



# wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 12:43 AM GMT

PDB ID : 4A1C  
Title : T.THERMOPHILA 60S RIBOSOMAL SUBUNIT IN COMPLEX WITH INITIATION FACTOR 6. THIS FILE CONTAINS 5S RRNA, 5.8S RRNA AND PROTEINS OF MOLECULE 4.  
Authors : Klinge, S.; Voigts-Hoffmann, F.; Leibundgut, M.; Arpagaus, S.; Ban, N.  
Deposited on : 2011-09-14  
Resolution : 3.52 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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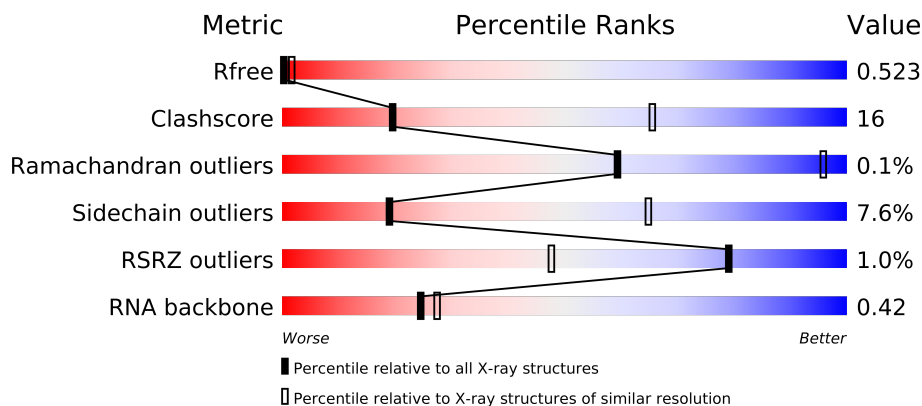
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.52 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	1256 (3.74-3.30)
Clashscore	79885	1020 (3.68-3.36)
Ramachandran outliers	78287	1082 (3.70-3.34)
Sidechain outliers	78261	1082 (3.70-3.34)
RSRZ outliers	66119	1256 (3.74-3.30)
RNA backbone	1838	1008 (4.26-2.76)

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. 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	2	154	
2	3	120	
3	A	264	
4	B	391	
5	C	410	
6	D	172	
7	E	188	
8	F	255	
9	G	123	
10	H	215	
11	I	198	

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Mol	Chain	Length	Quality of chain
12	J	141	
13	K	149	
14	L	204	
15	M	301	
16	N	181	
17	O	185	
18	P	157	
19	Q	183	
20	R	150	
21	S	135	
22	T	158	
23	U	124	
24	V	239	
25	W	111	
26	X	134	
27	Y	103	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
28	MG	0	197	-	X
28	MG	0	200	-	X
28	MG	0	228	-	X
28	MG	0	325	-	X
28	MG	0	347	-	X

## 2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 43522 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 5.8S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2	154	Total	C	N	O	P	0	0	0
			3300	1475	602	1069	154			

- Molecule 2 is a RNA chain called 5S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	3	120	Total	C	N	O	P	0	0	0
			2566	1145	463	838	120			

- Molecule 3 is a protein called RPL8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	257	Total	C	N	O	S	0	0	0
			1977	1226	400	343	8			

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	386	Total	C	N	O	S	0	0	0
			3080	1944	595	530	11			

- Molecule 5 is a protein called RPL4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	409	Total	C	N	O	S	0	0	0
			3172	1975	622	571	4			

- Molecule 6 is a protein called 60S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	169	Total	C	N	O	S	0	0	0
			1357	851	254	243	9			

- Molecule 7 is a protein called 60S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	186	Total	C	N	O	S	0	0	0
			1481	939	272	264	6			

- Molecule 8 is a protein called RPL7A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	231	Total	C	N	O	S	0	0	0
			1860	1191	341	327	1			

- Molecule 9 is a protein called RPLP0.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	G	123	Total	C	N	O	0	0	0
			711	465	123	123			

- Molecule 10 is a protein called 60S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	201	Total	C	N	O	S	0	0	0
			1620	1027	319	271	3			

- Molecule 11 is a protein called 60S RIBOSOMAL PROTEIN L13A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	198	Total	C	N	O	S	0	0	0
			1594	1019	308	263	4			

- Molecule 12 is a protein called RPL23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	138	Total	C	N	O	S	0	0	0
			1022	643	193	179	7			

- Molecule 13 is a protein called 60S RIBOSOMAL PROTEIN L27A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	148	Total	C	N	O	S	0	0	0
			1161	739	234	182	6			

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	203	Total	C	N	O	S	0	0	0
			1691	1061	351	275	4			

- Molecule 15 is a protein called 60S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	300	Total	C	N	O	S	0	0	0
			2424	1541	447	432	4			

- Molecule 16 is a protein called RPL18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	180	Total	C	N	O	S	0	0	0
			1441	909	280	249	3			

- Molecule 17 is a protein called RPL19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	O	153	Total	C	N	O	S	0	0	0
			1234	772	256	201	5			

- Molecule 18 is a protein called 60S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	156	Total	C	N	O	S	0	0	0
			1272	804	251	215	2			

- Molecule 19 is a protein called RPL17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	157	Total	C	N	O	S	0	0	0
			1239	771	249	216	3			

- Molecule 20 is a protein called RPL23A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	121	Total	C	N	O	S	0	0	0
			965	613	176	173	3			

- Molecule 21 is a protein called RPL26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	126	Total	C	N	O	S	0	0	0
			1013	638	200	173	2			

- Molecule 22 is a protein called RPL24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	61	Total	C	N	O	S	0	0	0
			510	331	100	76	3			

- Molecule 23 is a protein called RPL35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	123	Total	C	N	O	S	0	0	0
			990	629	196	165				

- Molecule 24 is a protein called 60S RIBOSOMAL PROTEIN L7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	234	Total	C	N	O	S	0	0	0
			1910	1221	362	323	4			

- Molecule 25 is a protein called 60S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	110	Total	C	N	O	S	0	0	0
			901	563	171	164	3			

- Molecule 26 is a protein called 60S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	X	125	Total	C	N	O	S	0	0	0
			1012	639	205	165	3			

- Molecule 27 is a protein called RPL37A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Y	102	Total	C	N	O	S	0	0	0
			786	502	148	131	5			

- Molecule 28 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	0	176	Total 176	Mg 176	0	0

- Molecule 29 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	Y	1	Total 1	Zn 1	0	0

- Molecule 30 is water.

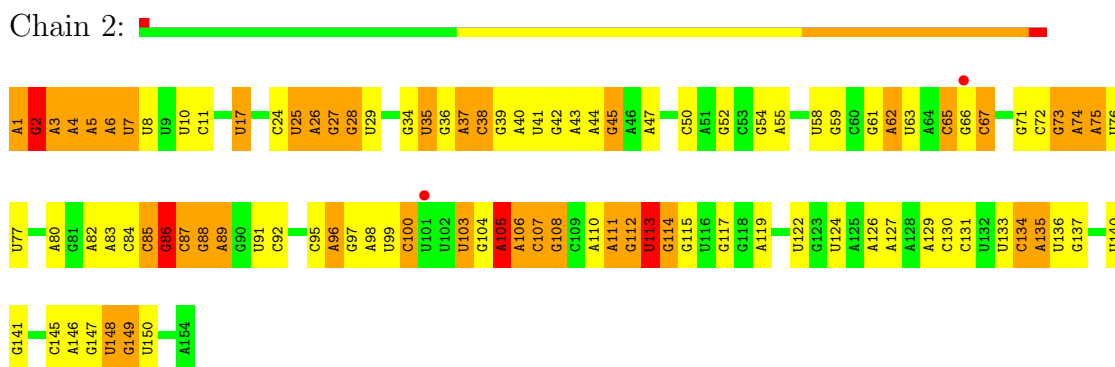
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	0	1056	Total 1056	O 1056	0	0



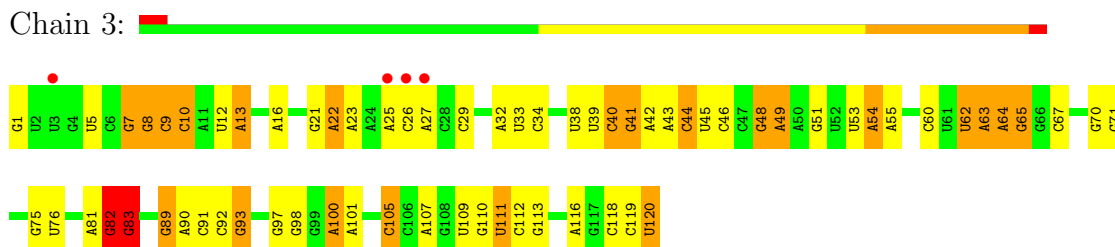
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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.

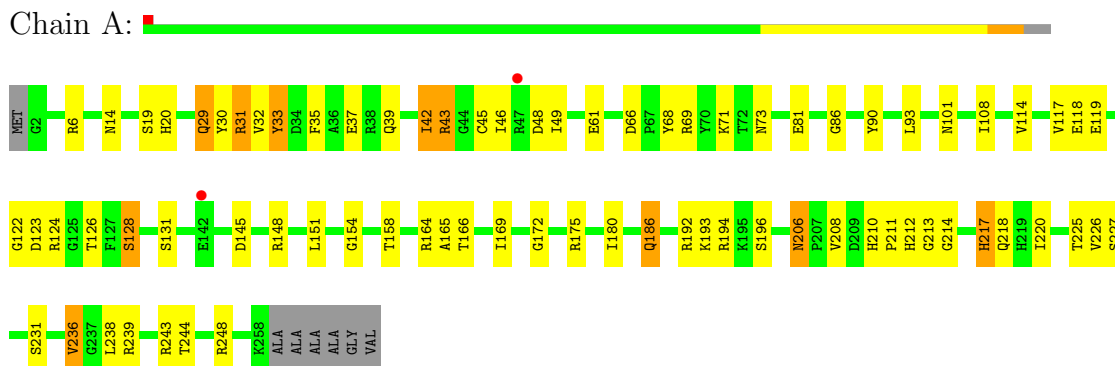
#### • Molecule 1: 5.8S rRNA



#### • Molecule 2: 5S rRNA

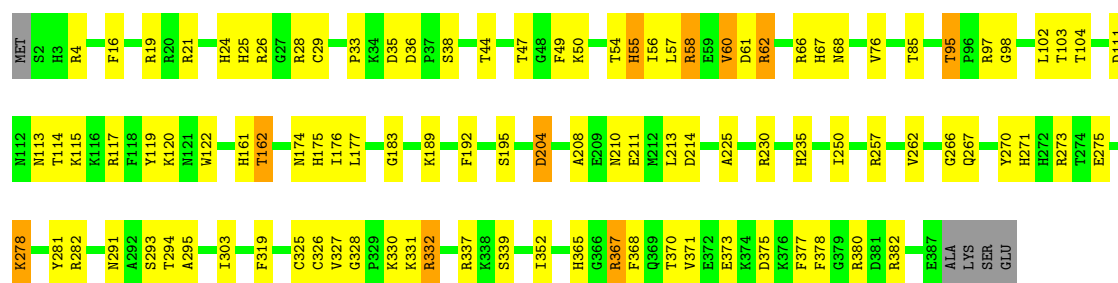


#### • Molecule 3: RPL8



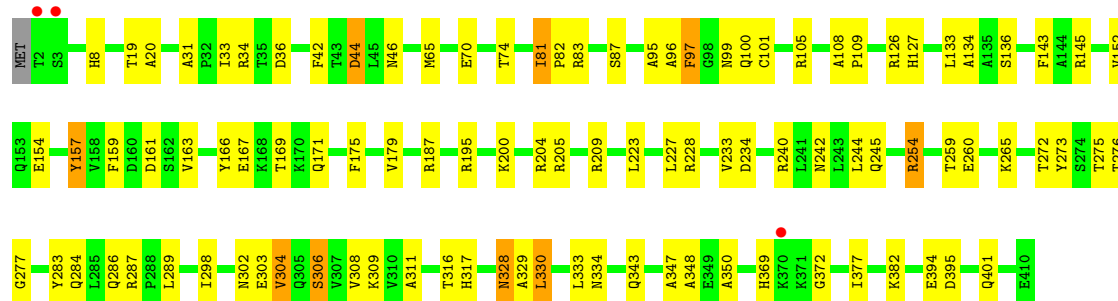
#### • Molecule 4: RIBOSOMAL PROTEIN L3





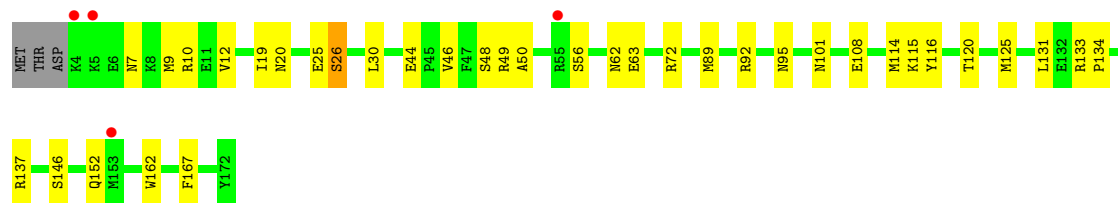
• Molecule 5: RPL4

Chain C:



• Molecule 6: 60S RIBOSOMAL PROTEIN L11

Chain D:



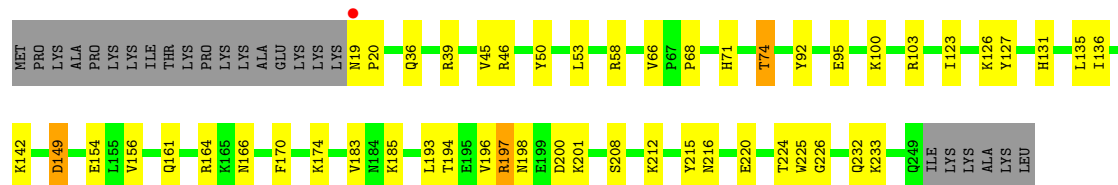
• Molecule 7: 60S RIBOSOMAL PROTEIN L9

Chain E:



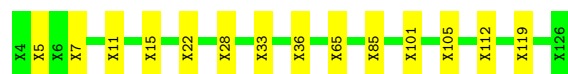
• Molecule 8: RPL7A

Chain F:



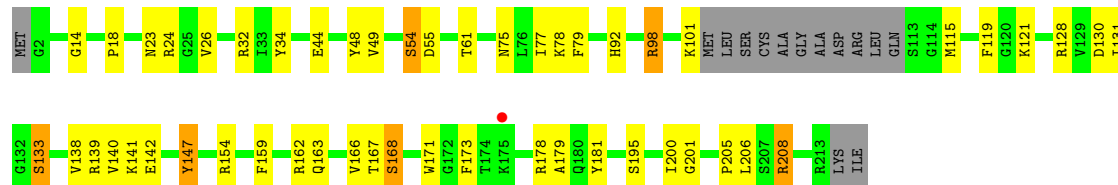
• Molecule 9: RPLP0

Chain G:



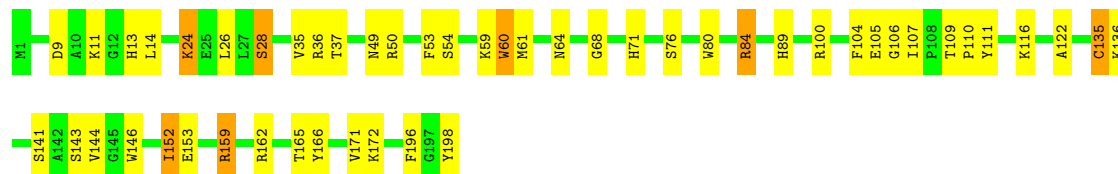
• Molecule 10: 60S RIBOSOMAL PROTEIN L10

Chain H:



• Molecule 11: 60S RIBOSOMAL PROTEIN L13A

Chain I:



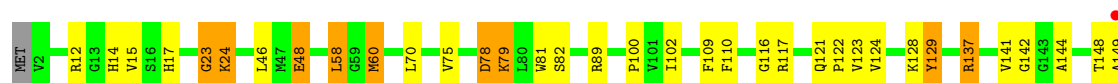
• Molecule 12: RPL23

Chain J:



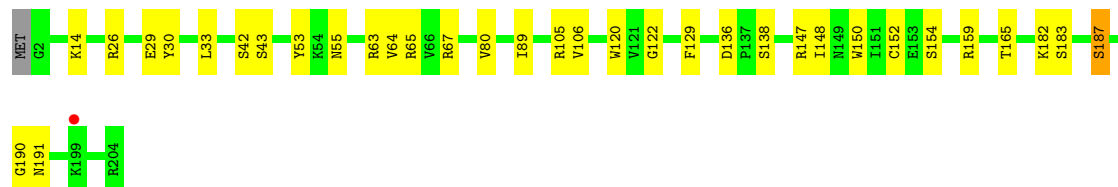
• Molecule 13: 60S RIBOSOMAL PROTEIN L27A

Chain K:



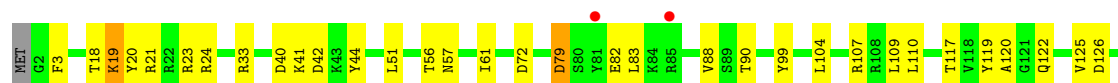
• Molecule 14: RIBOSOMAL PROTEIN L15

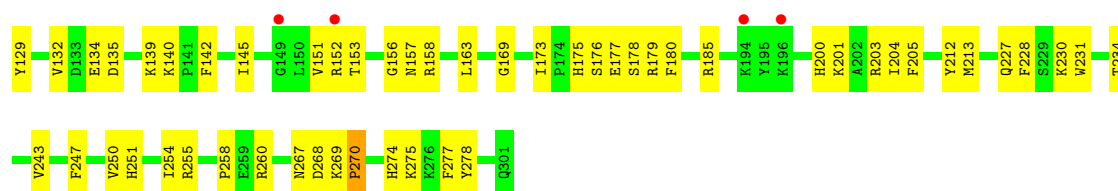
Chain L:



• Molecule 15: 60S RIBOSOMAL PROTEIN L5

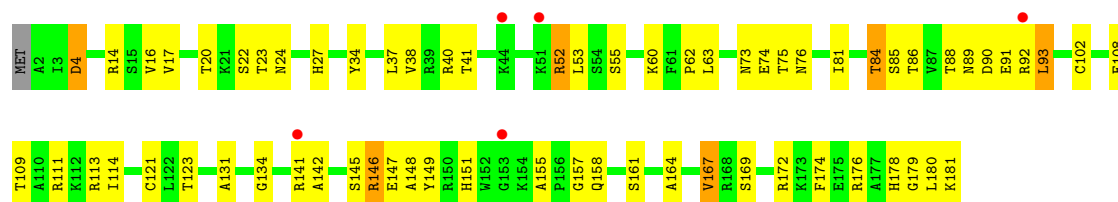
Chain M:





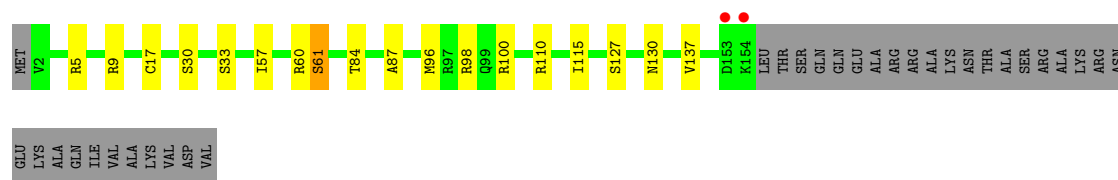
• Molecule 16: RPL18

Chain N:



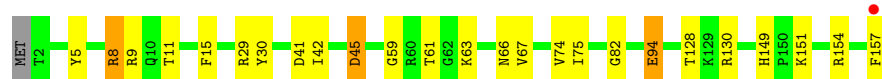
• Molecule 17: RPL19

Chain O:



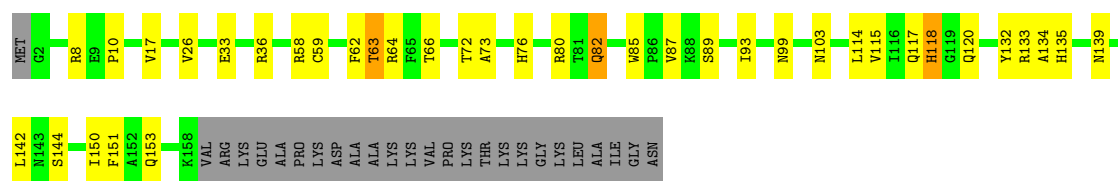
• Molecule 18: 60S RIBOSOMAL PROTEIN L21

Chain P:



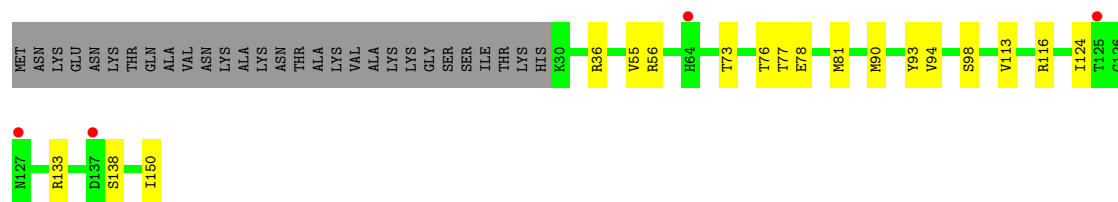
• Molecule 19: RPL17

Chain Q:

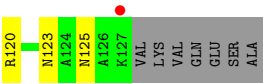


• Molecule 20: RPL23A

Chain R:

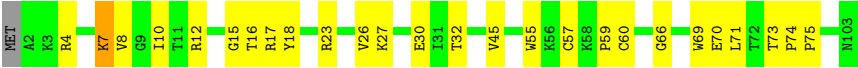






● Molecule 27: RPL37A

Chain Y:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	320.19Å 289.25Å 535.04Å 90.00° 91.22° 90.00°	Depositor
Resolution (Å)	20.00 – 3.52 39.96 – 3.52	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-3.52) 99.4 (39.96-3.52)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 3.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.216 , 0.244 0.526 , 0.523	Depositor DCC
$R_{free}$ test set	10000 reflections (0.85%)	DCC
Wilson B-factor (Å <sup>2</sup> )	96.9	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 76.0	EDS
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 1192534 reflections	Xtriage
$F_o, F_c$ correlation	0.45	EDS
Total number of atoms	43522	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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: ZN, 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	2	0.86	1/3696 (0.0%)	1.17	24/5761 (0.4%)
2	3	0.63	0/2870	0.98	10/4473 (0.2%)
3	A	0.60	0/2019	0.76	1/2712 (0.0%)
4	B	0.52	0/3144	0.72	0/4213
5	C	0.53	0/3222	0.69	1/4338 (0.0%)
6	D	0.47	0/1376	0.67	0/1833
7	E	0.50	0/1501	0.74	2/2015 (0.1%)
8	F	0.49	0/1893	0.66	0/2548
10	H	0.46	0/1652	0.67	0/2213
11	I	0.87	6/1624 (0.4%)	0.92	7/2176 (0.3%)
12	J	0.68	1/1038 (0.1%)	0.77	2/1394 (0.1%)
13	K	0.58	0/1189	0.74	0/1589
14	L	0.59	0/1727	0.73	0/2308
15	M	0.53	1/2469 (0.0%)	0.72	1/3306 (0.0%)
16	N	0.60	0/1464	0.78	1/1965 (0.1%)
17	O	0.50	0/1250	0.65	0/1660
18	P	0.54	0/1300	0.64	0/1743
19	Q	0.56	0/1259	0.78	1/1693 (0.1%)
20	R	0.52	0/981	0.67	0/1320
21	S	0.50	0/1028	0.63	0/1372
22	T	0.53	0/521	0.70	0/693
23	U	0.51	0/995	0.66	0/1318
24	V	0.49	0/1950	0.66	1/2614 (0.0%)
25	W	0.51	0/913	0.68	0/1222
26	X	0.56	0/1028	0.68	0/1371
27	Y	0.55	0/799	0.75	0/1069
All	All	0.59	9/42908 (0.0%)	0.79	51/58919 (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
8	F	0	1
13	K	0	2
19	Q	0	1
26	X	0	1
All	All	0	5

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	60	TRP	NE1-CE2	-18.39	1.13	1.37
11	I	60	TRP	CD2-CE2	13.85	1.57	1.41
11	I	60	TRP	CG-CD2	11.72	1.63	1.43
11	I	60	TRP	CD2-CE3	-7.63	1.28	1.40
15	M	117	THR	CA-CB	-7.02	1.35	1.53

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	I	60	TRP	CE2-CD2-CG	-18.64	92.39	107.30
11	I	60	TRP	NE1-CE2-CZ2	-11.79	117.43	130.40
1	2	95	C	C6-N1-C2	9.96	124.28	120.30
11	I	60	TRP	CD1-NE1-CE2	9.80	117.82	109.00
11	I	60	TRP	CD2-CE2-CZ2	-9.52	110.88	122.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	F	174	LYS	Peptide
13	K	23	GLY	Peptide
13	K	58	LEU	Peptide
19	Q	118	HIS	Peptide
26	X	8	HIS	Peptide

## 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	2	3300	0	11	72	0
2	3	2566	0	0	73	0
3	A	1977	0	0	41	0
4	B	3080	0	0	59	0
5	C	3172	0	0	68	0
6	D	1357	0	0	22	0
7	E	1481	0	0	14	0
8	F	1860	0	0	33	0
9	G	711	0	0	8	0
10	H	1620	0	0	30	0
11	I	1594	0	0	27	0
12	J	1022	0	0	13	0
13	K	1161	0	0	24	0
14	L	1691	0	0	19	0
15	M	2424	0	0	71	0
16	N	1441	0	0	44	0
17	O	1234	0	0	5	0
18	P	1272	0	0	18	0
19	Q	1239	0	0	18	0
20	R	965	0	0	9	0
21	S	1013	0	0	29	0
22	T	510	0	0	5	0
23	U	990	0	0	9	0
24	V	1910	0	0	28	0
25	W	901	0	0	5	0
26	X	1012	0	0	16	0
27	Y	786	0	0	13	0
28	0	176	0	0	0	0
29	Y	1	0	0	0	0
30	0	1056	0	0	25	0
All	All	43522	0	11	683	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 16.

The worst 5 of 683 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:C:395:ASP:OD1	18:P:154:ARG:NH2	1.80	1.15
26:X:15:ARG:O	30:0:5447:HOH:O	1.68	1.09
12:J:51:SER:OG	30:0:6869:HOH:O	1.71	1.08

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:218:GLN:O	30:0:6118:HOH:O	1.72	1.08
1:2:100:C:OP2	20:R:56:ARG:NH2	1.88	1.07

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	
3	A	255/264 (97%)	237 (93%)	18 (7%)	0	100	100
4	B	384/391 (98%)	370 (96%)	14 (4%)	0	100	100
5	C	407/410 (99%)	386 (95%)	21 (5%)	0	100	100
6	D	167/172 (97%)	156 (93%)	11 (7%)	0	100	100
7	E	184/188 (98%)	171 (93%)	13 (7%)	0	100	100
8	F	229/255 (90%)	219 (96%)	10 (4%)	0	100	100
10	H	197/215 (92%)	186 (94%)	11 (6%)	0	100	100
11	I	196/198 (99%)	189 (96%)	7 (4%)	0	100	100
12	J	136/141 (96%)	132 (97%)	4 (3%)	0	100	100
13	K	146/149 (98%)	135 (92%)	8 (6%)	3 (2%)	11	62
14	L	201/204 (98%)	193 (96%)	7 (4%)	1 (0%)	38	87
15	M	298/301 (99%)	285 (96%)	12 (4%)	1 (0%)	50	92
16	N	178/181 (98%)	168 (94%)	10 (6%)	0	100	100
17	O	151/185 (82%)	143 (95%)	8 (5%)	0	100	100
18	P	154/157 (98%)	147 (96%)	7 (4%)	0	100	100
19	Q	155/183 (85%)	147 (95%)	8 (5%)	0	100	100
20	R	119/150 (79%)	114 (96%)	5 (4%)	0	100	100
21	S	124/135 (92%)	118 (95%)	6 (5%)	0	100	100
22	T	59/158 (37%)	57 (97%)	2 (3%)	0	100	100
23	U	121/124 (98%)	112 (93%)	9 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	V	232/239 (97%)	216 (93%)	15 (6%)	1 (0%)	43	90
25	W	108/111 (97%)	102 (94%)	6 (6%)	0	100	100
26	X	123/134 (92%)	117 (95%)	6 (5%)	0	100	100
27	Y	100/103 (97%)	90 (90%)	10 (10%)	0	100	100
All	All	4424/4748 (93%)	4190 (95%)	228 (5%)	6 (0%)	59	96

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	K	24	LYS
13	K	15	VAL
13	K	46	LEU
14	L	187	SER
24	V	228	GLU

### 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	
3	A	196/198 (99%)	165 (84%)	31 (16%)	4	23
4	B	330/334 (99%)	306 (93%)	24 (7%)	20	66
5	C	325/326 (100%)	300 (92%)	25 (8%)	18	64
6	D	146/149 (98%)	136 (93%)	10 (7%)	22	70
7	E	163/165 (99%)	157 (96%)	6 (4%)	45	86
8	F	201/222 (90%)	194 (96%)	7 (4%)	48	88
10	H	169/180 (94%)	153 (90%)	16 (10%)	12	51
11	I	166/166 (100%)	150 (90%)	16 (10%)	12	51
12	J	107/108 (99%)	99 (92%)	8 (8%)	19	65
13	K	120/121 (99%)	110 (92%)	10 (8%)	16	59
14	L	174/175 (99%)	166 (95%)	8 (5%)	37	82
15	M	253/254 (100%)	240 (95%)	13 (5%)	33	80
16	N	159/160 (99%)	146 (92%)	13 (8%)	17	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	O	127/159 (80%)	117 (92%)	10 (8%)	18	62
18	P	134/135 (99%)	125 (93%)	9 (7%)	23	70
19	Q	128/148 (86%)	115 (90%)	13 (10%)	11	47
20	R	108/132 (82%)	103 (95%)	5 (5%)	37	82
21	S	113/120 (94%)	104 (92%)	9 (8%)	17	62
22	T	52/130 (40%)	46 (88%)	6 (12%)	8	39
23	U	105/106 (99%)	96 (91%)	9 (9%)	15	58
24	V	197/202 (98%)	187 (95%)	10 (5%)	33	80
25	W	100/101 (99%)	96 (96%)	4 (4%)	42	85
26	X	104/111 (94%)	88 (85%)	16 (15%)	4	24
27	Y	79/80 (99%)	73 (92%)	6 (8%)	19	65
All	All	3756/3982 (94%)	3472 (92%)	284 (8%)	19	65

5 of 284 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	I	116	LYS
14	L	154	SER
26	X	32	SER
11	I	152	ILE
13	K	17	HIS

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	2	154/154 (100%)	60 (38%)	13 (8%)
2	3	119/120 (99%)	38 (31%)	1 (0%)
All	All	273/274 (99%)	98 (35%)	14 (5%)

5 of 98 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	G
1	2	3	A

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Mol	Chain	Res	Type
1	2	4	A
1	2	5	A
1	2	6	A

5 of 14 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	88	G
1	2	91	U
1	2	112	G
1	2	43	A
1	2	111	A

## 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 177 ligands modelled in this entry, 177 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	2	154/154 (100%)	-0.03	2 (1%) 74 41	98, 146, 182, 210	0
2	3	120/120 (100%)	0.29	4 (3%) 44 21	95, 138, 175, 235	0
3	A	257/264 (97%)	-0.03	2 (0%) 83 53	60, 106, 157, 242	0
4	B	386/391 (98%)	-0.07	0 100 100	51, 82, 132, 217	0
5	C	409/410 (99%)	-0.01	3 (0%) 84 56	77, 143, 195, 252	0
6	D	169/172 (98%)	0.12	4 (2%) 56 27	96, 139, 182, 216	0
7	E	186/188 (98%)	-0.18	0 100 100	53, 91, 135, 220	0
8	F	231/255 (90%)	-0.06	1 (0%) 90 71	112, 166, 210, 233	0
9	G	0/123	-	-	-	-
10	H	201/215 (93%)	-0.03	1 (0%) 88 65	71, 118, 171, 203	0
11	I	198/198 (100%)	-0.17	0 100 100	53, 91, 151, 195	0
12	J	138/141 (97%)	-0.02	0 100 100	30, 60, 98, 186	0
13	K	148/149 (99%)	-0.08	1 (0%) 84 56	78, 129, 181, 208	0
14	L	203/204 (99%)	-0.10	1 (0%) 88 65	89, 133, 165, 205	0
15	M	300/301 (99%)	0.20	6 (2%) 62 31	98, 157, 204, 233	0
16	N	180/181 (99%)	0.04	5 (2%) 50 24	94, 139, 188, 248	0
17	O	153/185 (82%)	-0.21	2 (1%) 74 41	67, 109, 153, 262	0
18	P	156/157 (99%)	-0.02	1 (0%) 86 60	69, 122, 163, 222	0
19	Q	157/183 (85%)	0.00	0 100 100	60, 106, 157, 200	0
20	R	121/150 (80%)	0.12	4 (3%) 44 21	97, 138, 175, 191	0
21	S	126/135 (93%)	0.02	3 (2%) 56 27	101, 143, 186, 218	0
22	T	61/158 (38%)	-0.16	0 100 100	42, 76, 115, 138	0
23	U	123/124 (99%)	-0.06	3 (2%) 56 27	113, 157, 193, 233	0
24	V	234/239 (97%)	0.02	1 (0%) 90 71	75, 121, 173, 239	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	110/111 (99%)	-0.06	2 (1%) 65 34	63, 102, 183, 216	0
26	X	125/134 (93%)	-0.04	2 (1%) 68 36	73, 117, 162, 215	0
27	Y	102/103 (99%)	-0.36	0 100 100	53, 102, 189, 222	0
All	All	4748/5145 (92%)	-0.02	48 (1%) 79 48	30, 125, 186, 262	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	O	154	LYS	8.9
6	D	4	LYS	5.6
17	O	153	ASP	5.1
1	2	101	U	4.8
21	S	4	HIS	3.8

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

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

## 6.3 Carbohydrates ⓘ

There are no 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
28	MG	0	197	1/1	0.51	23.36	174,174,174,174	0
28	MG	0	347	1/1	0.28	12.71	171,171,171,171	0
28	MG	0	325	1/1	0.57	11.36	143,143,143,143	0
28	MG	0	228	1/1	0.23	7.00	114,114,114,114	0
28	MG	0	200	1/1	0.25	2.89	137,137,137,137	0
28	MG	0	70	1/1	0.18	0.45	181,181,181,181	0
28	MG	0	135	1/1	0.19	0.39	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
28	MG	0	204	1/1	0.15	0.31	86,86,86,86	0
28	MG	0	1	1/1	0.16	0.08	141,141,141,141	0
28	MG	0	345	1/1	0.21	-0.25	146,146,146,146	0
28	MG	0	100	1/1	0.20	-0.38	119,119,119,119	0
28	MG	0	145	1/1	0.21	-0.55	141,141,141,141	0
28	MG	0	8	1/1	0.19	-0.97	146,146,146,146	0
28	MG	0	63	1/1	0.11	-1.10	122,122,122,122	0
29	ZN	Y	104	1/1	0.06	-1.17	116,116,116,116	0
28	MG	0	314	1/1	0.18	-1.51	114,114,114,114	0
28	MG	0	359	1/1	0.09	-2.42	114,114,114,114	0
28	MG	0	74	1/1	0.09	-2.61	62,62,62,62	0
28	MG	0	66	1/1	0.12	-2.61	112,112,112,112	0
28	MG	0	117	1/1	0.15	-5.00	136,136,136,136	0
28	MG	0	373	1/1	0.08	-5.43	113,113,113,113	0
28	MG	0	140	1/1	0.09	-5.72	142,142,142,142	0
28	MG	0	183	1/1	0.14	-5.75	134,134,134,134	0
28	MG	0	277	1/1	0.07	-5.97	69,69,69,69	0
28	MG	0	174	1/1	0.05	-7.34	102,102,102,102	0
28	MG	0	94	1/1	0.24	-147.00	96,96,96,96	0
28	MG	0	317	1/1	0.16	-	212,212,212,212	0
28	MG	0	366	1/1	0.23	-	124,124,124,124	0
28	MG	0	244	1/1	0.18	-	104,104,104,104	0
28	MG	0	35	1/1	0.27	-	173,173,173,173	0
28	MG	0	300	1/1	0.26	-	121,121,121,121	0
28	MG	0	342	1/1	0.38	-	221,221,221,221	0
28	MG	0	242	1/1	0.32	-	166,166,166,166	0
28	MG	0	287	1/1	0.16	-	80,80,80,80	0
28	MG	0	233	1/1	0.17	-	81,81,81,81	0
28	MG	0	356	1/1	0.28	-	154,154,154,154	0
28	MG	0	202	1/1	0.41	-	121,121,121,121	0
28	MG	0	263	1/1	0.17	-	79,79,79,79	0
28	MG	0	371	1/1	0.55	-	131,131,131,131	0
28	MG	0	172	1/1	0.07	-	97,97,97,97	0
28	MG	0	12	1/1	0.25	-	111,111,111,111	0
28	MG	0	309	1/1	0.69	-	151,151,151,151	0
28	MG	0	272	1/1	0.10	-	82,82,82,82	0
28	MG	0	271	1/1	0.23	-	75,75,75,75	0
28	MG	0	60	1/1	0.12	-	114,114,114,114	0
28	MG	0	132	1/1	0.20	-	120,120,120,120	0
28	MG	0	285	1/1	0.07	-	64,64,64,64	0
28	MG	0	129	1/1	0.26	-	146,146,146,146	0
28	MG	0	376	1/1	0.16	-	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
28	MG	0	335	1/1	0.12	-	119,119,119,119	0
28	MG	0	362	1/1	0.12	-	156,156,156,156	0
28	MG	0	331	1/1	0.46	-	99,99,99,99	0
28	MG	0	14	1/1	0.16	-	132,132,132,132	0
28	MG	0	101	1/1	0.15	-	87,87,87,87	0
28	MG	0	141	1/1	0.23	-	157,157,157,157	0
28	MG	0	330	1/1	0.10	-	94,94,94,94	0
28	MG	0	11	1/1	0.09	-	118,118,118,118	0
28	MG	0	337	1/1	0.16	-	154,154,154,154	0
28	MG	0	320	1/1	0.12	-	107,107,107,107	0
28	MG	0	303	1/1	0.13	-	87,87,87,87	0
28	MG	0	217	1/1	0.12	-	123,123,123,123	0
28	MG	0	224	1/1	0.07	-	70,70,70,70	0
28	MG	0	166	1/1	0.34	-	147,147,147,147	0
28	MG	0	338	1/1	0.21	-	157,157,157,157	0
28	MG	0	99	1/1	0.16	-	77,77,77,77	0
28	MG	0	259	1/1	0.17	-	111,111,111,111	0
28	MG	0	239	1/1	0.08	-	162,162,162,162	0
28	MG	0	279	1/1	0.09	-	95,95,95,95	0
28	MG	0	96	1/1	0.06	-	108,108,108,108	0
28	MG	0	108	1/1	0.22	-	94,94,94,94	0
28	MG	0	374	1/1	0.44	-	146,146,146,146	0
28	MG	0	264	1/1	0.09	-	56,56,56,56	0
28	MG	0	316	1/1	0.37	-	123,123,123,123	0
28	MG	0	54	1/1	0.16	-	133,133,133,133	0
28	MG	0	241	1/1	0.05	-	108,108,108,108	0
28	MG	0	255	1/1	0.18	-	206,206,206,206	0
28	MG	0	227	1/1	0.12	-	103,103,103,103	0
28	MG	0	256	1/1	0.09	-	122,122,122,122	0
28	MG	0	308	1/1	0.66	-	110,110,110,110	0
28	MG	0	143	1/1	0.10	-	68,68,68,68	0
28	MG	0	193	1/1	0.17	-	107,107,107,107	0
28	MG	0	192	1/1	0.09	-	109,109,109,109	0
28	MG	0	273	1/1	0.06	-	110,110,110,110	0
28	MG	0	229	1/1	0.25	-	132,132,132,132	0
28	MG	0	247	1/1	0.07	-	105,105,105,105	0
28	MG	0	37	1/1	0.27	-	117,117,117,117	0
28	MG	0	350	1/1	0.48	-	174,174,174,174	0
28	MG	0	80	1/1	0.10	-	151,151,151,151	0
28	MG	0	270	1/1	0.12	-	60,60,60,60	0
28	MG	0	329	1/1	0.11	-	157,157,157,157	0
28	MG	0	162	1/1	0.05	-	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
28	MG	0	361	1/1	0.24	-	146,146,146,146	0
28	MG	0	153	1/1	0.12	-	78,78,78,78	0
28	MG	0	50	1/1	0.35	-	169,169,169,169	0
28	MG	0	363	1/1	0.18	-	120,120,120,120	0
28	MG	0	195	1/1	0.07	-	95,95,95,95	0
28	MG	0	321	1/1	0.29	-	167,167,167,167	0
28	MG	0	191	1/1	0.22	-	143,143,143,143	0
28	MG	0	112	1/1	0.20	-	132,132,132,132	0
28	MG	0	364	1/1	0.14	-	175,175,175,175	0
28	MG	0	268	1/1	0.30	-	141,141,141,141	0
28	MG	0	351	1/1	0.36	-	140,140,140,140	0
28	MG	0	64	1/1	0.11	-	141,141,141,141	0
28	MG	0	190	1/1	0.04	-	108,108,108,108	0
28	MG	0	328	1/1	0.43	-	139,139,139,139	0
28	MG	0	160	1/1	0.09	-	66,66,66,66	0
28	MG	0	92	1/1	0.37	-	98,98,98,98	0
28	MG	0	148	1/1	0.29	-	110,110,110,110	0
28	MG	0	226	1/1	0.04	-	52,52,52,52	0
28	MG	0	276	1/1	0.17	-	91,91,91,91	0
28	MG	0	150	1/1	0.17	-	98,98,98,98	0
28	MG	0	251	1/1	0.12	-	122,122,122,122	0
28	MG	0	137	1/1	0.15	-	102,102,102,102	0
28	MG	0	348	1/1	0.19	-	168,168,168,168	0
28	MG	0	340	1/1	0.31	-	162,162,162,162	0
28	MG	0	144	1/1	0.15	-	120,120,120,120	0
28	MG	0	211	1/1	0.32	-	124,124,124,124	0
28	MG	0	336	1/1	0.17	-	214,214,214,214	0
28	MG	0	307	1/1	0.15	-	79,79,79,79	0
28	MG	0	261	1/1	0.15	-	96,96,96,96	0
28	MG	0	354	1/1	0.07	-	128,128,128,128	0
28	MG	0	184	1/1	0.11	-	131,131,131,131	0
28	MG	0	25	1/1	0.25	-	193,193,193,193	0
28	MG	0	304	1/1	0.04	-	66,66,66,66	0
28	MG	0	163	1/1	0.06	-	113,113,113,113	0
28	MG	0	21	1/1	0.17	-	111,111,111,111	0
28	MG	0	267	1/1	0.10	-	65,65,65,65	0
28	MG	0	305	1/1	0.06	-	73,73,73,73	0
28	MG	0	102	1/1	0.24	-	82,82,82,82	0
28	MG	0	278	1/1	0.27	-	111,111,111,111	0
28	MG	0	152	1/1	0.06	-	156,156,156,156	0
28	MG	0	119	1/1	0.21	-	93,93,93,93	0
28	MG	0	34	1/1	0.32	-	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
28	MG	0	19	1/1	0.17	-	105,105,105,105	0
28	MG	0	130	1/1	0.24	-	93,93,93,93	0
28	MG	0	16	1/1	0.15	-	101,101,101,101	0
28	MG	0	139	1/1	0.09	-	79,79,79,79	0
28	MG	0	133	1/1	0.23	-	75,75,75,75	0
28	MG	0	97	1/1	0.20	-	105,105,105,105	0
28	MG	0	165	1/1	0.48	-	145,145,145,145	0
28	MG	0	142	1/1	0.11	-	65,65,65,65	0
28	MG	0	358	1/1	0.21	-	183,183,183,183	0
28	MG	0	56	1/1	0.39	-	113,113,113,113	0
28	MG	0	349	1/1	0.30	-	152,152,152,152	0
28	MG	0	181	1/1	0.09	-	69,69,69,69	0
28	MG	0	298	1/1	0.24	-	140,140,140,140	0
28	MG	0	306	1/1	0.45	-	129,129,129,129	0
28	MG	0	369	1/1	0.24	-	202,202,202,202	0
28	MG	0	274	1/1	0.05	-	82,82,82,82	0
28	MG	0	78	1/1	0.22	-	97,97,97,97	0
28	MG	0	252	1/1	0.13	-	108,108,108,108	0
28	MG	0	215	1/1	0.07	-	104,104,104,104	0
28	MG	0	346	1/1	0.13	-	150,150,150,150	0
28	MG	0	151	1/1	0.29	-	118,118,118,118	0
28	MG	0	154	1/1	0.07	-	108,108,108,108	0
28	MG	0	77	1/1	0.23	-	113,113,113,113	0
28	MG	0	222	1/1	0.28	-	123,123,123,123	0
28	MG	0	171	1/1	0.14	-	90,90,90,90	0
28	MG	0	269	1/1	0.18	-	50,50,50,50	0
28	MG	0	120	1/1	0.09	-	116,116,116,116	0
28	MG	0	208	1/1	0.18	-	140,140,140,140	0
28	MG	0	291	1/1	0.30	-	143,143,143,143	0
28	MG	0	98	1/1	0.13	-	83,83,83,83	0
28	MG	0	375	1/1	0.20	-	128,128,128,128	0
28	MG	0	110	1/1	0.06	-	91,91,91,91	0
28	MG	0	368	1/1	0.17	-	152,152,152,152	0
28	MG	0	186	1/1	0.15	-	78,78,78,78	0
28	MG	0	294	1/1	0.09	-	120,120,120,120	0
28	MG	0	357	1/1	0.18	-	137,137,137,137	0
28	MG	0	206	1/1	0.17	-	119,119,119,119	0
28	MG	0	18	1/1	0.08	-	143,143,143,143	0
28	MG	0	280	1/1	0.11	-	75,75,75,75	0
28	MG	0	341	1/1	0.20	-	153,153,153,153	0
28	MG	0	355	1/1	0.17	-	136,136,136,136	0
28	MG	0	33	1/1	0.45	-	192,192,192,192	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
28	MG	0	236	1/1	0.17	-	134,134,134,134	0
28	MG	0	365	1/1	0.33	-	188,188,188,188	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.