



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2019 – 01:30 PM EST

PDB ID : 2UXB  
Title : Crystal structure of an extended tRNA anticodon stem loop in complex with its cognate mRNA GGGU in the context of the *Thermus thermophilus* 30S subunit.  
Authors : Dunham, C.M.; Selmer, M.; Phelps, S.S.; Kelley, A.C.; Suzuki, T.; Joseph, S.; Ramakrishnan, V.  
Deposited on : 2007-03-28  
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

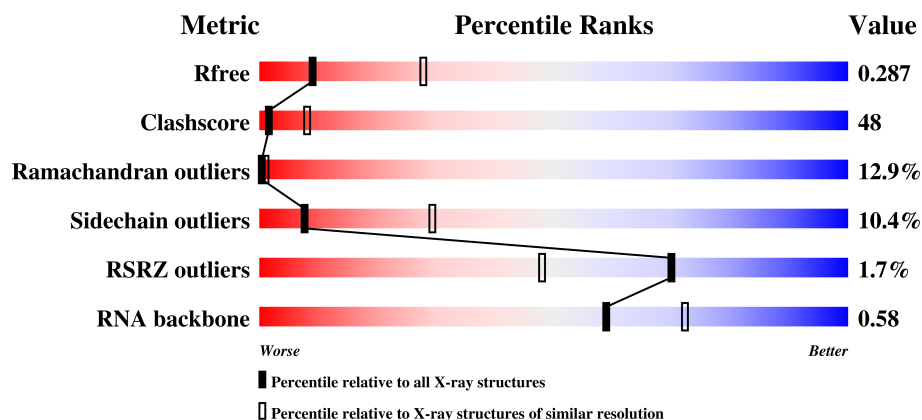
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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.



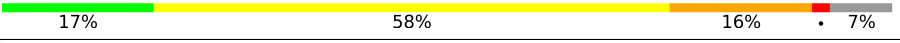

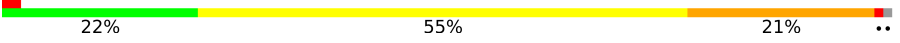
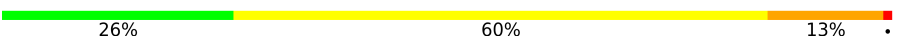
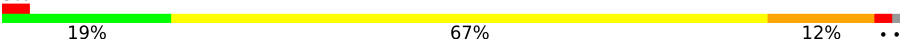

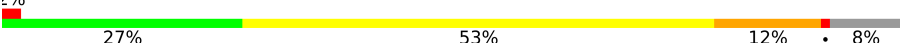
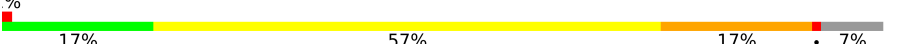

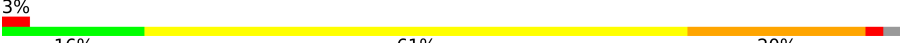

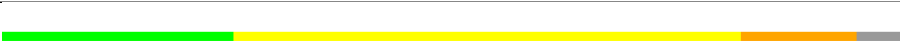
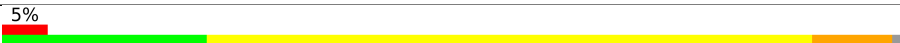
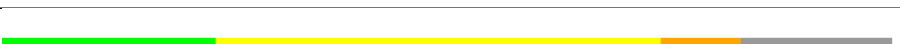
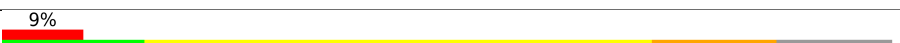

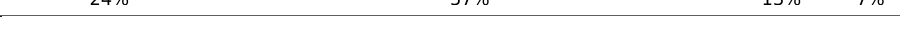
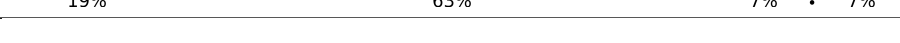
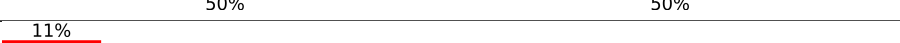
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	1115 (3.12-3.08)
Clashscore	122126	1042 (3.10-3.10)
Ramachandran outliers	120053	1010 (3.10-3.10)
Sidechain outliers	120020	1010 (3.10-3.10)
RSRZ outliers	108989	1089 (3.12-3.08)
RNA backbone	2636	1015 (3.44-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	1522	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 19%, green 66%, orange 14%, red 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>19%</span> <span>66%</span> <span>14%</span> <span>..</span> </div> </div>
2	B	256	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 18%, green 58%, orange 13%, red 1%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>18%</span> <span>58%</span> <span>13%</span> <span>•</span> <span>8%</span> </div> </div>
3	C	239	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 20%, yellow 49%, orange 16%, red 1%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>20%</span> <span>49%</span> <span>16%</span> <span>•</span> <span>13%</span> </div> </div>
4	D	209	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 19%, green 60%, orange 19%, red 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>19%</span> <span>60%</span> <span>19%</span> <span>•</span> </div> </div>

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Mol	Chain	Length	Quality of chain
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	X	4	
23	Y	18	

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
25	MG	G	3005	-	-	-	X
25	MG	G	3006	-	-	-	X
25	MG	G	3012	-	-	-	X
25	MG	G	3013	-	-	-	X
25	MG	G	3018	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	G	3021	-	-	-	X
25	MG	G	3025	-	-	-	X
25	MG	G	3027	-	-	-	X
25	MG	G	3028	-	-	-	X
25	MG	G	3029	-	-	-	X
25	MG	G	3031	-	-	-	X
25	MG	G	3032	-	-	-	X
25	MG	G	3038	-	-	-	X
25	MG	G	3040	-	-	-	X
25	MG	G	3041	-	-	-	X
25	MG	G	3043	-	-	-	X
25	MG	G	3052	-	-	-	X
25	MG	G	3054	-	-	-	X
25	MG	G	3055	-	-	-	X
25	MG	G	3056	-	-	-	X
25	MG	G	3059	-	-	-	X
25	MG	G	3068	-	-	-	X
25	MG	G	3069	-	-	-	X
25	MG	G	3071	-	-	-	X
25	MG	G	3074	-	-	-	X
25	MG	G	3076	-	-	-	X
25	MG	G	3080	-	-	-	X
25	MG	G	3082	-	-	-	X
25	MG	G	3087	-	-	-	X
25	MG	G	3088	-	-	-	X
25	MG	G	3089	-	-	-	X
25	MG	G	3091	-	-	-	X
25	MG	G	3099	-	-	-	X
25	MG	G	3103	-	-	-	X
25	MG	G	3122	-	-	-	X
25	MG	G	3130	-	-	-	X
26	K	G	3138	-	-	-	X
26	K	G	3140	-	-	-	X
26	K	G	3142	-	-	-	X

## 2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 52165 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 RNA chain called 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1513	Total	C	N	O	P	0	0	0
			32514	14472	6016	10513	1513			

- Molecule 2 is a protein called RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	0	0	0
			1011	639	198	174			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	58	ARG	HIS	conflict	UNP P80374

- Molecule 10 is a protein called RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	1
			793	498	157	137	1			

- Molecule 11 is a protein called RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 14 is a protein called RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLN	GLU	conflict	UNP Q5SHP7

- Molecule 18 is a protein called RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	73	Total	C	N	O		0	0	0
			597	380	118	99				

- Molecule 19 is a protein called RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	1
			648	414	120	112	2			

- Molecule 20 is a protein called RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	41	VAL	ILE	conflict	UNP P80380

- Molecule 21 is a protein called RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called A-SITE MESSENGER RNA FRAGMENT GGGU.

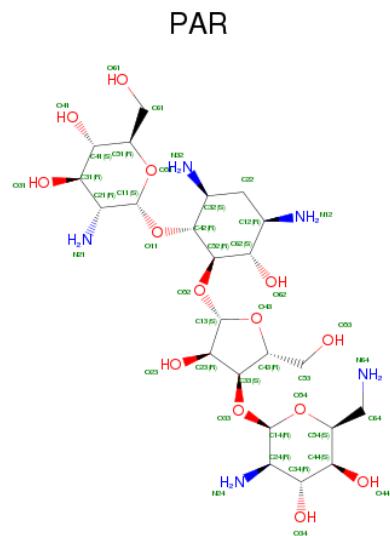
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	X	4	Total	C	N	O	P	0	0	0
			86	39	17	27	3			

- Molecule 23 is a RNA chain called ANTICODON STEM-LOOP OF TRANSFER RNA WITH ANTICODON ACCC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Y	7	Total	C	N	O	P	0	0	0
			143	66	26	45	6			

- Molecule 24 is PAROMOMYCIN (three-letter code: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	G	131	Total Mg 131 131	0	0

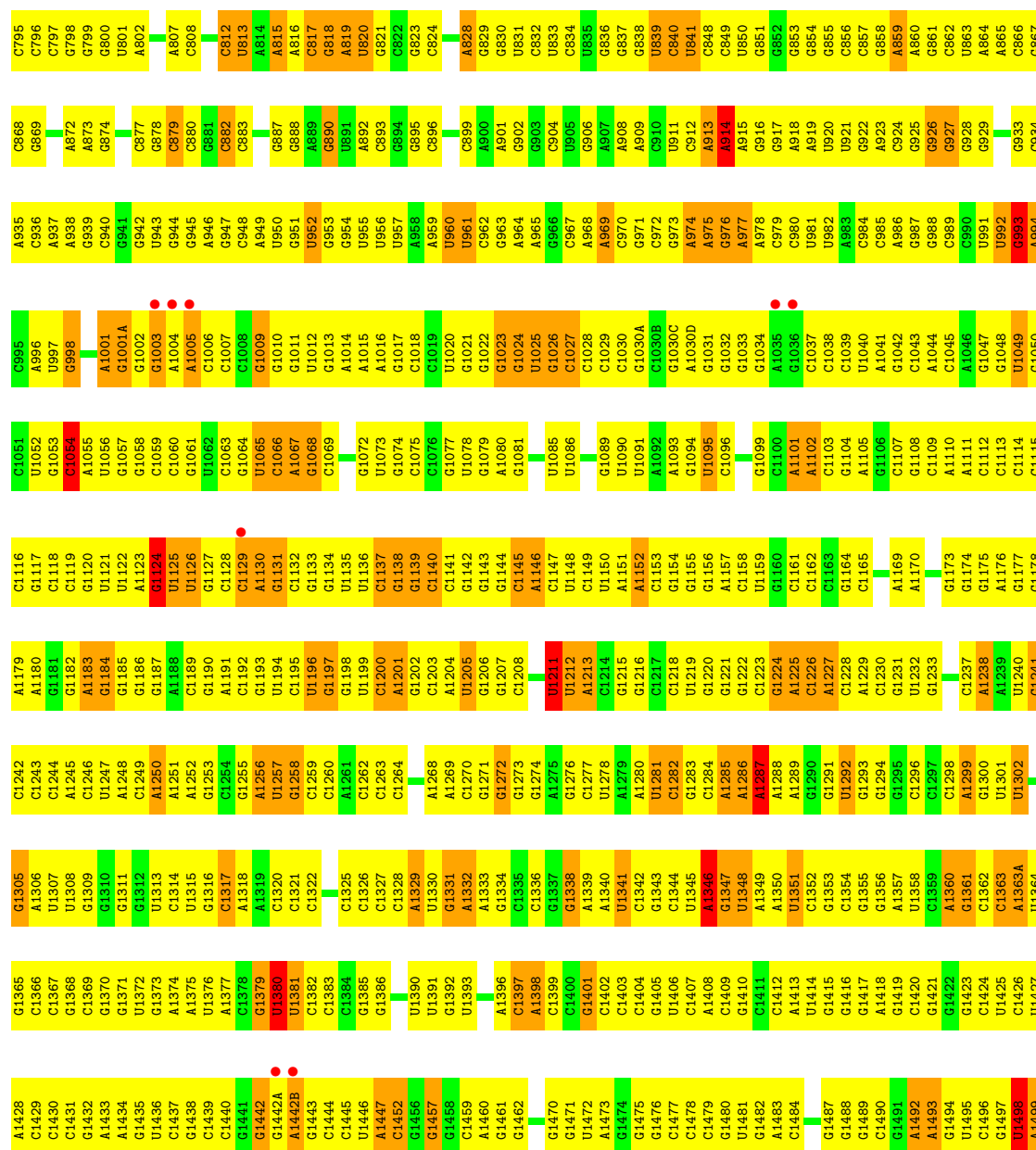
- Molecule 26 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	G	10	Total K 10 10	0	0

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	G	2	Total Zn 2 2	0	0

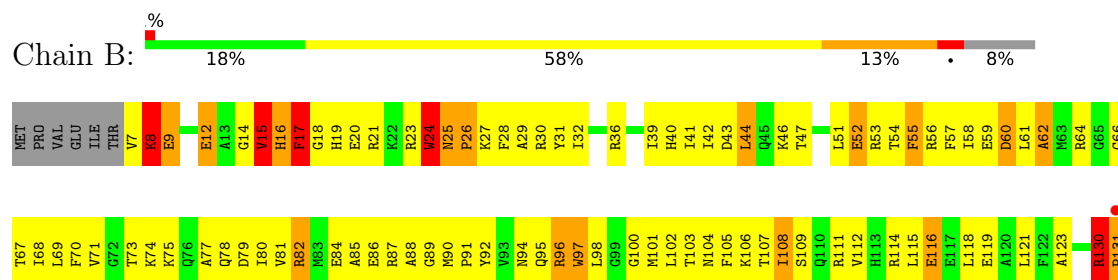


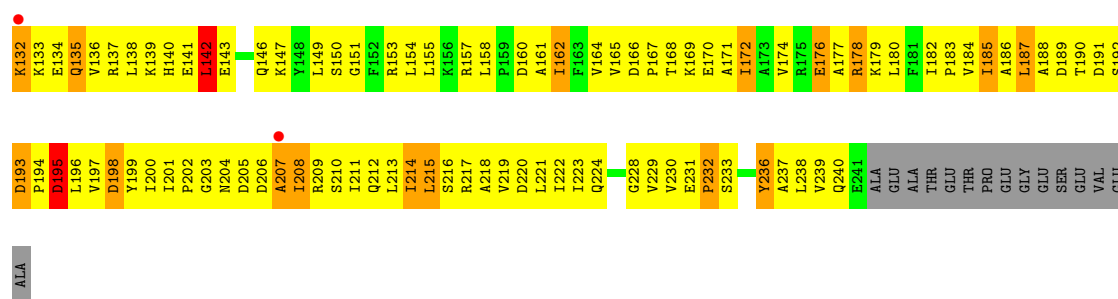


• Molecule 2: RIBOSOMAL PROTEIN S2

Chain B:

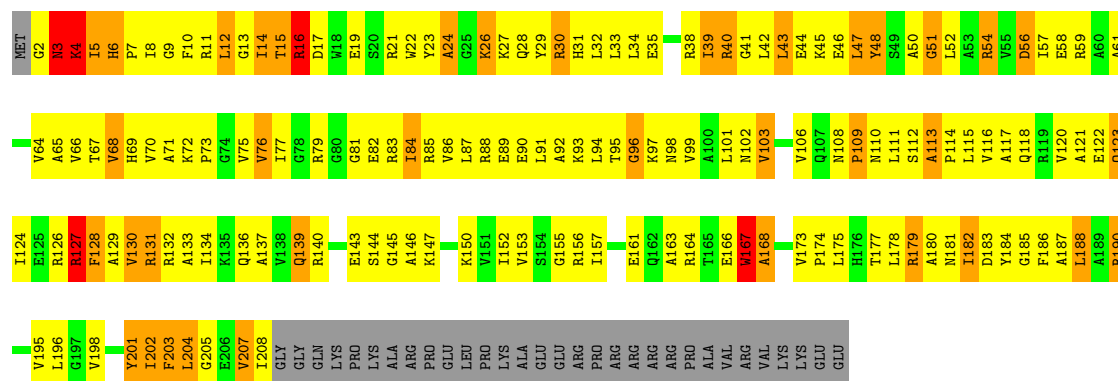
18% 58% 13% 8%





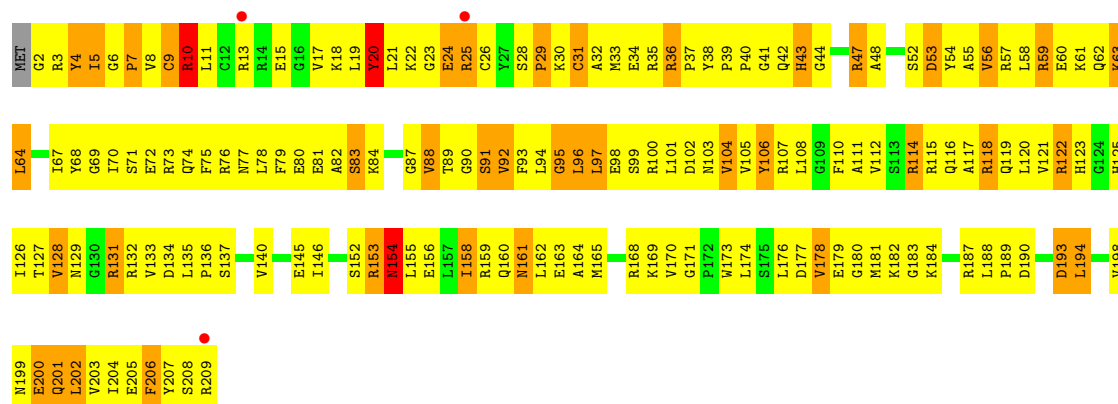
### • Molecule 3: RIBOSOMAL PROTEIN S3

Chain C: 20% 49% 16% 13%



### • Molecule 4: RIBOSOMAL PROTEIN S4

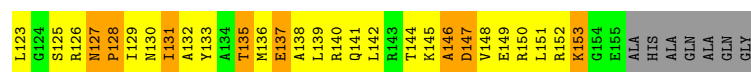
Chain D: 19% 60% 19%



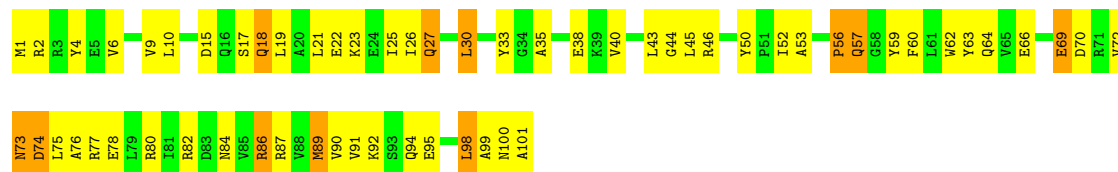
### • Molecule 5: RIBOSOMAL PROTEIN S5

Chain E: 17% 58% 16% 7%

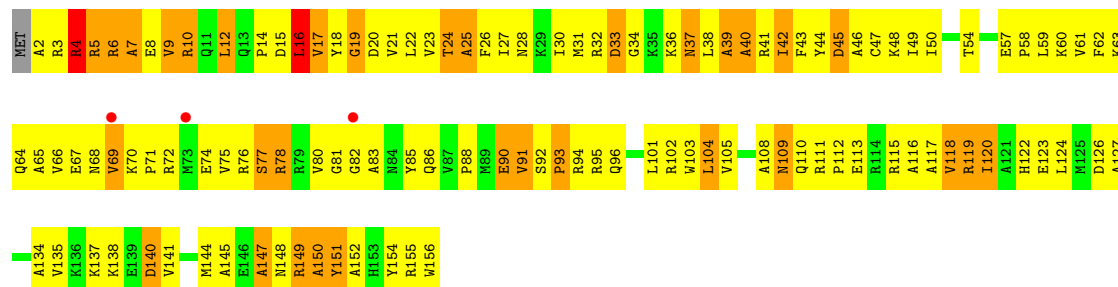




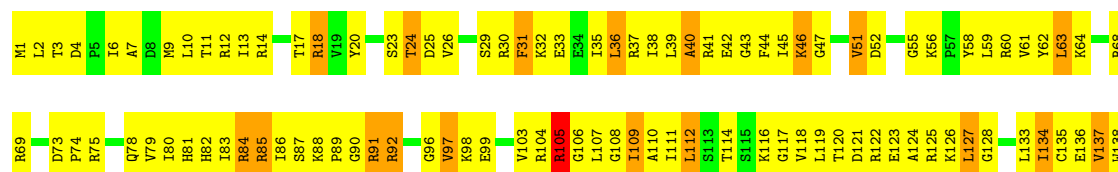
● Molecule 6: RIBOSOMAL PROTEIN S6



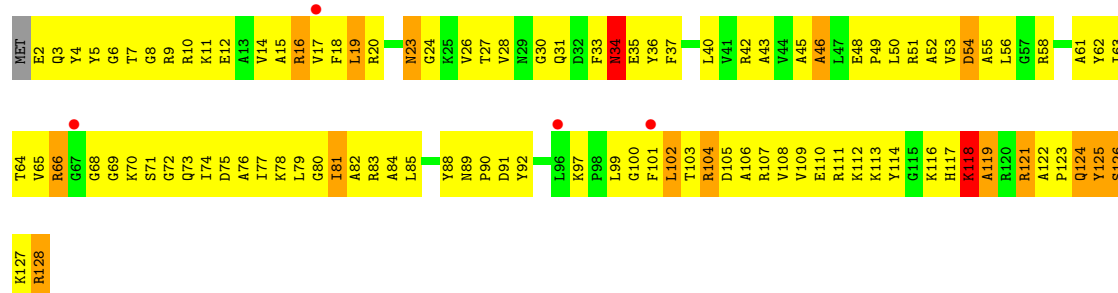
● Molecule 7: RIBOSOMAL PROTEIN S7



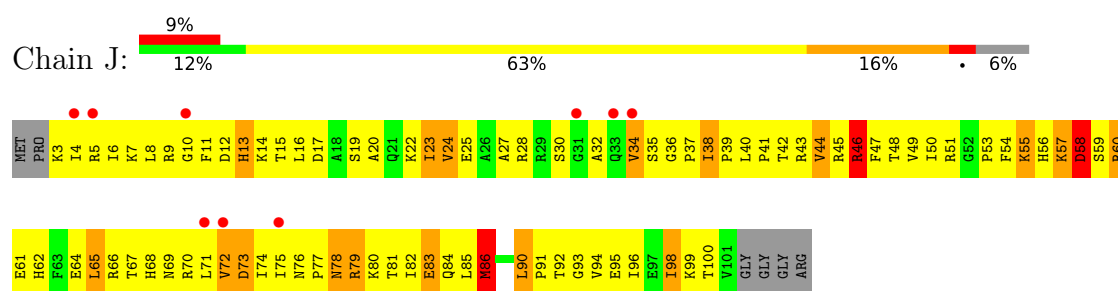
● Molecule 8: RIBOSOMAL PROTEIN S8



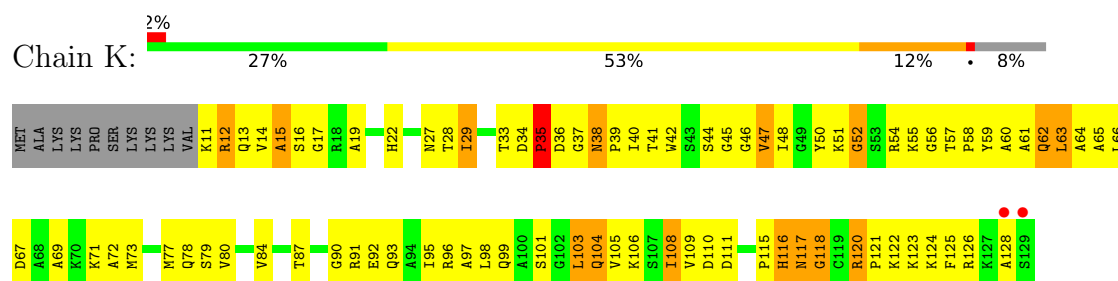
● Molecule 9: RIBOSOMAL PROTEIN S9



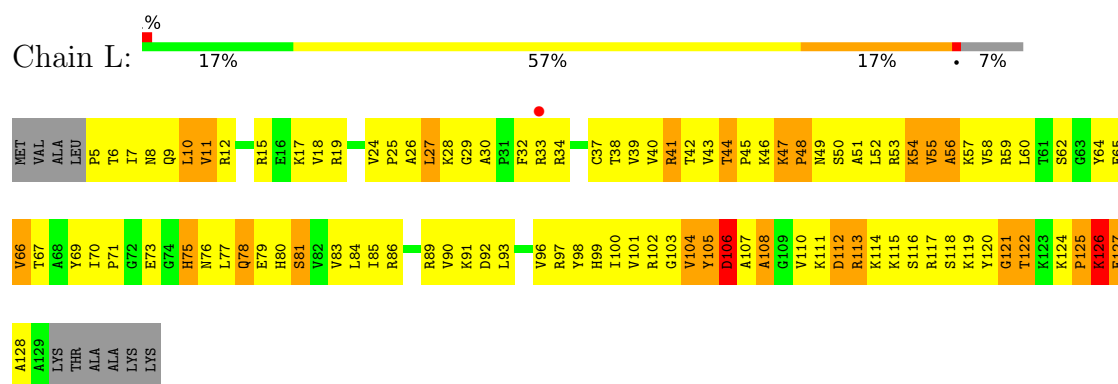
● Molecule 10: RIBOSOMAL PROTEIN S10



• Molecule 11: RIBOSOMAL PROTEIN S11



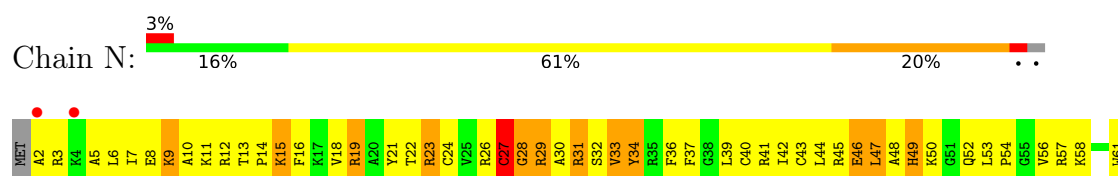
• Molecule 12: RIBOSOMAL PROTEIN S12



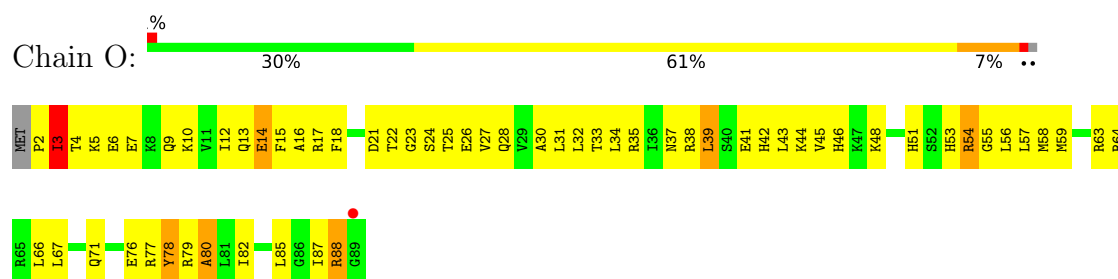
• Molecule 13: RIBOSOMAL PROTEIN S13



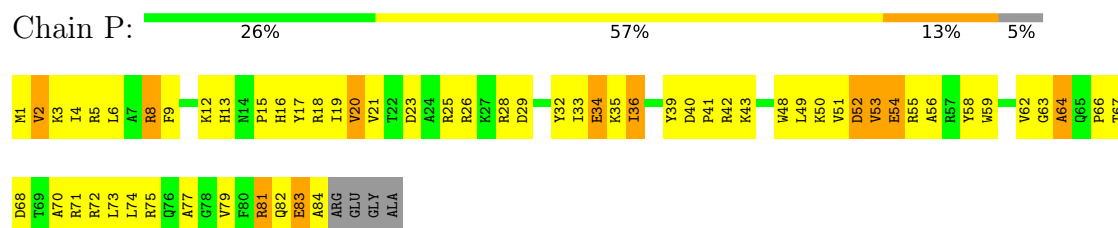
• Molecule 14: RIBOSOMAL PROTEIN S14



• Molecule 15: RIBOSOMAL PROTEIN S15



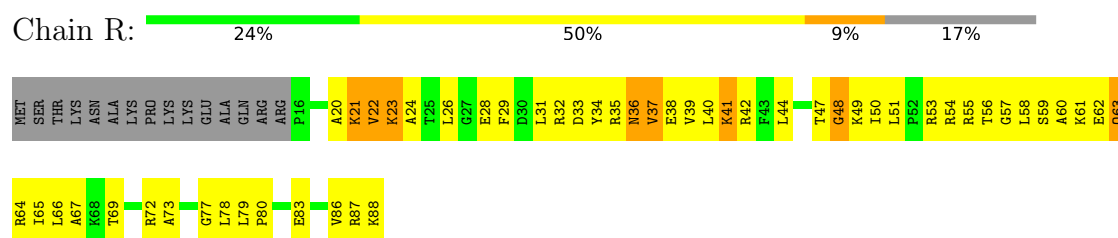
- Molecule 16: RIBOSOMAL PROTEIN S16



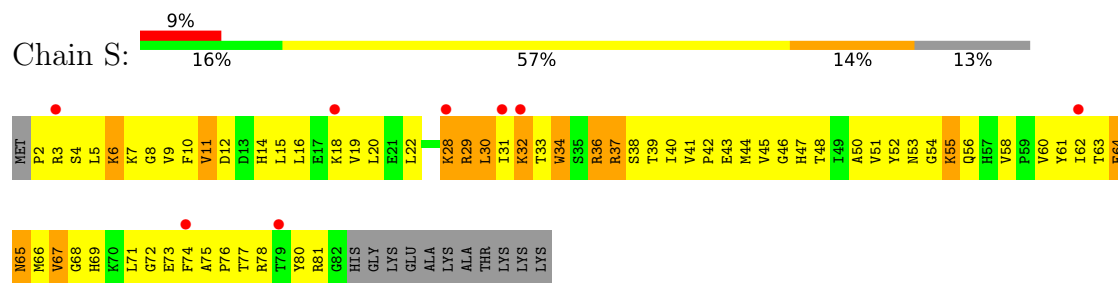
- Molecule 17: RIBOSOMAL PROTEIN S17



- Molecule 18: RIBOSOMAL PROTEIN S18

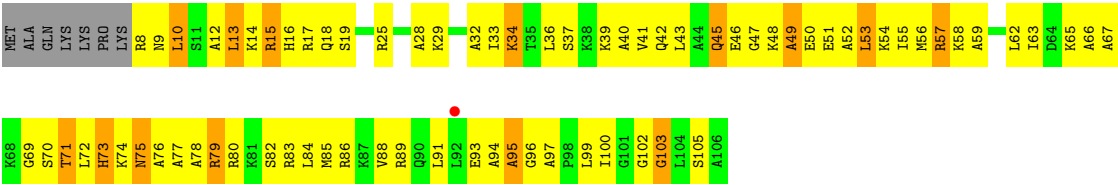


- Molecule 19: RIBOSOMAL PROTEIN S19

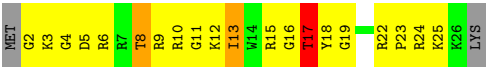


- Molecule 20: RIBOSOMAL PROTEIN S20





● Molecule 21: RIBOSOMAL PROTEIN THX



● Molecule 22: A-SITE MESSENGER RNA FRAGMENT GGGU



● Molecule 23: ANTICODON STEM-LOOP OF TRANSFER RNA WITH ANTICODON ACCC





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	401.95Å 401.95Å 174.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 3.10 47.93 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (29.88-3.10) 98.0 (47.93-3.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.295 , 0.328 0.240 , 0.287	Depositor DCC
$R_{free}$ test set	13830 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.7	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.19 , 58.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	52165	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

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

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, ZN, PAR, 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	A	0.58	1/36393 (0.0%)	0.75	28/56797 (0.0%)
2	B	0.39	0/1936	0.66	0/2611
3	C	0.34	0/1637	0.62	0/2207
4	D	0.36	0/1733	0.63	0/2318
5	E	0.52	0/1163	0.77	1/1566 (0.1%)
6	F	0.34	0/856	0.62	0/1154
7	G	0.33	0/1276	0.59	0/1709
8	H	0.57	0/1136	0.84	0/1527
9	I	0.36	0/1029	0.66	0/1378
10	J	0.36	0/806	0.65	0/1084
11	K	0.41	0/900	0.71	0/1213
12	L	0.43	0/987	0.75	0/1322
13	M	0.35	0/1008	0.64	0/1347
14	N	0.37	0/501	0.64	0/664
15	O	0.42	0/745	0.66	0/992
16	P	0.48	0/717	0.77	0/965
17	Q	0.50	0/870	0.73	0/1159
18	R	0.38	0/603	0.67	0/799
19	S	0.34	0/662	0.62	0/892
20	T	0.40	0/764	0.71	0/1006
21	U	0.51	0/213	0.74	0/279
22	X	0.46	0/96	0.81	0/149
23	Y	0.54	0/159	0.81	0/245
All	All	0.53	1/56190 (0.0%)	0.73	29/83383 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	41

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1532	U	O3'-P	-6.99	1.52	1.61

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1532	U	P-O3'-C3'	26.85	151.92	119.70
1	A	1532	U	OP2-P-O3'	-14.62	73.05	105.20
1	A	1532	U	OP1-P-O3'	11.12	129.67	105.20
1	A	1498	U	C2'-C3'-O3'	9.82	131.11	109.50
1	A	1532	U	C4'-C3'-O3'	9.72	132.44	113.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1498	U	C3'

5 of 41 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	G	Sidechain
1	A	189(G)	G	Sidechain
1	A	250	A	Sidechain
1	A	280	C	Sidechain
1	A	297	G	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	32514	0	16412	1687	0
2	B	1901	0	1951	322	0
3	C	1613	0	1677	287	0
4	D	1703	0	1764	242	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1147	0	1207	158	0
6	F	843	0	857	82	0
7	G	1257	0	1296	170	0
8	H	1116	0	1177	143	0
9	I	1011	0	1043	187	0
10	J	793	0	835	183	0
11	K	885	0	904	129	0
12	L	971	0	1057	174	0
13	M	997	0	1072	117	0
14	N	492	0	531	103	0
15	O	734	0	771	87	0
16	P	701	0	720	97	0
17	Q	857	0	930	111	0
18	R	597	0	666	84	0
19	S	648	0	673	85	0
20	T	762	0	859	101	0
21	U	209	0	221	34	0
22	X	86	0	45	6	0
23	Y	143	0	78	15	0
24	A	42	0	45	2	0
25	G	131	0	0	0	0
26	G	10	0	0	0	0
27	G	2	0	0	0	0
All	All	52165	0	36791	4225	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 48.

The worst 5 of 4225 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)
1:A:1539:C:C5	7:G:81:GLY:O	1.88	1.24
1:A:1347:G:N2	1:A:1373:G:H2'	1.58	1.19
1:A:1442(A):G:H5''	1:A:1442(B):A:H5'	1.28	1.15
11:K:48:ILE:HD13	11:K:63:LEU:HB2	1.27	1.15
1:A:1347:G:H22	1:A:1373:G:H2'	1.09	1.15

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	233/256 (91%)	134 (58%)	72 (31%)	27 (12%)	0	2
3	C	205/239 (86%)	116 (57%)	42 (20%)	47 (23%)	0	0
4	D	206/209 (99%)	125 (61%)	47 (23%)	34 (16%)	0	0
5	E	149/162 (92%)	109 (73%)	25 (17%)	15 (10%)	0	4
6	F	99/101 (98%)	72 (73%)	24 (24%)	3 (3%)	5	26
7	G	153/156 (98%)	78 (51%)	44 (29%)	31 (20%)	0	0
8	H	136/138 (99%)	105 (77%)	23 (17%)	8 (6%)	2	11
9	I	125/128 (98%)	80 (64%)	34 (27%)	11 (9%)	1	5
10	J	97/105 (92%)	56 (58%)	24 (25%)	17 (18%)	0	0
11	K	117/129 (91%)	83 (71%)	25 (21%)	9 (8%)	1	6
12	L	123/135 (91%)	70 (57%)	33 (27%)	20 (16%)	0	0
13	M	123/126 (98%)	74 (60%)	29 (24%)	20 (16%)	0	0
14	N	58/61 (95%)	31 (53%)	18 (31%)	9 (16%)	0	0
15	O	86/89 (97%)	43 (50%)	38 (44%)	5 (6%)	2	11
16	P	82/88 (93%)	52 (63%)	22 (27%)	8 (10%)	1	4
17	Q	102/105 (97%)	70 (69%)	26 (26%)	6 (6%)	2	11
18	R	71/88 (81%)	47 (66%)	15 (21%)	9 (13%)	0	1
19	S	79/93 (85%)	47 (60%)	17 (22%)	15 (19%)	0	0
20	T	97/106 (92%)	52 (54%)	37 (38%)	8 (8%)	1	6
21	U	23/27 (85%)	17 (74%)	3 (13%)	3 (13%)	0	1
All	All	2364/2541 (93%)	1461 (62%)	598 (25%)	305 (13%)	0	1

5 of 305 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	GLU

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Mol	Chain	Res	Type
2	B	15	VAL
2	B	16	HIS
2	B	17	PHE
2	B	24	TRP

### 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	
2	B	202/220 (92%)	176 (87%)	26 (13%)	5	20
3	C	160/188 (85%)	145 (91%)	15 (9%)	9	35
4	D	180/181 (99%)	161 (89%)	19 (11%)	7	28
5	E	115/123 (94%)	97 (84%)	18 (16%)	3	12
6	F	90/90 (100%)	79 (88%)	11 (12%)	5	21
7	G	126/127 (99%)	115 (91%)	11 (9%)	11	40
8	H	119/119 (100%)	102 (86%)	17 (14%)	3	15
9	I	98/99 (99%)	86 (88%)	12 (12%)	5	21
10	J	87/92 (95%)	80 (92%)	7 (8%)	13	44
11	K	90/99 (91%)	81 (90%)	9 (10%)	8	31
12	L	104/111 (94%)	95 (91%)	9 (9%)	11	40
13	M	100/101 (99%)	92 (92%)	8 (8%)	13	44
14	N	49/50 (98%)	43 (88%)	6 (12%)	5	21
15	O	79/80 (99%)	72 (91%)	7 (9%)	11	38
16	P	72/74 (97%)	67 (93%)	5 (7%)	17	50
17	Q	96/97 (99%)	90 (94%)	6 (6%)	20	53
18	R	64/77 (83%)	63 (98%)	1 (2%)	65	87
19	S	71/80 (89%)	66 (93%)	5 (7%)	16	49
20	T	76/82 (93%)	64 (84%)	12 (16%)	3	12
21	U	19/22 (86%)	16 (84%)	3 (16%)	3	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1997/2112 (95%)	1790 (90%)	207 (10%)	8 29

5 of 207 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	24	THR
8	H	133	LEU
19	S	61	TYR
7	G	126	ASP
8	H	63	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	100	ASN
9	I	34	ASN
17	Q	94	ASN
7	G	37	ASN
7	G	122	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1511/1522 (99%)	217 (14%)	50 (3%)
22	X	3/4 (75%)	1 (33%)	0
23	Y	6/18 (33%)	1 (16%)	0
All	All	1520/1544 (98%)	219 (14%)	50 (3%)

5 of 219 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G

5 of 50 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	687	A
1	A	960	U
1	A	1498	U
1	A	701	C
1	A	812	C

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 144 ligands modelled in this entry, 143 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
24	PAR	A	3001	-	44,45,45	1.38	5 (11%)	62,67,67	1.13	6 (9%)

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
24	PAR	A	3001	-	-	0/18/94/94	0/4/4/4

All (5) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	3001	PAR	C11-C21	2.40	1.57	1.52
24	A	3001	PAR	C31-C21	2.44	1.56	1.53
24	A	3001	PAR	C52-C42	2.98	1.58	1.52
24	A	3001	PAR	C34-C24	3.09	1.57	1.53
24	A	3001	PAR	O54-C14	3.20	1.50	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	3001	PAR	O52-C13-O43	-2.46	108.77	111.43
24	A	3001	PAR	O11-C11-C21	2.00	111.81	108.24
24	A	3001	PAR	C11-O51-C51	2.13	117.91	113.71
24	A	3001	PAR	O52-C13-C23	2.77	113.70	107.96
24	A	3001	PAR	C14-O54-C54	2.97	119.56	113.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	3001	PAR	2	0

## 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	1513/1522 (99%)	-0.38	12 (0%) 86 72	18, 65, 147, 201	0
2	B	235/256 (91%)	-0.34	3 (1%) 77 59	27, 82, 159, 197	0
3	C	207/239 (86%)	-0.34	0 100 100	41, 101, 167, 197	0
4	D	208/209 (99%)	-0.28	3 (1%) 75 56	28, 78, 139, 160	0
5	E	151/162 (93%)	-0.68	0 100 100	14, 46, 91, 164	0
6	F	101/101 (100%)	-0.55	0 100 100	42, 83, 133, 151	0
7	G	155/156 (99%)	-0.22	3 (1%) 66 45	36, 97, 162, 197	0
8	H	138/138 (100%)	-0.80	0 100 100	9, 35, 83, 108	0
9	I	127/128 (99%)	-0.04	4 (3%) 49 26	23, 98, 159, 190	0
10	J	99/105 (94%)	0.37	9 (9%) 9 3	41, 139, 192, 197	0
11	K	119/129 (92%)	-0.44	2 (1%) 70 48	19, 64, 129, 178	0
12	L	125/135 (92%)	-0.28	1 (0%) 86 72	5, 75, 133, 187	0
13	M	125/126 (99%)	0.40	12 (9%) 8 3	36, 86, 165, 197	0
14	N	60/61 (98%)	0.07	2 (3%) 46 24	42, 92, 187, 193	0
15	O	88/89 (98%)	-0.59	1 (1%) 80 64	21, 55, 102, 154	0
16	P	84/88 (95%)	-0.43	0 100 100	24, 48, 91, 140	0
17	Q	104/105 (99%)	-0.35	5 (4%) 30 13	17, 49, 117, 197	0
18	R	73/88 (82%)	-0.54	0 100 100	29, 64, 142, 187	0
19	S	81/93 (87%)	0.45	8 (9%) 7 2	84, 133, 174, 197	0
20	T	99/106 (93%)	-0.36	1 (1%) 82 67	33, 63, 121, 151	0
21	U	25/27 (92%)	-0.07	0 100 100	47, 69, 115, 123	0
22	X	4/4 (100%)	-0.30	0 100 100	87, 92, 100, 115	0
23	Y	7/18 (38%)	1.27	2 (28%) 0 0	88, 120, 170, 196	0
All	All	3928/4085 (96%)	-0.32	68 (1%) 70 48	5, 72, 157, 201	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1534	A	13.6
13	M	124	PRO	11.3
13	M	123	ALA	11.3
13	M	121	LYS	10.5
13	M	122	LYS	10.4

## 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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	G	3041	1/1	0.41	3.13	116,116,116,116	0
25	MG	G	3043	1/1	0.43	0.62	105,105,105,105	0
25	MG	G	3068	1/1	0.46	1.14	102,102,102,102	0
25	MG	G	3052	1/1	0.50	0.68	99,99,99,99	0
25	MG	G	3122	1/1	0.53	0.62	77,77,77,77	0
25	MG	G	3013	1/1	0.56	1.73	103,103,103,103	0
25	MG	G	3027	1/1	0.56	1.89	89,89,89,89	0
25	MG	G	3018	1/1	0.56	0.70	96,96,96,96	0
25	MG	G	3130	1/1	0.59	0.50	47,47,47,47	0
26	K	G	3142	1/1	0.60	0.85	156,156,156,156	0
26	K	G	3138	1/1	0.60	1.18	146,146,146,146	0
25	MG	G	3066	1/1	0.64	0.37	102,102,102,102	0
25	MG	G	3082	1/1	0.64	1.40	121,121,121,121	0
25	MG	G	3028	1/1	0.66	0.77	90,90,90,90	0
25	MG	G	3025	1/1	0.67	2.04	113,113,113,113	0
25	MG	G	3071	1/1	0.67	0.78	89,89,89,89	0
25	MG	G	3031	1/1	0.69	0.70	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
25	MG	G	3080	1/1	0.69	2.44	108,108,108,108	0
25	MG	G	3034	1/1	0.70	0.30	103,103,103,103	0
25	MG	G	3005	1/1	0.70	0.93	95,95,95,95	0
25	MG	G	3040	1/1	0.70	2.31	121,121,121,121	0
25	MG	G	3029	1/1	0.71	0.42	112,112,112,112	0
25	MG	G	3059	1/1	0.71	0.55	93,93,93,93	0
25	MG	G	3038	1/1	0.72	1.04	99,99,99,99	0
25	MG	G	3110	1/1	0.72	0.34	44,44,44,44	0
25	MG	G	3091	1/1	0.73	1.43	110,110,110,110	0
25	MG	G	3073	1/1	0.74	0.34	93,93,93,93	0
25	MG	G	3088	1/1	0.75	1.21	113,113,113,113	0
25	MG	G	3006	1/1	0.75	0.86	92,92,92,92	0
25	MG	G	3076	1/1	0.76	0.70	143,143,143,143	0
26	K	G	3140	1/1	0.76	1.07	161,161,161,161	0
25	MG	G	3069	1/1	0.76	1.49	97,97,97,97	0
25	MG	G	3087	1/1	0.77	0.91	102,102,102,102	0
25	MG	G	3032	1/1	0.77	1.53	107,107,107,107	0
25	MG	G	3055	1/1	0.77	1.00	91,91,91,91	0
25	MG	G	3054	1/1	0.78	1.29	95,95,95,95	0
25	MG	G	3102	1/1	0.78	0.26	53,53,53,53	0
25	MG	G	3012	1/1	0.78	1.12	101,101,101,101	0
25	MG	G	3099	1/1	0.78	1.13	102,102,102,102	0
25	MG	G	3089	1/1	0.79	1.05	106,106,106,106	0
25	MG	G	3056	1/1	0.79	0.81	113,113,113,113	0
25	MG	G	3103	1/1	0.79	0.53	52,52,52,52	0
25	MG	G	3074	1/1	0.79	1.96	112,112,112,112	0
25	MG	G	3021	1/1	0.80	1.37	108,108,108,108	0
25	MG	G	3079	1/1	0.80	1.05	128,128,128,128	0
25	MG	G	3070	1/1	0.80	0.35	106,106,106,106	0
25	MG	G	3113	1/1	0.81	0.32	31,31,31,31	0
26	K	G	3137	1/1	0.81	0.43	123,123,123,123	0
25	MG	G	3081	1/1	0.81	1.12	110,110,110,110	0
25	MG	G	3044	1/1	0.81	1.62	109,109,109,109	0
25	MG	G	3072	1/1	0.81	0.53	61,61,61,61	0
25	MG	G	3078	1/1	0.82	0.77	118,118,118,118	0
25	MG	G	3026	1/1	0.82	0.95	108,108,108,108	0
25	MG	G	3085	1/1	0.82	0.99	116,116,116,116	0
25	MG	G	3015	1/1	0.82	0.58	87,87,87,87	0
25	MG	G	3023	1/1	0.82	1.09	91,91,91,91	0
25	MG	G	3092	1/1	0.83	0.99	97,97,97,97	0
25	MG	G	3061	1/1	0.84	1.45	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	G	3033	1/1	0.84	0.68	84,84,84,84	0
25	MG	G	3009	1/1	0.84	0.81	90,90,90,90	0
25	MG	G	3042	1/1	0.84	1.13	103,103,103,103	0
25	MG	G	3117	1/1	0.84	0.40	53,53,53,53	0
25	MG	G	3075	1/1	0.84	1.49	134,134,134,134	0
25	MG	G	3014	1/1	0.85	1.01	101,101,101,101	0
25	MG	G	3111	1/1	0.85	0.27	54,54,54,54	0
25	MG	G	3086	1/1	0.85	1.31	102,102,102,102	0
25	MG	G	3022	1/1	0.85	1.76	126,126,126,126	0
25	MG	G	3057	1/1	0.86	1.24	86,86,86,86	0
25	MG	G	3123	1/1	0.86	0.20	35,35,35,35	0
26	K	G	3135	1/1	0.86	0.52	135,135,135,135	0
25	MG	G	3118	1/1	0.86	0.24	46,46,46,46	0
25	MG	G	3116	1/1	0.87	0.22	43,43,43,43	0
25	MG	G	3129	1/1	0.87	0.12	48,48,48,48	0
25	MG	G	3046	1/1	0.87	0.57	77,77,77,77	0
25	MG	G	3047	1/1	0.88	1.07	87,87,87,87	0
25	MG	G	3098	1/1	0.88	0.50	81,81,81,81	0
25	MG	G	3096	1/1	0.88	0.23	43,43,43,43	0
25	MG	G	3101	1/1	0.88	0.24	56,56,56,56	0
25	MG	G	3024	1/1	0.88	0.59	102,102,102,102	0
25	MG	G	3020	1/1	0.88	1.26	115,115,115,115	0
25	MG	G	3008	1/1	0.89	0.76	100,100,100,100	0
25	MG	G	3125	1/1	0.89	0.54	60,60,60,60	0
25	MG	G	3077	1/1	0.89	1.65	103,103,103,103	0
25	MG	G	3037	1/1	0.89	0.40	90,90,90,90	0
25	MG	G	3062	1/1	0.89	0.45	114,114,114,114	0
25	MG	G	3083	1/1	0.89	0.88	162,162,162,162	0
25	MG	G	3049	1/1	0.89	0.26	78,78,78,78	0
25	MG	G	3067	1/1	0.89	1.40	102,102,102,102	0
25	MG	G	3109	1/1	0.89	0.19	57,57,57,57	0
25	MG	G	3003	1/1	0.90	1.73	102,102,102,102	0
25	MG	G	3060	1/1	0.90	0.67	91,91,91,91	0
26	K	G	3139	1/1	0.90	1.16	150,150,150,150	0
25	MG	G	3063	1/1	0.90	1.10	96,96,96,96	0
25	MG	G	3108	1/1	0.91	0.30	58,58,58,58	0
25	MG	G	3127	1/1	0.91	0.27	49,49,49,49	0
25	MG	G	3048	1/1	0.91	0.59	100,100,100,100	0
25	MG	G	3104	1/1	0.91	0.42	47,47,47,47	0
25	MG	G	3120	1/1	0.91	0.57	59,59,59,59	0
25	MG	G	3016	1/1	0.91	1.22	93,93,93,93	0
25	MG	G	3035	1/1	0.91	0.70	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
26	K	G	3141	1/1	0.91	0.58	145,145,145,145	0
26	K	G	3134	1/1	0.91	0.33	131,131,131,131	0
25	MG	G	3114	1/1	0.92	0.15	38,38,38,38	0
25	MG	G	3030	1/1	0.92	0.59	83,83,83,83	0
25	MG	G	3119	1/1	0.92	0.10	47,47,47,47	0
25	MG	G	3084	1/1	0.92	0.69	97,97,97,97	0
25	MG	G	3053	1/1	0.92	0.68	96,96,96,96	0
25	MG	G	3051	1/1	0.93	0.34	80,80,80,80	0
25	MG	G	3121	1/1	0.93	0.26	56,56,56,56	0
25	MG	G	3112	1/1	0.93	0.14	51,51,51,51	0
26	K	G	3136	1/1	0.93	0.31	105,105,105,105	0
25	MG	G	3002	1/1	0.93	0.33	79,79,79,79	0
25	MG	G	3019	1/1	0.93	0.81	92,92,92,92	0
24	PAR	A	3001	42/42	0.93	0.20	67,70,81,87	0
25	MG	G	3097	1/1	0.93	0.82	100,100,100,100	0
25	MG	G	3004	1/1	0.94	0.37	89,89,89,89	0
25	MG	G	3115	1/1	0.94	0.16	49,49,49,49	0
25	MG	G	3039	1/1	0.94	1.47	96,96,96,96	0
25	MG	G	3095	1/1	0.94	0.56	74,74,74,74	0
25	MG	G	3065	1/1	0.94	0.64	87,87,87,87	0
25	MG	G	3090	1/1	0.94	1.29	123,123,123,123	0
25	MG	G	3036	1/1	0.94	1.26	96,96,96,96	0
27	ZN	G	3143	1/1	0.94	0.43	118,118,118,118	0
25	MG	G	3094	1/1	0.95	0.18	49,49,49,49	0
25	MG	G	3126	1/1	0.95	0.14	45,45,45,45	0
25	MG	G	3106	1/1	0.95	0.33	39,39,39,39	0
25	MG	G	3010	1/1	0.95	1.06	103,103,103,103	0
25	MG	G	3100	1/1	0.95	0.78	45,45,45,45	0
25	MG	G	3050	1/1	0.95	1.59	97,97,97,97	0
25	MG	G	3128	1/1	0.95	0.19	58,58,58,58	0
25	MG	G	3011	1/1	0.96	0.57	106,106,106,106	0
25	MG	G	3124	1/1	0.96	0.18	35,35,35,35	0
25	MG	G	3017	1/1	0.96	1.17	110,110,110,110	0
25	MG	G	3131	1/1	0.97	0.17	30,30,30,30	0
25	MG	G	3105	1/1	0.97	0.12	44,44,44,44	0
25	MG	G	3093	1/1	0.97	0.47	71,71,71,71	0
26	K	G	3133	1/1	0.97	0.40	107,107,107,107	0
25	MG	G	3132	1/1	0.97	0.21	51,51,51,51	0
25	MG	G	3064	1/1	0.97	0.86	83,83,83,83	0
25	MG	G	3058	1/1	0.97	0.90	89,89,89,89	0
25	MG	G	3045	1/1	0.97	1.12	87,87,87,87	0
25	MG	G	3007	1/1	0.99	0.58	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	G	3107	1/1	0.99	0.11	59,59,59,59	0
27	ZN	G	3144	1/1	0.99	0.26	97,97,97,97	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.