



# wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 10:26 AM GMT

PDB ID : 3OTO  
Title : Crystal Structure of the 30S ribosomal subunit from a KsgA mutant of *Thermus thermophilus* (HB8)  
Authors : Demirci, H.; Murphy IV, F.; Belardinelli, R.; Kelley, A.C.; Ramakrishnan, V.; Gregory, S.T.; Dahlberg, A.E.; Jorgl, G.  
Deposited on : 2010-09-13  
Resolution : 3.69 Å(reported)

This is a wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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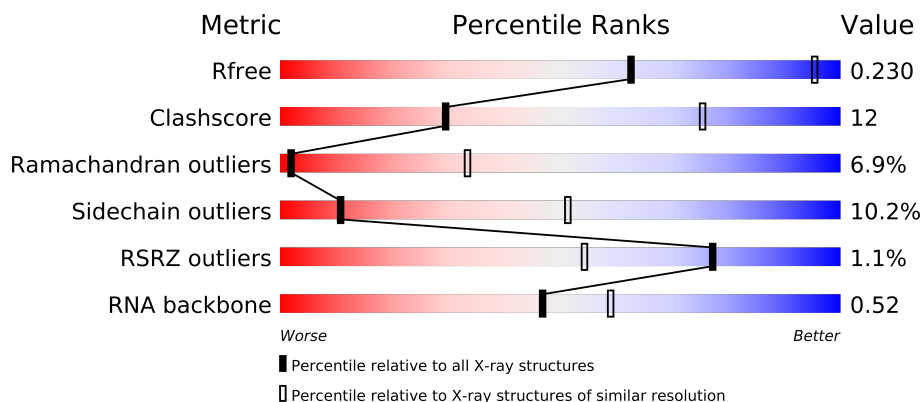
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.69 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.









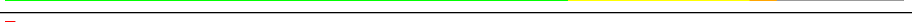

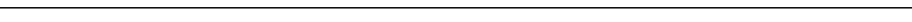
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1098 (4.00-3.40)
Clashscore	79885	1009 (3.94-3.46)
Ramachandran outliers	78287	1016 (3.98-3.42)
Sidechain outliers	78261	1014 (3.98-3.42)
RSRZ outliers	66119	1099 (4.00-3.40)
RNA backbone	1838	1008 (4.52-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1522	
2	B	256	
3	C	239	
4	D	209	
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	

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Mol	Chain	Length	Quality of chain
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	

## 2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 51775 atoms, of which 0 are hydrogen and 0 are deuterium.

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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1513	Total	C	N	O	P	0	0	0
			32511	14472	6016	10511	1512			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	0
			1873	1195	335	338	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 4 is a protein called 30S 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 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 6 is a protein called 30S 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 30S 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 30S 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 30S RIBOSOMAL PROTEIN S9.

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

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 11 is a protein called 30S 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 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	115	Total	C	N	O	S	0	0	0
			921	569	190	160	2			

- Molecule 14 is a protein called 30S 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 30S 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 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 17 is a protein called 30S 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			

- Molecule 18 is a protein called 30S 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 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

- Molecule 20 is a protein called 30S 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	SEE REMARK 999	UNP P80380

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	D	1	Total	Zn	0	0
			1	1		
22	N	1	Total	Zn	0	0
			1	1		

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	B	1	Total	Mg	0	0
			1	1		
23	A	91	Total	Mg	0	0
			91	91		
23	D	1	Total	Mg	0	0
			1	1		
23	M	1	Total	Mg	0	0
			1	1		

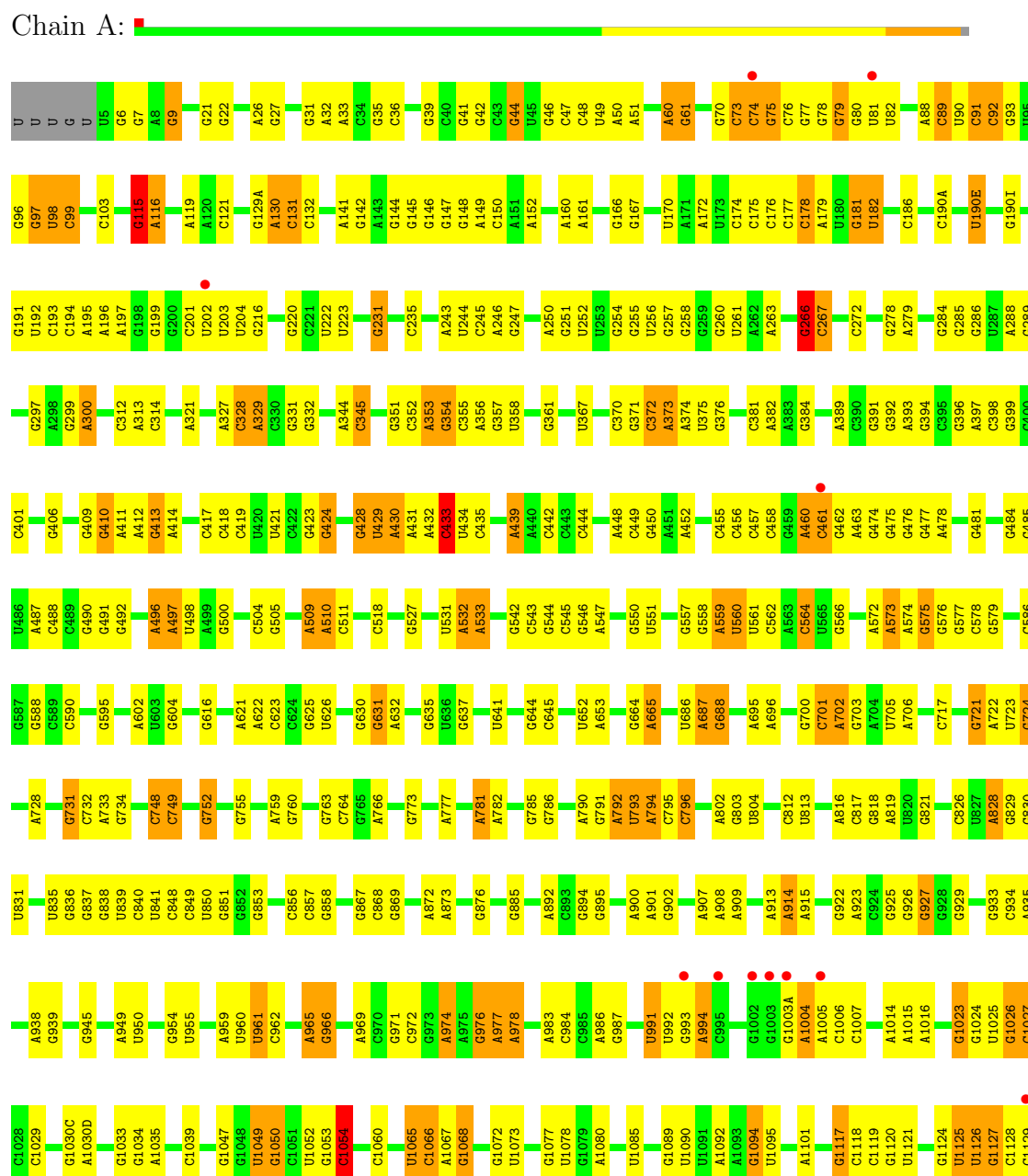
- Molecule 24 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	41	Total	K	0	0
			41	41		
24	E	1	Total	K	0	0
			1	1		

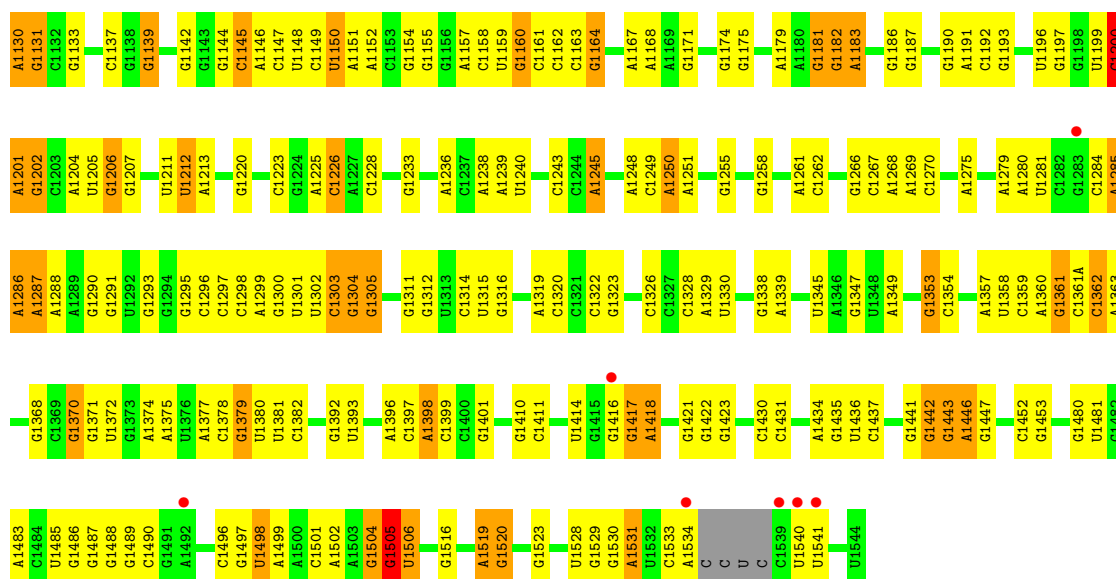
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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: 16S rRNA

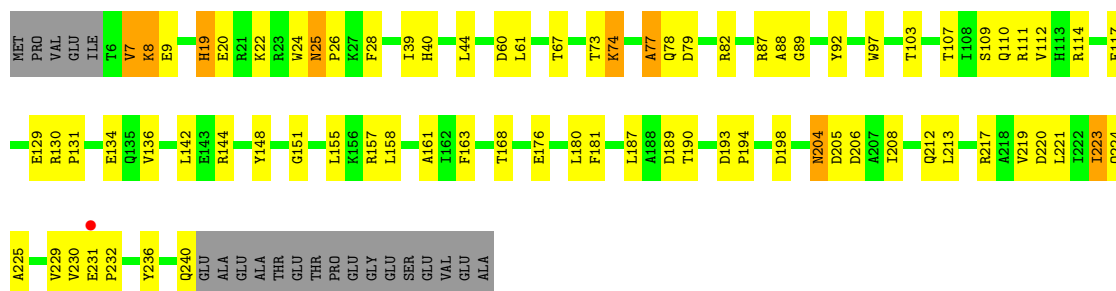






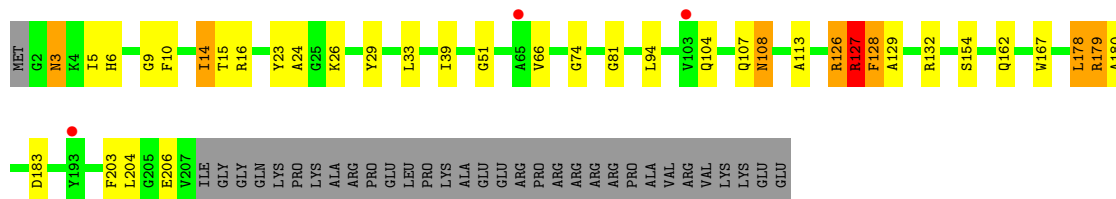
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain B:



• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain C:



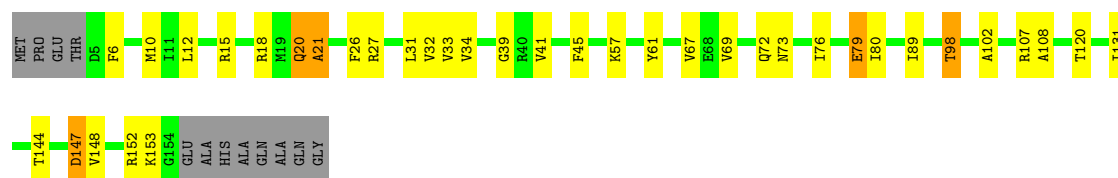
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain D:



• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain E:



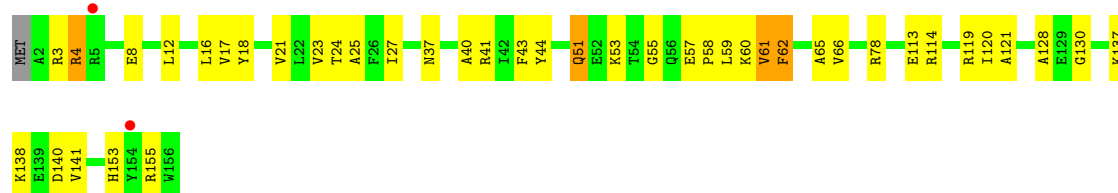
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain F:



- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain G:



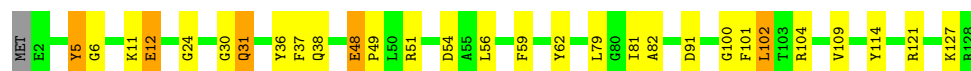
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain H:



- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain I:



- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain J:



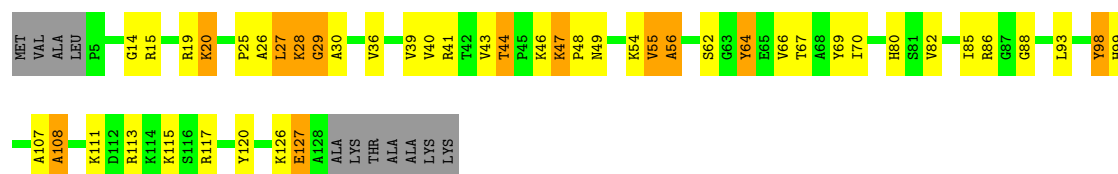
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K:



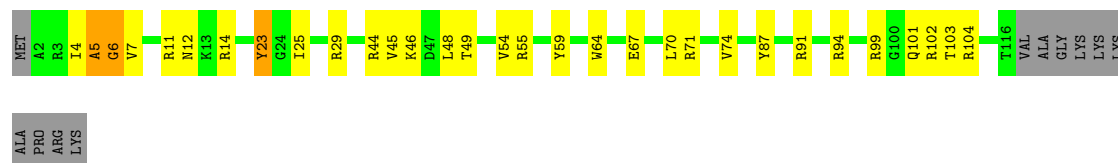
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain L: 



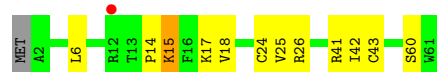
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M: 



• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain N: 



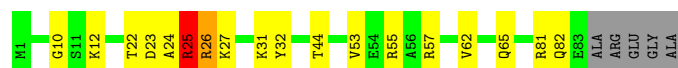
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain O: 



• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain P: 



• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain Q: 



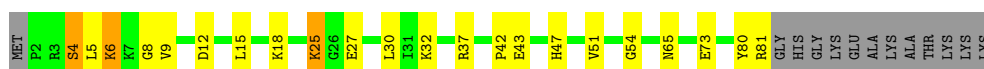
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain R: 



• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain S: 



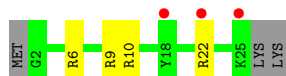
- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain T:



- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain U:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	402.09Å 402.09Å 173.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 3.69 29.84 – 3.69	Depositor EDS
% Data completeness (in resolution range)	92.7 (29.84-3.69) 97.8 (29.84-3.69)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 3.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.173 , 0.231 0.175 , 0.230	Depositor DCC
$R_{free}$ test set	7425 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	112.1	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 57.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 148377 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	51775	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	127.0	wwPDB-VP

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, MG, ZN

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	0.45	0/36390	0.81	19/56793 (0.0%)
2	B	0.32	0/1908	0.49	0/2577
3	C	0.25	0/1636	0.44	0/2205
4	D	0.31	0/1733	0.47	0/2318
5	E	0.39	0/1162	0.58	0/1564
6	F	0.29	0/856	0.47	0/1154
7	G	0.26	0/1276	0.44	0/1709
8	H	0.42	0/1136	0.59	0/1527
9	I	0.28	0/1029	0.46	0/1378
10	J	0.27	0/805	0.47	0/1082
11	K	0.32	0/900	0.50	0/1213
12	L	0.34	0/986	0.55	0/1320
13	M	0.27	0/931	0.49	0/1248
14	N	0.26	0/501	0.46	0/664
15	O	0.33	0/745	0.51	0/992
16	P	0.33	0/716	0.52	0/963
17	Q	0.39	0/870	0.59	0/1159
18	R	0.30	0/603	0.50	0/799
19	S	0.23	0/661	0.45	0/890
20	T	0.31	0/764	0.50	0/1006
21	U	0.28	0/212	0.51	0/277
All	All	0.41	0/55820	0.73	19/82838 (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	0

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1505	G	C4-N9-C1'	8.15	137.09	126.50
1	A	1505	G	C6-C5-N7	-6.83	126.30	130.40
1	A	1505	G	C8-N9-C1'	-6.33	118.77	127.00
1	A	1505	G	N7-C8-N9	6.30	116.25	113.10
1	A	235	C	C6-N1-C2	5.81	122.62	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	410	G	C3'

There are no planarity outliers.

## 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32511	0	0	433	0
2	B	1873	0	0	27	0
3	C	1612	0	0	14	0
4	D	1703	0	0	12	0
5	E	1146	0	0	14	0
6	F	843	0	0	4	0
7	G	1257	0	0	15	0
8	H	1116	0	0	12	0
9	I	1011	0	0	9	0
10	J	792	0	0	5	0
11	K	885	0	0	7	0
12	L	970	0	0	24	0
13	M	921	0	0	12	0
14	N	492	0	0	4	0
15	O	734	0	0	9	0
16	P	700	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Q	857	0	0	8	0
18	R	597	0	0	4	0
19	S	647	0	0	4	0
20	T	762	0	0	14	0
21	U	208	0	0	2	0
22	D	1	0	0	0	0
22	N	1	0	0	0	0
23	A	91	0	0	0	0
23	B	1	0	0	0	0
23	D	1	0	0	0	0
23	M	1	0	0	0	0
24	A	41	0	0	0	0
24	E	1	0	0	0	0
All	All	51775	0	0	605	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

The worst 5 of 605 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:79:G:C2	1:A:80:G:N7	2.51	0.79
1:A:80:G:C2	1:A:81:U:C4	2.73	0.76
1:A:1361:G:C6	1:A:1361(A):C:N4	2.55	0.76
1:A:75:G:C2	1:A:76:C:C4	2.78	0.72
1:A:77:G:N1	1:A:92:C:N4	2.40	0.70

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%)	168 (72%)	45 (19%)	20 (9%)	1	25
3	C	204/239 (85%)	152 (74%)	37 (18%)	15 (7%)	2	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	206/209 (99%)	168 (82%)	32 (16%)	6 (3%)	7	60
5	E	148/162 (91%)	119 (80%)	26 (18%)	3 (2%)	11	68
6	F	99/101 (98%)	80 (81%)	17 (17%)	2 (2%)	11	68
7	G	153/156 (98%)	105 (69%)	34 (22%)	14 (9%)	1	24
8	H	136/138 (99%)	115 (85%)	15 (11%)	6 (4%)	4	48
9	I	125/128 (98%)	86 (69%)	28 (22%)	11 (9%)	1	25
10	J	96/105 (91%)	60 (62%)	22 (23%)	14 (15%)	0	10
11	K	117/129 (91%)	85 (73%)	22 (19%)	10 (8%)	1	26
12	L	122/135 (90%)	87 (71%)	22 (18%)	13 (11%)	1	17
13	M	113/126 (90%)	91 (80%)	16 (14%)	6 (5%)	3	42
14	N	58/61 (95%)	40 (69%)	13 (22%)	5 (9%)	1	25
15	O	86/89 (97%)	70 (81%)	13 (15%)	3 (4%)	6	56
16	P	81/88 (92%)	63 (78%)	11 (14%)	7 (9%)	1	25
17	Q	102/105 (97%)	86 (84%)	14 (14%)	2 (2%)	11	68
18	R	71/88 (81%)	53 (75%)	14 (20%)	4 (6%)	3	40
19	S	78/93 (84%)	47 (60%)	19 (24%)	12 (15%)	0	8
20	T	97/106 (92%)	60 (62%)	28 (29%)	9 (9%)	1	23
21	U	22/27 (82%)	17 (77%)	5 (23%)	0	100	100
All	All	2347/2541 (92%)	1752 (75%)	433 (18%)	162 (7%)	2	33

5 of 162 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
3	C	15	THR
3	C	29	TYR
3	C	127	ARG

### 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	194/220 (88%)	173 (89%)	21 (11%)	9	48
3	C	160/188 (85%)	148 (92%)	12 (8%)	19	67
4	D	180/181 (99%)	166 (92%)	14 (8%)	18	65
5	E	115/123 (94%)	98 (85%)	17 (15%)	4	30
6	F	90/90 (100%)	81 (90%)	9 (10%)	11	52
7	G	126/127 (99%)	116 (92%)	10 (8%)	18	65
8	H	119/119 (100%)	104 (87%)	15 (13%)	7	39
9	I	98/99 (99%)	87 (89%)	11 (11%)	9	45
10	J	87/92 (95%)	80 (92%)	7 (8%)	17	64
11	K	90/99 (91%)	80 (89%)	10 (11%)	9	46
12	L	104/111 (94%)	90 (86%)	14 (14%)	6	35
13	M	93/101 (92%)	81 (87%)	12 (13%)	6	38
14	N	49/50 (98%)	47 (96%)	2 (4%)	41	85
15	O	79/80 (99%)	69 (87%)	10 (13%)	6	38
16	P	72/74 (97%)	63 (88%)	9 (12%)	7	40
17	Q	96/97 (99%)	92 (96%)	4 (4%)	40	84
18	R	64/77 (83%)	57 (89%)	7 (11%)	9	47
19	S	71/80 (89%)	64 (90%)	7 (10%)	11	53
20	T	76/82 (93%)	67 (88%)	9 (12%)	8	42
21	U	19/22 (86%)	17 (90%)	2 (10%)	10	49
All	All	1982/2112 (94%)	1780 (90%)	202 (10%)	11	51

5 of 202 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	85	ARG
10	J	57	LYS
19	S	18	LYS
8	H	102	ARG
9	I	79	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1511/1522 (99%)	281 (18%)	35 (2%)

5 of 281 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	G
1	A	31	G
1	A	32	A
1	A	33	A

5 of 35 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	560	U
1	A	812	C
1	A	1504	G
1	A	687	A
1	A	701	C

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 138 ligands modelled in this entry, 138 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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1513/1522 (99%)	-0.31	18 (1%) 75 52	50, 108, 253, 361	0
2	B	235/256 (91%)	-0.29	1 (0%) 90 78	65, 115, 197, 256	0
3	C	206/239 (86%)	-0.08	3 (1%) 70 46	116, 170, 237, 271	0
4	D	208/209 (99%)	-0.19	0 100 100	63, 111, 160, 175	0
5	E	150/162 (92%)	-0.30	0 100 100	51, 78, 114, 154	0
6	F	101/101 (100%)	-0.29	0 100 100	87, 129, 155, 177	0
7	G	155/156 (99%)	-0.14	2 (1%) 74 50	99, 152, 220, 233	0
8	H	138/138 (100%)	-0.37	0 100 100	41, 72, 104, 137	0
9	I	127/128 (99%)	-0.10	0 100 100	78, 171, 216, 224	0
10	J	98/105 (93%)	0.29	6 (6%) 21 14	122, 178, 274, 291	0
11	K	119/129 (92%)	-0.19	1 (0%) 83 63	62, 106, 146, 183	0
12	L	124/135 (91%)	-0.18	0 100 100	48, 107, 143, 174	0
13	M	115/126 (91%)	-0.15	0 100 100	96, 136, 170, 180	0
14	N	60/61 (98%)	0.17	1 (1%) 67 44	125, 157, 213, 229	0
15	O	88/89 (98%)	-0.30	0 100 100	54, 95, 133, 171	0
16	P	83/88 (94%)	-0.32	0 100 100	69, 99, 137, 199	0
17	Q	104/105 (99%)	-0.16	4 (3%) 38 25	54, 83, 125, 223	0
18	R	73/88 (82%)	-0.29	0 100 100	65, 99, 164, 209	0
19	S	80/93 (86%)	0.13	0 100 100	149, 183, 219, 231	0
20	T	99/106 (93%)	-0.32	1 (1%) 79 57	76, 107, 165, 190	0
21	U	24/27 (88%)	0.65	3 (12%) 5 5	121, 141, 162, 171	0
All	All	3900/4063 (95%)	-0.23	40 (1%) 77 57	41, 116, 222, 361	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	128	ALA	7.7
1	A	1541	U	6.7
17	Q	104	LYS	5.9
1	A	1540	U	5.7
10	J	33	GLN	5.6

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
23	MG	A	1610	1/1	0.28	-	47,47,47,47	0
24	K	A	1647	1/1	0.18	-	85,85,85,85	0
23	MG	A	1613	1/1	0.17	-	39,39,39,39	0
23	MG	A	1620	1/1	0.89	-	92,92,92,92	0
24	K	A	1633	1/1	0.20	-	135,135,135,135	0
24	K	A	1648	1/1	0.24	-	63,63,63,63	0
24	K	A	1658	1/1	0.66	-	107,107,107,107	0
23	MG	A	1582	1/1	0.82	-	83,83,83,83	0
23	MG	A	1576	1/1	0.50	-	78,78,78,78	0
23	MG	A	1627	1/1	0.49	-	39,39,39,39	0
24	K	A	1665	1/1	0.32	-	79,79,79,79	0
24	K	A	1666	1/1	0.55	-	74,74,74,74	0
23	MG	A	1614	1/1	0.15	-	56,56,56,56	0
23	MG	A	1617	1/1	0.30	-	78,78,78,78	0
23	MG	A	1621	1/1	0.10	-	58,58,58,58	0
23	MG	A	1571	1/1	0.41	-	67,67,67,67	0
24	K	A	1660	1/1	0.20	-	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1572	1/1	0.36	-	35,35,35,35	0
24	K	A	1637	1/1	0.43	-	129,129,129,129	0
23	MG	A	1623	1/1	0.35	-	77,77,77,77	0
23	MG	A	1545	1/1	0.21	-	75,75,75,75	0
23	MG	A	1605	1/1	1.18	-	56,56,56,56	0
23	MG	A	1601	1/1	0.27	-	78,78,78,78	0
23	MG	A	1565	1/1	0.39	-	87,87,87,87	0
23	MG	A	1597	1/1	0.24	-	47,47,47,47	0
23	MG	A	1585	1/1	0.25	-	78,78,78,78	0
24	K	A	1662	1/1	0.29	-	92,92,92,92	0
23	MG	M	127	1/1	0.43	-	76,76,76,76	0
23	MG	A	1594	1/1	0.13	-	46,46,46,46	0
23	MG	A	1629	1/1	0.42	-	61,61,61,61	0
24	K	A	1635	1/1	0.57	-	149,149,149,149	0
23	MG	A	1625	1/1	0.23	-	93,93,93,93	0
23	MG	A	1558	1/1	0.43	-	81,81,81,81	0
23	MG	A	1588	1/1	0.21	-	59,59,59,59	0
23	MG	A	1567	1/1	0.20	-	70,70,70,70	0
23	MG	A	1561	1/1	0.12	-	59,59,59,59	0
23	MG	A	1579	1/1	0.23	-	29,29,29,29	0
23	MG	A	1546	1/1	0.78	-	76,76,76,76	0
23	MG	A	1548	1/1	1.02	-	81,81,81,81	0
23	MG	A	1619	1/1	0.40	-	91,91,91,91	0
24	K	A	1631	1/1	0.38	-	110,110,110,110	0
23	MG	A	1563	1/1	0.24	-	20,20,20,20	0
23	MG	A	1616	1/1	0.39	-	49,49,49,49	0
24	K	A	1671	1/1	0.47	-	79,79,79,79	0
24	K	A	1636	1/1	0.67	-	116,116,116,116	0
24	K	A	1640	1/1	0.49	-	108,108,108,108	0
23	MG	A	1554	1/1	0.61	-	59,59,59,59	0
23	MG	A	1622	1/1	0.55	-	87,87,87,87	0
24	K	A	1649	1/1	0.26	-	75,75,75,75	0
23	MG	A	1609	1/1	0.71	-	96,96,96,96	0
23	MG	A	1607	1/1	0.55	-	65,65,65,65	0
23	MG	A	1628	1/1	0.39	-	65,65,65,65	0
23	MG	A	86	1/1	0.21	-	59,59,59,59	0
23	MG	A	1569	1/1	0.20	-	59,59,59,59	0
24	K	A	1632	1/1	0.17	-	102,102,102,102	0
23	MG	A	1556	1/1	0.43	-	93,93,93,93	0
24	K	E	163	1/1	0.34	-	115,115,115,115	0
24	K	A	1670	1/1	0.34	-	107,107,107,107	0
24	K	A	1644	1/1	0.47	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1559	1/1	0.84	-	53,53,53,53	0
23	MG	A	1611	1/1	0.17	-	56,56,56,56	0
24	K	A	1657	1/1	0.55	-	83,83,83,83	0
23	MG	A	1564	1/1	0.33	-	59,59,59,59	0
24	K	A	1653	1/1	0.14	-	98,98,98,98	0
23	MG	A	1603	1/1	0.49	-	100,100,100,100	0
23	MG	A	1573	1/1	0.37	-	70,70,70,70	0
23	MG	B	257	1/1	0.37	-	77,77,77,77	0
23	MG	A	1547	1/1	0.48	-	86,86,86,86	0
24	K	A	1645	1/1	0.33	-	75,75,75,75	0
23	MG	D	211	1/1	0.14	-	73,73,73,73	0
23	MG	A	1581	1/1	0.47	-	68,68,68,68	0
23	MG	A	1599	1/1	0.64	-	65,65,65,65	0
23	MG	A	1552	1/1	0.20	-	80,80,80,80	0
23	MG	A	1586	1/1	0.30	-	48,48,48,48	0
24	K	A	1661	1/1	0.14	-	79,79,79,79	0
23	MG	A	1555	1/1	0.26	-	95,95,95,95	0
24	K	A	1638	1/1	0.40	-	143,143,143,143	0
23	MG	A	1590	1/1	0.32	-	39,39,39,39	0
23	MG	A	1560	1/1	0.47	-	89,89,89,89	0
23	MG	A	1618	1/1	0.45	-	64,64,64,64	0
23	MG	A	1553	1/1	0.65	-	94,94,94,94	0
23	MG	A	1574	1/1	0.90	-	68,68,68,68	0
24	K	A	1667	1/1	0.37	-	80,80,80,80	0
24	K	A	1669	1/1	0.47	-	98,98,98,98	0
23	MG	A	1608	1/1	0.36	-	72,72,72,72	0
24	K	A	1654	1/1	0.35	-	85,85,85,85	0
23	MG	A	1551	1/1	0.56	-	50,50,50,50	0
23	MG	A	1602	1/1	0.45	-	63,63,63,63	0
23	MG	A	94	1/1	0.30	-	66,66,66,66	0
23	MG	A	1589	1/1	0.23	-	79,79,79,79	0
24	K	A	1656	1/1	0.40	-	105,105,105,105	0
23	MG	A	85	1/1	0.36	-	35,35,35,35	0
23	MG	A	1570	1/1	0.71	-	34,34,34,34	0
24	K	A	1639	1/1	0.65	-	81,81,81,81	0
23	MG	A	1593	1/1	0.56	-	87,87,87,87	0
23	MG	A	1578	1/1	0.51	-	50,50,50,50	0
23	MG	A	1549	1/1	0.51	-	59,59,59,59	0
23	MG	A	1557	1/1	0.84	-	90,90,90,90	0
24	K	A	1659	1/1	0.31	-	76,76,76,76	0
23	MG	A	1562	1/1	0.72	-	54,54,54,54	0
24	K	A	1642	1/1	0.41	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1630	1/1	0.30	-	41,41,41,41	0
23	MG	A	1584	1/1	0.55	-	52,52,52,52	0
23	MG	A	1615	1/1	0.20	-	55,55,55,55	0
23	MG	A	1587	1/1	0.40	-	37,37,37,37	0
24	K	A	1651	1/1	0.43	-	138,138,138,138	0
24	K	A	1663	1/1	0.54	-	99,99,99,99	0
22	ZN	N	141	1/1	0.07	-	150,150,150,150	0
23	MG	A	1575	1/1	0.58	-	32,32,32,32	0
24	K	A	1646	1/1	0.54	-	82,82,82,82	0
23	MG	A	1612	1/1	0.23	-	81,81,81,81	0
23	MG	A	100	1/1	0.22	-	126,126,126,126	0
23	MG	A	1606	1/1	0.35	-	65,65,65,65	0
23	MG	A	1577	1/1	0.59	-	63,63,63,63	0
23	MG	A	1580	1/1	0.40	-	79,79,79,79	0
23	MG	A	1583	1/1	0.39	-	67,67,67,67	0
23	MG	A	1626	1/1	0.13	-	62,62,62,62	0
24	K	A	1634	1/1	0.21	-	134,134,134,134	0
23	MG	A	1550	1/1	0.21	-	52,52,52,52	0
24	K	A	1652	1/1	0.21	-	100,100,100,100	0
23	MG	A	1596	1/1	1.22	-	54,54,54,54	0
23	MG	A	1624	1/1	0.09	-	38,38,38,38	0
23	MG	A	1604	1/1	0.19	-	52,52,52,52	0
24	K	A	1664	1/1	0.22	-	111,111,111,111	0
23	MG	A	1591	1/1	0.34	-	82,82,82,82	0
24	K	A	1668	1/1	0.45	-	95,95,95,95	0
23	MG	A	1568	1/1	0.12	-	17,17,17,17	0
23	MG	A	1566	1/1	0.41	-	90,90,90,90	0
23	MG	A	71	1/1	0.87	-	74,74,74,74	0
24	K	A	1650	1/1	0.12	-	86,86,86,86	0
24	K	A	1643	1/1	0.29	-	122,122,122,122	0
22	ZN	D	210	1/1	0.32	-	85,85,85,85	0
24	K	A	1655	1/1	0.47	-	102,102,102,102	0
23	MG	A	1600	1/1	0.62	-	72,72,72,72	0
23	MG	A	1595	1/1	0.18	-	33,33,33,33	0
24	K	A	1641	1/1	0.69	-	97,97,97,97	0
23	MG	A	1592	1/1	0.35	-	63,63,63,63	0
23	MG	A	1598	1/1	0.66	-	73,73,73,73	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.