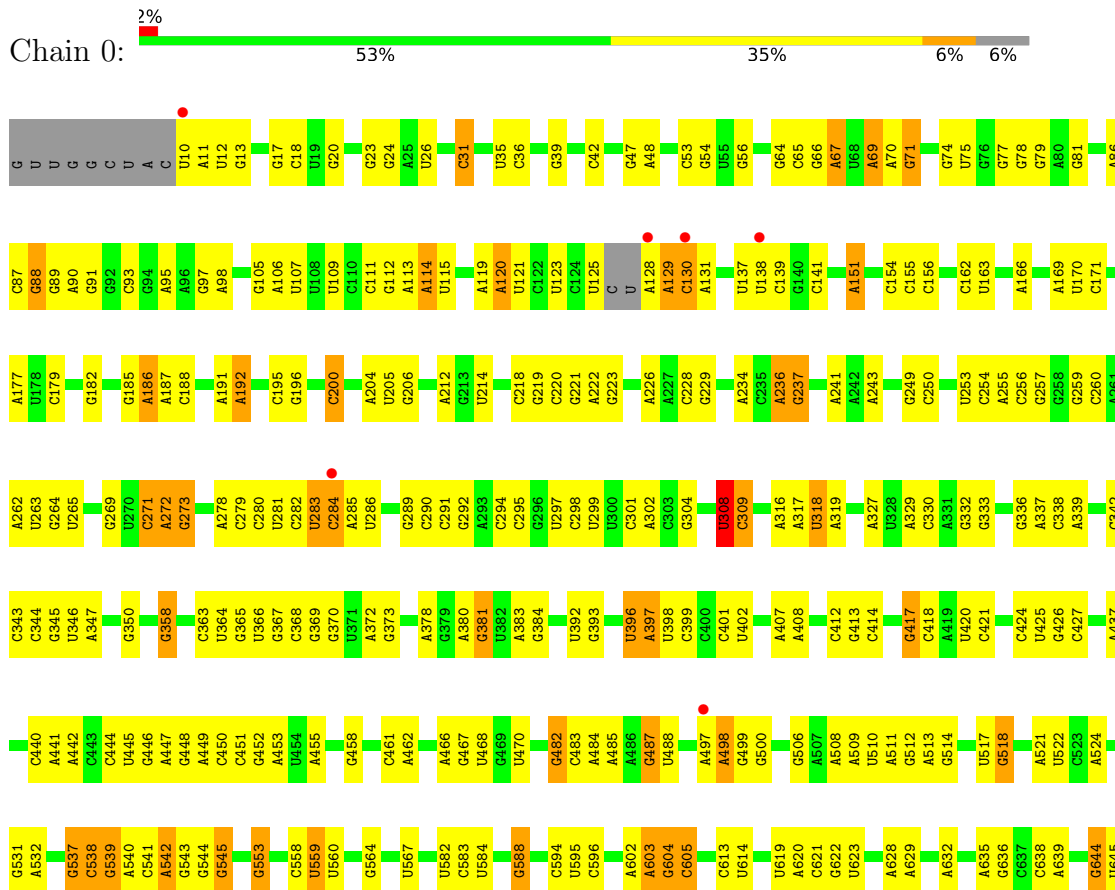
- Molecule 28: 50S ribosomal protein L39e



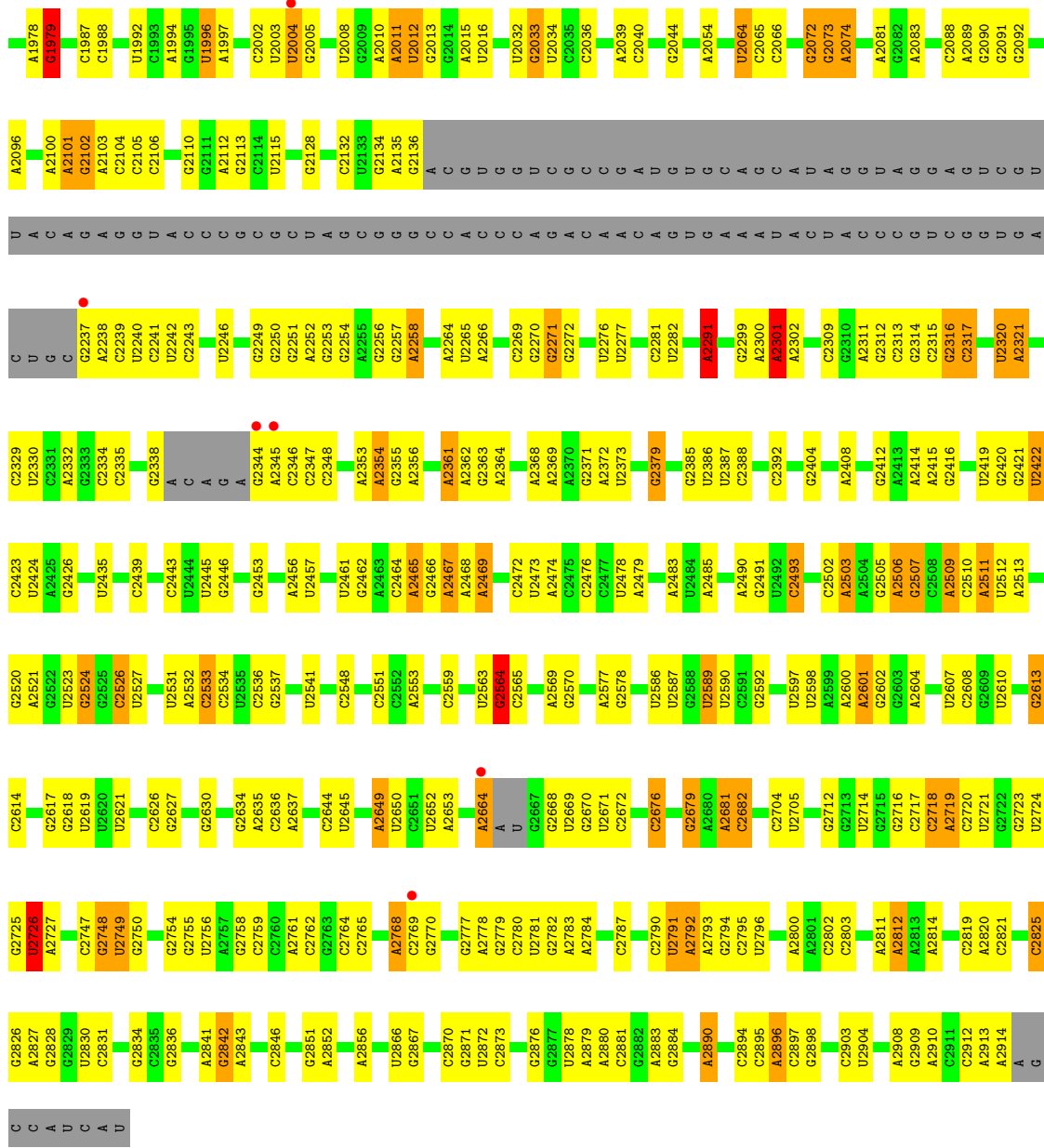
- Molecule 29: 50S ribosomal protein L44E



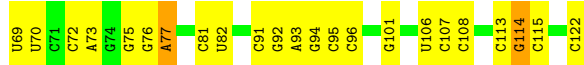
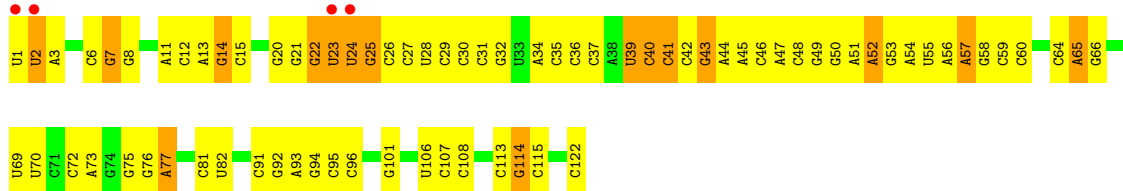
- Molecule 30: 23S ribosomal RNA







• 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, $\alpha$ , $\beta$ , $\gamma$	212.83Å 299.90Å 576.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.83 – 2.70 49.83 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.7 (49.83-2.70) 92.7 (49.83-2.70)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.40Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.184 , 0.226 0.175 , 0.215	Depositor DCC
$R_{free}$ test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.5	Xtrriage
Anisotropy	0.113	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 74.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	99122	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% 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: NA, UR3, OMG, PSU, CL, 1MA, MG, SR, K, CD, OMU

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	0.42	0/1786	0.99	9/2408 (0.4%)
2	B	0.42	0/2690	1.02	16/3652 (0.4%)
3	C	0.44	0/1885	0.94	5/2552 (0.2%)
4	D	0.39	0/1111	0.93	6/1498 (0.4%)
5	E	0.38	0/1382	0.87	3/1880 (0.2%)
6	F	0.39	0/901	0.95	2/1224 (0.2%)
7	G	0.36	0/241	0.85	0/324
8	H	0.38	0/1302	0.92	4/1743 (0.2%)
9	I	0.36	0/526	0.86	0/716
10	J	0.42	0/1136	0.95	7/1530 (0.5%)
11	K	0.40	0/1004	0.95	4/1351 (0.3%)
12	L	0.38	0/1130	0.94	4/1509 (0.3%)
13	M	0.42	0/1582	0.89	3/2116 (0.1%)
14	N	0.37	0/1474	1.01	10/1999 (0.5%)
15	O	0.42	0/874	0.94	3/1181 (0.3%)
16	P	0.39	0/1147	0.85	0/1528
17	Q	0.42	0/749	1.02	5/1005 (0.5%)
18	R	1.29	7/1172 (0.6%)	1.40	8/1578 (0.5%)
19	S	0.36	0/648	0.89	2/875 (0.2%)
20	T	0.39	0/958	0.94	4/1289 (0.3%)
21	U	0.40	0/417	0.86	1/562 (0.2%)
22	V	0.39	0/502	0.97	3/675 (0.4%)
23	W	0.47	1/1219 (0.1%)	0.98	4/1655 (0.2%)
24	X	0.45	0/664	0.99	3/895 (0.3%)
25	Y	0.43	0/1146	0.91	3/1536 (0.2%)
26	Z	0.38	0/584	0.94	1/781 (0.1%)
27	1	0.40	0/438	0.84	0/578
28	2	0.41	0/401	0.77	0/529
29	3	0.38	0/771	0.87	6/1024 (0.6%)
30	0	0.37	0/65957	0.60	14/102867 (0.0%)
31	9	0.36	0/2904	0.59	2/4526 (0.0%)
All	All	0.41	8/98701 (0.0%)	0.72	132/147586 (0.1%)

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
30	0	0	42
31	9	0	1
All	All	1	43

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.40	2.86	1.49
18	R	150	PRO	CA-C	-17.39	1.16	1.52
18	R	150	PRO	CG-CD	13.53	1.96	1.50
18	R	150	PRO	N-CA	12.91	1.66	1.47
18	R	150	PRO	C-O	11.73	1.47	1.23

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-28.56	55.83	110.10
18	R	150	PRO	N-CA-C	-20.16	61.69	112.10
18	R	150	PRO	N-CA-CB	12.25	116.48	103.00
18	R	150	PRO	CA-N-CD	12.10	128.94	112.00
14	N	163	PHE	N-CA-C	-8.93	102.18	113.43

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	221	G	Sidechain
30	0	26	U	Sidechain
30	0	396	U	Sidechain
30	0	458	G	Sidechain
30	0	48	A	Sidechain

## 5.2 Too-close contacts [i](#)

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	77	0
2	B	2625	0	2533	95	0
3	C	1860	0	1813	57	0
4	D	1094	0	1085	44	0
5	E	1357	0	1266	26	0
6	F	890	0	843	26	0
7	G	240	0	231	6	0
8	H	1282	0	1292	39	0
9	I	519	0	500	15	0
10	J	1120	0	1098	32	0
11	K	994	0	1027	36	0
12	L	1118	0	1076	23	0
13	M	1558	0	1573	43	0
14	N	1445	0	1401	46	0
15	O	865	0	873	15	0
16	P	1136	0	1123	28	0
17	Q	735	0	729	14	0
18	R	1149	0	1122	33	0
19	S	641	0	605	10	0
20	T	950	0	924	19	0
21	U	410	0	364	19	0
22	V	499	0	511	17	0
23	W	1196	0	1137	57	0
24	X	654	0	653	23	0
25	Y	1130	0	1133	36	0
26	Z	573	0	531	17	0
27	1	431	0	426	22	0
28	2	396	0	413	18	0
29	3	755	0	728	20	0
30	0	59020	0	29806	1146	0
31	9	2599	0	1325	104	0
32	0	85	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	2	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	2	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	0	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	2	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	J	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	66	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	2	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	5951	0	0	153	0
38	1	52	0	0	3	0
38	2	37	0	0	2	0
38	3	68	0	0	5	0
38	9	147	0	0	8	0
38	A	111	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	B	153	0	0	13	0
38	C	165	0	0	11	0
38	D	46	0	0	2	0
38	E	44	0	0	2	0
38	F	23	0	0	1	0
38	G	19	0	0	0	0
38	H	71	0	0	6	0
38	I	10	0	0	2	0
38	J	54	0	0	2	0
38	K	56	0	0	2	0
38	L	80	0	0	6	0
38	M	130	0	0	5	0
38	N	59	0	0	5	0
38	O	41	0	0	3	0
38	P	61	0	0	1	0
38	Q	51	0	0	2	0
38	R	78	0	0	3	0
38	S	33	0	0	2	0
38	T	37	0	0	2	0
38	U	25	0	0	3	0
38	V	11	0	0	0	0
38	W	63	0	0	4	0
38	X	28	0	0	1	0
38	Y	91	0	0	6	0
38	Z	28	0	0	3	0
All	All	99122	0	59907	1956	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 1956 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	1.44
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.12
30:0:1160:G:C5'	30:0:1161:A:H5'	1.81	1.10
31:9:56:A:H2'	31:9:57:A:H5''	1.33	1.08
30:0:871:G:C8	30:0:871:G:H5'	1.87	1.07

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/240 (98%)	212 (90%)	18 (8%)	5 (2%)	5	15
2	B	335/338 (99%)	306 (91%)	26 (8%)	3 (1%)	14	35
3	C	244/246 (99%)	228 (93%)	16 (7%)	0	100	100
4	D	134/177 (76%)	112 (84%)	19 (14%)	3 (2%)	5	14
5	E	170/178 (96%)	161 (95%)	9 (5%)	0	100	100
6	F	117/120 (98%)	107 (92%)	9 (8%)	1 (1%)	14	35
7	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
8	H	156/177 (88%)	149 (96%)	6 (4%)	1 (1%)	21	44
9	I	68/162 (42%)	55 (81%)	10 (15%)	3 (4%)	2	4
10	J	140/145 (97%)	131 (94%)	9 (6%)	0	100	100
11	K	130/132 (98%)	125 (96%)	5 (4%)	0	100	100
12	L	141/165 (86%)	127 (90%)	13 (9%)	1 (1%)	18	41
13	M	192/196 (98%)	182 (95%)	9 (5%)	1 (0%)	24	48
14	N	184/187 (98%)	168 (91%)	13 (7%)	3 (2%)	7	20
15	O	113/116 (97%)	109 (96%)	4 (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%)	140 (95%)	8 (5%)	0	100	100
19	S	79/85 (93%)	78 (99%)	1 (1%)	0	100	100
20	T	117/120 (98%)	110 (94%)	6 (5%)	1 (1%)	14	35
21	U	51/67 (76%)	47 (92%)	4 (8%)	0	100	100
22	V	63/71 (89%)	60 (95%)	2 (3%)	1 (2%)	7	20
23	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
24	X	80/92 (87%)	73 (91%)	6 (8%)	1 (1%)	9	25
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%)	61 (86%)	8 (11%)	2 (3%)	4	9
27	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	11	29
All	All	3705/4472 (83%)	3458 (93%)	220 (6%)	27 (1%)	18	41

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	37	VAL
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/182 (98%)	169 (94%)	10 (6%)	19	44
2	B	282/283 (100%)	266 (94%)	16 (6%)	18	43
3	C	193/193 (100%)	178 (92%)	15 (8%)	11	29
4	D	117/148 (79%)	109 (93%)	8 (7%)	14	35
5	E	152/156 (97%)	146 (96%)	6 (4%)	28	57
6	F	93/94 (99%)	93 (100%)	0	100	100
7	G	27/282 (10%)	26 (96%)	1 (4%)	30	59
8	H	134/145 (92%)	125 (93%)	9 (7%)	15	36
9	I	58/130 (45%)	57 (98%)	1 (2%)	53	79
10	J	118/121 (98%)	112 (95%)	6 (5%)	21	48
11	K	106/106 (100%)	103 (97%)	3 (3%)	38	68
12	L	113/127 (89%)	110 (97%)	3 (3%)	39	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	158/160 (99%)	152 (96%)	6 (4%)	29	58
14	N	149/150 (99%)	142 (95%)	7 (5%)	23	51
15	O	93/94 (99%)	90 (97%)	3 (3%)	34	64
16	P	113/117 (97%)	109 (96%)	4 (4%)	32	61
17	Q	79/80 (99%)	77 (98%)	2 (2%)	42	71
18	R	117/122 (96%)	111 (95%)	6 (5%)	21	48
19	S	71/74 (96%)	71 (100%)	0	100	100
20	T	105/106 (99%)	99 (94%)	6 (6%)	18	43
21	U	44/53 (83%)	43 (98%)	1 (2%)	44	73
22	V	51/57 (90%)	50 (98%)	1 (2%)	48	76
23	W	130/130 (100%)	123 (95%)	7 (5%)	20	45
24	X	66/74 (89%)	59 (89%)	7 (11%)	6	17
25	Y	120/196 (61%)	115 (96%)	5 (4%)	26	55
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%)	43	72
29	3	79/79 (100%)	75 (95%)	4 (5%)	21	48
All	All	3095/3646 (85%)	2957 (96%)	138 (4%)	24	52

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	W	26	ILE
23	W	142	ASP
25	Y	189	ASN
4	D	170	TYR
4	D	149	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
18	R	113	HIS
23	W	28	HIS
18	R	140	GLN
21	U	39	ASN

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Mol	Chain	Res	Type
23	W	141	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	244 (8%)	32 (1%)
31	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3045 (94%)	260 (9%)	33 (1%)

5 of 260 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 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	2649	A
30	0	2718	C
31	9	65	A
30	0	1080	C
30	0	877	G

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

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	OMG	0	2588	30	23,26,27	0.32	0	32,38,41	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	OMU	0	2587	30	19,22,23	0.33	0	25,31,34	0.36	0
30	1MA	0	628	35,30	21,25,26	0.69	1 (4%)	30,37,40	0.69	1 (3%)
30	PSU	0	2621	30	18,21,22	1.53	2 (11%)	21,30,33	1.37	3 (14%)
30	UR3	0	2619	30	19,22,23	0.45	0	26,32,35	0.71	1 (3%)

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	OMG	0	2588	30	-	0/9/27/28	0/3/3/3
30	OMU	0	2587	30	-	0/9/27/28	0/2/2/2
30	1MA	0	628	35,30	-	2/7/25/26	0/3/3/3
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	UR3	0	2619	30	-	0/7/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	5.08	1.43	1.36
30	0	2621	PSU	C6-C5	2.61	1.38	1.35
30	0	628	1MA	C6-N6	2.32	1.33	1.28

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	C6-C5-C4	3.62	120.62	118.17
30	0	2621	PSU	O2-C2-N1	2.92	125.80	122.79
30	0	2621	PSU	C6-N1-C2	-2.84	120.06	122.69
30	0	2619	UR3	C4-N3-C2	2.81	126.84	124.58
30	0	628	1MA	N1-C2-N3	2.76	129.27	126.00

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	0	628	1MA	C2'-C1'-N9-C8
30	0	628	1MA	C2'-C1'-N9-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	237/240 (98%)	0.09	8 (3%) 48 44	26, 50, 86, 109	0
2	B	337/338 (99%)	0.17	6 (1%) 67 65	28, 51, 79, 93	0
3	C	246/246 (100%)	-0.02	3 (1%) 76 75	21, 43, 69, 77	0
4	D	140/177 (79%)	1.61	37 (26%) 1 1	56, 98, 124, 134	0
5	E	172/178 (96%)	0.56	14 (8%) 18 15	43, 66, 87, 91	0
6	F	119/120 (99%)	0.78	11 (9%) 14 12	47, 70, 99, 114	0
7	G	29/348 (8%)	1.38	5 (17%) 4 3	75, 93, 103, 106	0
8	H	160/177 (90%)	0.27	8 (5%) 34 30	34, 54, 92, 100	0
9	I	70/162 (43%)	2.79	51 (72%) 0 0	129, 145, 162, 163	0
10	J	142/145 (97%)	0.14	4 (2%) 55 51	34, 48, 70, 91	0
11	K	132/132 (100%)	0.00	0 100 100	31, 49, 72, 78	0
12	L	145/165 (87%)	0.61	16 (11%) 10 9	24, 63, 111, 125	0
13	M	194/196 (98%)	-0.16	2 (1%) 79 78	28, 40, 55, 64	0
14	N	186/187 (99%)	0.75	20 (10%) 11 9	39, 61, 111, 121	0
15	O	115/116 (99%)	0.30	2 (1%) 69 67	36, 51, 69, 79	0
16	P	143/149 (95%)	0.22	3 (2%) 63 61	37, 53, 67, 76	0
17	Q	95/96 (98%)	-0.04	1 (1%) 78 76	33, 43, 59, 76	0
18	R	150/155 (96%)	-0.24	1 (0%) 84 83	30, 43, 62, 77	0
19	S	81/85 (95%)	0.16	1 (1%) 76 75	38, 57, 78, 89	0
20	T	119/120 (99%)	0.28	2 (1%) 69 67	37, 54, 86, 111	0
21	U	53/67 (79%)	0.16	0 100 100	40, 54, 72, 80	0
22	V	65/71 (91%)	1.02	11 (16%) 4 3	51, 71, 116, 122	0
23	W	154/154 (100%)	0.12	2 (1%) 75 73	32, 48, 64, 77	0
24	X	82/92 (89%)	0.46	8 (9%) 13 11	39, 58, 83, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	142/241 (58%)	-0.06	3 (2%) 63 61	23, 43, 66, 86	0
26	Z	73/116 (62%)	0.96	10 (13%) 6 5	49, 67, 83, 95	0
27	1	56/57 (98%)	-0.68	0 100 100	25, 31, 39, 47	0
28	2	46/50 (92%)	0.68	5 (10%) 10 9	31, 59, 88, 100	0
29	3	92/92 (100%)	0.15	2 (2%) 62 59	33, 55, 68, 83	0
30	0	2749/2923 (94%)	-0.51	55 (2%) 65 62	19, 42, 87, 162	0
31	9	122/122 (100%)	0.05	4 (3%) 49 45	35, 61, 85, 146	0
All	All	6646/7517 (88%)	-0.02	295 (4%) 39 35	19, 49, 98, 163	0

The worst 5 of 295 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	1	THR	10.8
9	I	128	THR	8.5
31	9	1	U	7.4
4	D	174	VAL	6.1
9	I	113	SER	6.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
30	UR3	0	2619	21/22	0.97	0.07	34,37,39,43	0
30	OMU	0	2587	21/22	0.98	0.06	29,32,34,36	0
30	OMG	0	2588	24/25	0.98	0.06	28,32,34,36	0
30	1MA	0	628	23/24	0.98	0.06	22,25,28,28	0
30	PSU	0	2621	20/21	0.98	0.05	24,26,33,33	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands i

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
35	NA	0	8548	1/1	0.65	0.38	59,59,59,59	0
35	NA	0	8573	1/1	0.68	0.24	69,69,69,69	0
34	SR	0	9001	1/1	0.69	0.14	171,171,171,171	0
34	SR	0	8976	1/1	0.73	0.24	194,194,194,194	0
34	SR	9	9003	1/1	0.75	0.19	169,169,169,169	0
34	SR	0	9006	1/1	0.76	0.27	200,200,200,200	0
34	SR	0	8983	1/1	0.76	0.18	177,177,177,177	0
35	NA	0	8557	1/1	0.77	0.34	68,68,68,68	0
35	NA	0	8571	1/1	0.77	0.24	73,73,73,73	0
34	SR	9	8980	1/1	0.77	0.14	177,177,177,177	0
34	SR	J	8986	1/1	0.79	0.30	200,200,200,200	0
34	SR	0	8979	1/1	0.79	0.20	199,199,199,199	0
34	SR	0	8971	1/1	0.79	0.18	165,165,165,165	0
34	SR	0	8991	1/1	0.79	0.23	188,188,188,188	0
34	SR	0	9004	1/1	0.80	0.34	200,200,200,200	0
35	NA	0	8559	1/1	0.81	0.39	71,71,71,71	0
34	SR	0	8997	1/1	0.81	0.24	190,190,190,190	0
34	SR	0	8922	1/1	0.81	0.21	160,160,160,160	0
35	NA	0	8546	1/1	0.82	0.30	77,77,77,77	0
35	NA	R	8575	1/1	0.82	0.29	82,82,82,82	0
34	SR	0	8947	1/1	0.83	0.19	178,178,178,178	0
34	SR	0	8919	1/1	0.83	0.17	173,173,173,173	0
34	SR	0	8996	1/1	0.83	0.27	200,200,200,200	0
32	MG	9	8074	1/1	0.83	0.21	74,74,74,74	0
34	SR	0	8944	1/1	0.83	0.20	161,161,161,161	0
35	NA	0	8525	1/1	0.83	0.20	79,79,79,79	0
35	NA	9	8543	1/1	0.83	0.21	47,47,47,47	0
35	NA	0	8554	1/1	0.84	0.25	63,63,63,63	0
35	NA	0	8574	1/1	0.84	0.39	61,61,61,61	0
34	SR	A	8977	1/1	0.84	0.12	158,158,158,158	0
32	MG	0	8071	1/1	0.85	0.30	53,53,53,53	0
35	NA	0	8567	1/1	0.86	0.37	65,65,65,65	0
32	MG	A	8051	1/1	0.86	0.12	72,72,72,72	0
35	NA	0	8506	1/1	0.86	0.16	66,66,66,66	0
34	SR	0	8939	1/1	0.86	0.14	146,146,146,146	0
34	SR	0	8959	1/1	0.86	0.17	159,159,159,159	0
34	SR	0	8988	1/1	0.87	0.10	158,158,158,158	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	SR	0	9002	1/1	0.87	0.21	175,175,175,175	0
35	NA	0	8562	1/1	0.87	0.42	62,62,62,62	0
34	SR	0	8974	1/1	0.87	0.18	166,166,166,166	0
32	MG	0	8073	1/1	0.88	0.27	79,79,79,79	0
34	SR	B	8987	1/1	0.88	0.37	200,200,200,200	0
32	MG	0	8037	1/1	0.88	0.19	89,89,89,89	0
34	SR	0	9000	1/1	0.88	0.23	157,157,157,157	0
35	NA	0	8564	1/1	0.89	0.14	63,63,63,63	0
32	MG	T	8057	1/1	0.89	0.11	58,58,58,58	0
32	MG	0	8083	1/1	0.89	0.11	55,55,55,55	0
35	NA	0	8522	1/1	0.89	0.18	58,58,58,58	0
34	SR	0	8993	1/1	0.89	0.12	165,165,165,165	0
34	SR	0	8927	1/1	0.89	0.14	150,150,150,150	0
34	SR	0	8968	1/1	0.90	0.12	146,146,146,146	0
32	MG	0	8092	1/1	0.90	0.16	51,51,51,51	0
34	SR	0	8960	1/1	0.90	0.17	141,141,141,141	0
34	SR	0	8998	1/1	0.90	0.21	171,171,171,171	0
35	NA	0	8558	1/1	0.90	0.17	44,44,44,44	0
34	SR	0	8962	1/1	0.90	0.19	164,164,164,164	0
35	NA	0	8561	1/1	0.90	0.37	68,68,68,68	0
32	MG	0	8049	1/1	0.91	0.21	65,65,65,65	0
32	MG	0	8031	1/1	0.91	0.12	55,55,55,55	0
33	CL	N	8807	1/1	0.91	0.12	68,68,68,68	0
34	SR	0	8951	1/1	0.91	0.10	132,132,132,132	0
34	SR	0	8955	1/1	0.91	0.20	189,189,189,189	0
35	NA	0	8560	1/1	0.91	0.26	92,92,92,92	0
34	SR	0	8957	1/1	0.91	0.15	188,188,188,188	0
35	NA	0	8511	1/1	0.91	0.22	63,63,63,63	0
35	NA	0	8518	1/1	0.91	0.27	65,65,65,65	0
34	SR	0	8958	1/1	0.91	0.08	86,86,86,86	0
35	NA	0	8523	1/1	0.91	0.08	29,29,29,29	0
34	SR	0	8981	1/1	0.91	0.17	153,153,153,153	0
35	NA	0	8541	1/1	0.91	0.12	50,50,50,50	0
34	SR	0	8933	1/1	0.91	0.15	127,127,127,127	0
35	NA	0	8514	1/1	0.92	0.11	41,41,41,41	0
34	SR	0	8994	1/1	0.92	0.46	198,198,198,198	0
34	SR	0	8982	1/1	0.92	0.42	189,189,189,189	0
34	SR	0	8924	1/1	0.92	0.14	134,134,134,134	0
34	SR	0	8965	1/1	0.92	0.10	117,117,117,117	0
35	NA	0	8533	1/1	0.92	0.08	55,55,55,55	0
35	NA	0	8535	1/1	0.92	0.18	46,46,46,46	0
35	NA	R	8532	1/1	0.92	0.11	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8544	1/1	0.92	0.21	64,64,64,64	0
34	SR	0	8989	1/1	0.92	0.19	168,168,168,168	0
34	SR	F	9005	1/1	0.92	0.13	122,122,122,122	0
34	SR	0	8915	1/1	0.92	0.10	115,115,115,115	0
35	NA	0	8555	1/1	0.93	0.23	61,61,61,61	0
32	MG	0	8033	1/1	0.93	0.10	51,51,51,51	0
32	MG	0	8036	1/1	0.93	0.11	49,49,49,49	0
34	SR	0	8953	1/1	0.93	0.12	143,143,143,143	0
34	SR	0	8970	1/1	0.93	0.09	115,115,115,115	0
32	MG	0	8081	1/1	0.93	0.13	64,64,64,64	0
34	SR	0	9007	1/1	0.93	0.26	200,200,200,200	0
32	MG	0	8063	1/1	0.93	0.14	69,69,69,69	0
35	NA	0	8565	1/1	0.93	0.13	57,57,57,57	0
34	SR	0	8975	1/1	0.93	0.10	120,120,120,120	0
35	NA	0	8569	1/1	0.93	0.17	53,53,53,53	0
34	SR	0	8995	1/1	0.93	0.10	117,117,117,117	0
34	SR	0	8916	1/1	0.93	0.13	98,98,98,98	0
34	SR	B	8950	1/1	0.93	0.10	101,101,101,101	0
34	SR	0	8946	1/1	0.93	0.10	102,102,102,102	0
35	NA	9	8572	1/1	0.93	0.12	64,64,64,64	0
37	K	0	8401	1/1	0.93	0.14	88,88,88,88	0
37	K	0	8402	1/1	0.93	0.15	62,62,62,62	0
33	CL	L	8810	1/1	0.94	0.11	50,50,50,50	0
35	NA	0	8552	1/1	0.94	0.11	59,59,59,59	0
35	NA	0	8553	1/1	0.94	0.16	67,67,67,67	0
32	MG	0	8068	1/1	0.94	0.08	64,64,64,64	0
32	MG	0	8069	1/1	0.94	0.19	65,65,65,65	0
35	NA	0	8556	1/1	0.94	0.22	41,41,41,41	0
34	SR	0	8985	1/1	0.94	0.22	118,118,118,118	0
32	MG	0	8040	1/1	0.94	0.20	84,84,84,84	0
34	SR	0	8938	1/1	0.94	0.09	139,139,139,139	0
35	NA	0	8505	1/1	0.94	0.41	45,45,45,45	0
34	SR	0	8963	1/1	0.94	0.09	105,105,105,105	0
35	NA	0	8509	1/1	0.94	0.14	50,50,50,50	0
34	SR	0	8992	1/1	0.94	0.32	125,125,125,125	0
34	SR	0	8964	1/1	0.94	0.08	110,110,110,110	0
32	MG	0	8030	1/1	0.94	0.15	60,60,60,60	0
34	SR	0	8967	1/1	0.94	0.08	116,116,116,116	0
34	SR	0	8941	1/1	0.94	0.09	113,113,113,113	0
32	MG	0	8053	1/1	0.94	0.10	53,53,53,53	0
32	MG	0	8060	1/1	0.94	0.09	54,54,54,54	0
32	MG	0	8089	1/1	0.94	0.10	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8039	1/1	0.94	0.07	64,64,64,64	0
32	MG	0	8066	1/1	0.94	0.09	57,57,57,57	0
34	SR	0	8920	1/1	0.94	0.08	113,113,113,113	0
34	SR	0	8969	1/1	0.95	0.18	134,134,134,134	0
35	NA	0	8508	1/1	0.95	0.07	39,39,39,39	0
34	SR	0	8943	1/1	0.95	0.09	104,104,104,104	0
32	MG	0	8082	1/1	0.95	0.07	56,56,56,56	0
34	SR	0	8973	1/1	0.95	0.09	121,121,121,121	0
35	NA	0	8516	1/1	0.95	0.07	28,28,28,28	0
33	CL	0	8805	1/1	0.95	0.12	58,58,58,58	0
35	NA	0	8520	1/1	0.95	0.14	54,54,54,54	0
35	NA	0	8521	1/1	0.95	0.12	54,54,54,54	0
34	SR	0	8928	1/1	0.95	0.11	125,125,125,125	0
32	MG	0	8080	1/1	0.95	0.07	66,66,66,66	0
33	CL	B	8819	1/1	0.95	0.08	50,50,50,50	0
35	NA	0	8527	1/1	0.95	0.12	43,43,43,43	0
35	NA	0	8531	1/1	0.95	0.07	41,41,41,41	0
35	NA	J	8538	1/1	0.95	0.12	57,57,57,57	0
34	SR	0	8954	1/1	0.95	0.07	94,94,94,94	0
33	CL	J	8801	1/1	0.95	0.08	54,54,54,54	0
35	NA	0	8542	1/1	0.95	0.13	42,42,42,42	0
35	NA	S	8510	1/1	0.95	0.08	34,34,34,34	0
35	NA	0	8502	1/1	0.95	0.12	55,55,55,55	0
35	NA	0	8547	1/1	0.95	0.22	51,51,51,51	0
32	MG	0	8079	1/1	0.95	0.09	50,50,50,50	0
33	CL	O	8808	1/1	0.96	0.11	62,62,62,62	0
35	NA	0	8545	1/1	0.96	0.14	38,38,38,38	0
33	CL	Y	8820	1/1	0.96	0.08	38,38,38,38	0
32	MG	0	8085	1/1	0.96	0.17	73,73,73,73	0
34	SR	0	8931	1/1	0.96	0.06	94,94,94,94	0
35	NA	0	8549	1/1	0.96	0.17	58,58,58,58	0
35	NA	0	8550	1/1	0.96	0.11	55,55,55,55	0
33	CL	0	8813	1/1	0.96	0.06	44,44,44,44	0
34	SR	0	8934	1/1	0.96	0.19	108,108,108,108	0
34	SR	0	8937	1/1	0.96	0.05	103,103,103,103	0
34	SR	A	8929	1/1	0.96	0.13	113,113,113,113	0
35	NA	0	8513	1/1	0.96	0.12	45,45,45,45	0
32	MG	0	8038	1/1	0.96	0.05	68,68,68,68	0
32	MG	0	8090	1/1	0.96	0.09	55,55,55,55	0
32	MG	0	8076	1/1	0.96	0.07	32,32,32,32	0
35	NA	0	8519	1/1	0.96	0.07	36,36,36,36	0
32	MG	0	8093	1/1	0.96	0.04	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
34	SR	0	8972	1/1	0.96	0.18	112,112,112,112	0
32	MG	0	8018	1/1	0.96	0.11	36,36,36,36	0
34	SR	0	8914	1/1	0.96	0.13	107,107,107,107	0
32	MG	0	8035	1/1	0.96	0.12	62,62,62,62	0
35	NA	0	8568	1/1	0.96	0.08	53,53,53,53	0
32	MG	B	8042	1/1	0.96	0.07	47,47,47,47	0
35	NA	0	8528	1/1	0.96	0.09	40,40,40,40	0
35	NA	0	8530	1/1	0.96	0.10	47,47,47,47	0
33	CL	J	8821	1/1	0.96	0.07	59,59,59,59	0
32	MG	0	8017	1/1	0.96	0.10	23,23,23,23	0
34	SR	0	8956	1/1	0.96	0.07	128,128,128,128	0
35	NA	Q	8540	1/1	0.96	0.10	41,41,41,41	0
32	MG	0	8059	1/1	0.96	0.05	35,35,35,35	0
34	SR	0	8990	1/1	0.97	0.07	113,113,113,113	0
32	MG	0	8088	1/1	0.97	0.04	34,34,34,34	0
35	NA	0	8507	1/1	0.97	0.06	40,40,40,40	0
34	SR	0	8942	1/1	0.97	0.07	115,115,115,115	0
34	SR	0	8966	1/1	0.97	0.06	100,100,100,100	0
35	NA	0	8551	1/1	0.97	0.12	47,47,47,47	0
34	SR	0	8917	1/1	0.97	0.06	95,95,95,95	0
33	CL	0	8815	1/1	0.97	0.09	58,58,58,58	0
34	SR	0	8945	1/1	0.97	0.06	105,105,105,105	0
33	CL	0	8816	1/1	0.97	0.12	54,54,54,54	0
35	NA	0	8517	1/1	0.97	0.14	31,31,31,31	0
34	SR	0	8921	1/1	0.97	0.06	84,84,84,84	0
34	SR	0	8949	1/1	0.97	0.08	90,90,90,90	0
33	CL	0	8817	1/1	0.97	0.05	50,50,50,50	0
32	MG	0	8062	1/1	0.97	0.10	47,47,47,47	0
34	SR	0	8926	1/1	0.97	0.08	107,107,107,107	0
33	CL	J	8802	1/1	0.97	0.04	56,56,56,56	0
35	NA	0	8563	1/1	0.97	0.11	65,65,65,65	0
34	SR	0	8978	1/1	0.97	0.06	108,108,108,108	0
32	MG	0	8024	1/1	0.97	0.22	61,61,61,61	0
35	NA	0	8566	1/1	0.97	0.18	58,58,58,58	0
32	MG	0	8091	1/1	0.97	0.17	54,54,54,54	0
35	NA	C	8503	1/1	0.97	0.04	31,31,31,31	0
32	MG	0	8077	1/1	0.97	0.04	35,35,35,35	0
32	MG	0	8078	1/1	0.97	0.04	43,43,43,43	0
34	SR	0	8984	1/1	0.97	0.06	105,105,105,105	0
35	NA	0	8537	1/1	0.97	0.04	32,32,32,32	0
34	SR	S	8961	1/1	0.97	0.06	113,113,113,113	0
32	MG	0	8056	1/1	0.97	0.07	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	CL	A	8809	1/1	0.97	0.08	60,60,60,60	0
35	NA	0	8504	1/1	0.97	0.06	33,33,33,33	0
34	SR	A	8930	1/1	0.98	0.05	100,100,100,100	0
32	MG	0	8034	1/1	0.98	0.06	36,36,36,36	0
32	MG	0	8070	1/1	0.98	0.04	40,40,40,40	0
32	MG	0	8055	1/1	0.98	0.03	30,30,30,30	0
32	MG	K	8054	1/1	0.98	0.03	37,37,37,37	0
34	SR	0	8936	1/1	0.98	0.03	84,84,84,84	0
32	MG	0	8075	1/1	0.98	0.04	49,49,49,49	0
35	NA	0	8512	1/1	0.98	0.06	38,38,38,38	0
34	SR	R	8912	1/1	0.98	0.05	73,73,73,73	0
32	MG	0	8032	1/1	0.98	0.04	36,36,36,36	0
35	NA	0	8515	1/1	0.98	0.07	35,35,35,35	0
34	SR	3	8999	1/1	0.98	0.05	93,93,93,93	0
34	SR	0	8908	1/1	0.98	0.04	80,80,80,80	0
34	SR	0	8910	1/1	0.98	0.09	84,84,84,84	0
33	CL	3	8804	1/1	0.98	0.05	53,53,53,53	0
32	MG	0	8044	1/1	0.98	0.05	46,46,46,46	0
33	CL	0	8811	1/1	0.98	0.07	58,58,58,58	0
32	MG	0	8046	1/1	0.98	0.04	28,28,28,28	0
34	SR	0	8948	1/1	0.98	0.06	77,77,77,77	0
35	NA	0	8524	1/1	0.98	0.09	41,41,41,41	0
34	SR	0	8918	1/1	0.98	0.06	76,76,76,76	0
35	NA	0	8526	1/1	0.98	0.06	46,46,46,46	0
33	CL	0	8814	1/1	0.98	0.05	48,48,48,48	0
32	MG	0	8047	1/1	0.98	0.16	44,44,44,44	0
35	NA	0	8529	1/1	0.98	0.15	38,38,38,38	0
35	NA	M	8539	1/1	0.98	0.05	33,33,33,33	0
35	NA	0	8570	1/1	0.98	0.05	44,44,44,44	0
32	MG	0	8064	1/1	0.98	0.05	43,43,43,43	0
32	MG	0	8016	1/1	0.98	0.04	43,43,43,43	0
34	SR	0	8923	1/1	0.98	0.04	85,85,85,85	0
35	NA	0	8536	1/1	0.98	0.08	44,44,44,44	0
33	CL	0	8822	1/1	0.98	0.23	74,74,74,74	0
36	CD	O	8705	1/1	0.98	0.04	83,83,83,83	0
35	NA	0	8501	1/1	0.98	0.08	24,24,24,24	0
32	MG	0	8052	1/1	0.98	0.04	38,38,38,38	0
32	MG	B	8043	1/1	0.99	0.03	48,48,48,48	0
32	MG	Y	8086	1/1	0.99	0.03	33,33,33,33	0
34	SR	0	8940	1/1	0.99	0.03	70,70,70,70	0
32	MG	0	8001	1/1	0.99	0.04	29,29,29,29	0
32	MG	0	8048	1/1	0.99	0.04	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8019	1/1	0.99	0.05	20,20,20,20	0
32	MG	0	8084	1/1	0.99	0.06	27,27,27,27	0
35	NA	0	8534	1/1	0.99	0.03	25,25,25,25	0
32	MG	0	8020	1/1	0.99	0.09	38,38,38,38	0
32	MG	0	8087	1/1	0.99	0.03	31,31,31,31	0
32	MG	0	8022	1/1	0.99	0.04	32,32,32,32	0
32	MG	0	8023	1/1	0.99	0.03	18,18,18,18	0
32	MG	0	8002	1/1	0.99	0.02	21,21,21,21	0
32	MG	0	8026	1/1	0.99	0.02	27,27,27,27	0
34	SR	1	8913	1/1	0.99	0.07	78,78,78,78	0
34	SR	0	9008	1/1	0.99	0.04	85,85,85,85	0
34	SR	1	8952	1/1	0.99	0.05	74,74,74,74	0
32	MG	0	8027	1/1	0.99	0.03	39,39,39,39	0
34	SR	0	8901	1/1	0.99	0.03	73,73,73,73	0
34	SR	0	8904	1/1	0.99	0.06	49,49,49,49	0
34	SR	0	8905	1/1	0.99	0.14	54,54,54,54	0
34	SR	0	8906	1/1	0.99	0.08	52,52,52,52	0
34	SR	0	8907	1/1	0.99	0.11	53,53,53,53	0
32	MG	0	8061	1/1	0.99	0.04	29,29,29,29	0
34	SR	0	8909	1/1	0.99	0.04	75,75,75,75	0
32	MG	0	8029	1/1	0.99	0.15	52,52,52,52	0
34	SR	0	8911	1/1	0.99	0.03	74,74,74,74	0
32	MG	0	8003	1/1	0.99	0.04	26,26,26,26	0
32	MG	0	8006	1/1	0.99	0.04	23,23,23,23	0
32	MG	0	8065	1/1	0.99	0.04	47,47,47,47	0
32	MG	0	8007	1/1	0.99	0.03	27,27,27,27	0
32	MG	0	8067	1/1	0.99	0.02	26,26,26,26	0
32	MG	0	8008	1/1	0.99	0.04	23,23,23,23	0
33	CL	M	8818	1/1	0.99	0.03	33,33,33,33	0
32	MG	0	8009	1/1	0.99	0.08	19,19,19,19	0
32	MG	0	8010	1/1	0.99	0.02	23,23,23,23	0
33	CL	R	8806	1/1	0.99	0.03	42,42,42,42	0
32	MG	0	8011	1/1	0.99	0.04	24,24,24,24	0
34	SR	0	8925	1/1	0.99	0.06	84,84,84,84	0
32	MG	0	8072	1/1	0.99	0.05	53,53,53,53	0
33	CL	0	8803	1/1	0.99	0.09	50,50,50,50	0
32	MG	0	8012	1/1	0.99	0.05	22,22,22,22	0
32	MG	0	8013	1/1	0.99	0.04	24,24,24,24	0
33	CL	0	8812	1/1	0.99	0.06	40,40,40,40	0
32	MG	0	8014	1/1	0.99	0.03	19,19,19,19	0
34	SR	0	8935	1/1	0.99	0.04	68,68,68,68	0
36	CD	Z	8703	1/1	0.99	0.03	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8015	1/1	0.99	0.03	27,27,27,27	0
32	MG	0	8041	1/1	0.99	0.04	19,19,19,19	0
34	SR	3	8932	1/1	1.00	0.02	67,67,67,67	0
32	MG	0	8004	1/1	1.00	0.03	21,21,21,21	0
32	MG	0	8005	1/1	1.00	0.06	29,29,29,29	0
34	SR	0	8902	1/1	1.00	0.02	58,58,58,58	0
34	SR	0	8903	1/1	1.00	0.07	45,45,45,45	0
32	MG	0	8045	1/1	1.00	0.04	39,39,39,39	0
32	MG	0	8025	1/1	1.00	0.02	31,31,31,31	0
32	MG	0	8058	1/1	1.00	0.02	25,25,25,25	0
36	CD	U	8701	1/1	1.00	0.02	51,51,51,51	0
32	MG	0	8021	1/1	1.00	0.03	31,31,31,31	0
36	CD	1	8702	1/1	1.00	0.05	53,53,53,53	0
36	CD	3	8704	1/1	1.00	0.02	64,64,64,64	0
32	MG	A	8050	1/1	1.00	0.02	24,24,24,24	0
32	MG	0	8028	1/1	1.00	0.01	18,18,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.