



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 02:55 AM GMT

PDB ID : 3UXT  
Title : The structure of thermorubin in complex with the 70S ribosome from *Thermus thermophilus*. This file contains the 30S subunit of one 70S ribosome. The entire crystal structure contains two 70S ribosomes.<sup>†</sup>  
Authors : Bulkley, D.; Johnson, F.A.; Steitz, T.A.  
Deposited on : 2011-12-05  
Resolution : 3.20 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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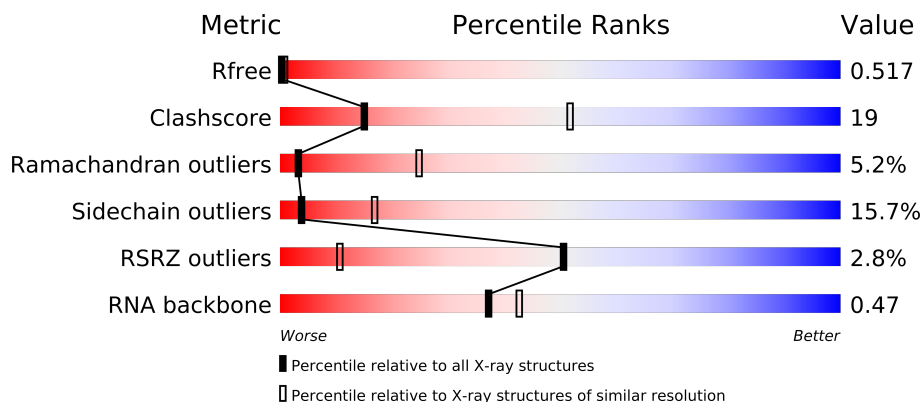
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.20 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.









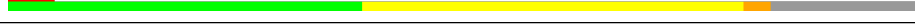


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)
RNA backbone	1838	1002 (3.72-2.68)

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	1521	
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	132	

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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 21 unique types of molecules in this entry. The entry contains 49743 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1498	Total	C	N	O	P	0	0	0
			32208	14334	5974	10402	1498			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	U	DELETION	GB AP008226.1

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	229	Total	C	N	O	S	0	0	0
			1777	1134	318	320	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
			1450	906	279	264	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
			1520	960	283	272	5			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	148	Total	C	N	O	S	0	0	0
			1105	699	204	198	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	100	Total	C	N	O	S	0	0	0
			781	495	137	146	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
			1167	727	224	210	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
			1045	665	188	190	2			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	125	Total	C	N	O	0	0	0
			852	533	163	156			

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 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	96	Total	C	N	O	0	0	0
			659	408	131	120			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	75	LEU	ILE	CONFLICT	UNP Q5SHN7

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	114	Total	C	N	O	S	0	0	0
			828	516	155	154	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	122	Total	C	N	O	S	0	0	0
			909	570	179	159	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	114	Total	C	N	O	S	0	0	0
			801	494	164	142	1			

- 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
			478	303	99	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
			724	453	143	126	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	82	Total	C	N	O	S	0	0	0
			651	416	123	111	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	68	Total	C	N	O	0	0	0
			514	329	98	87			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	78	Total	C	N	O	S	0	0	0
			544	342	105	95	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	96	Total	C	N	O	S	0	0	0
			708	435	151	120	2			

- Molecule 21 is a protein called 30S ribosomal protein THX.

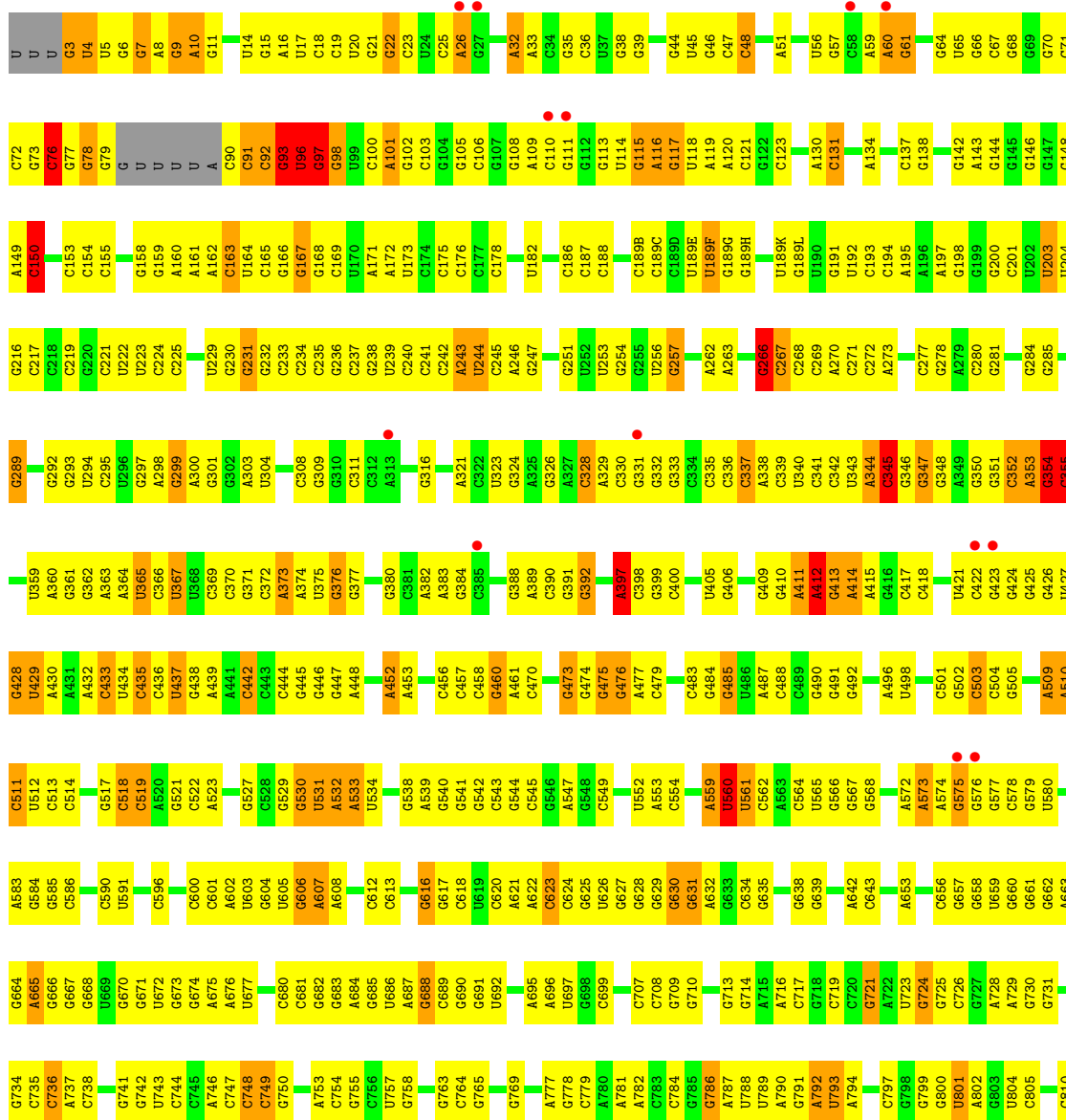
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	23	Total	C	N	O	0	0	0
			199	122	48	29			

### 3 Residue-property plots

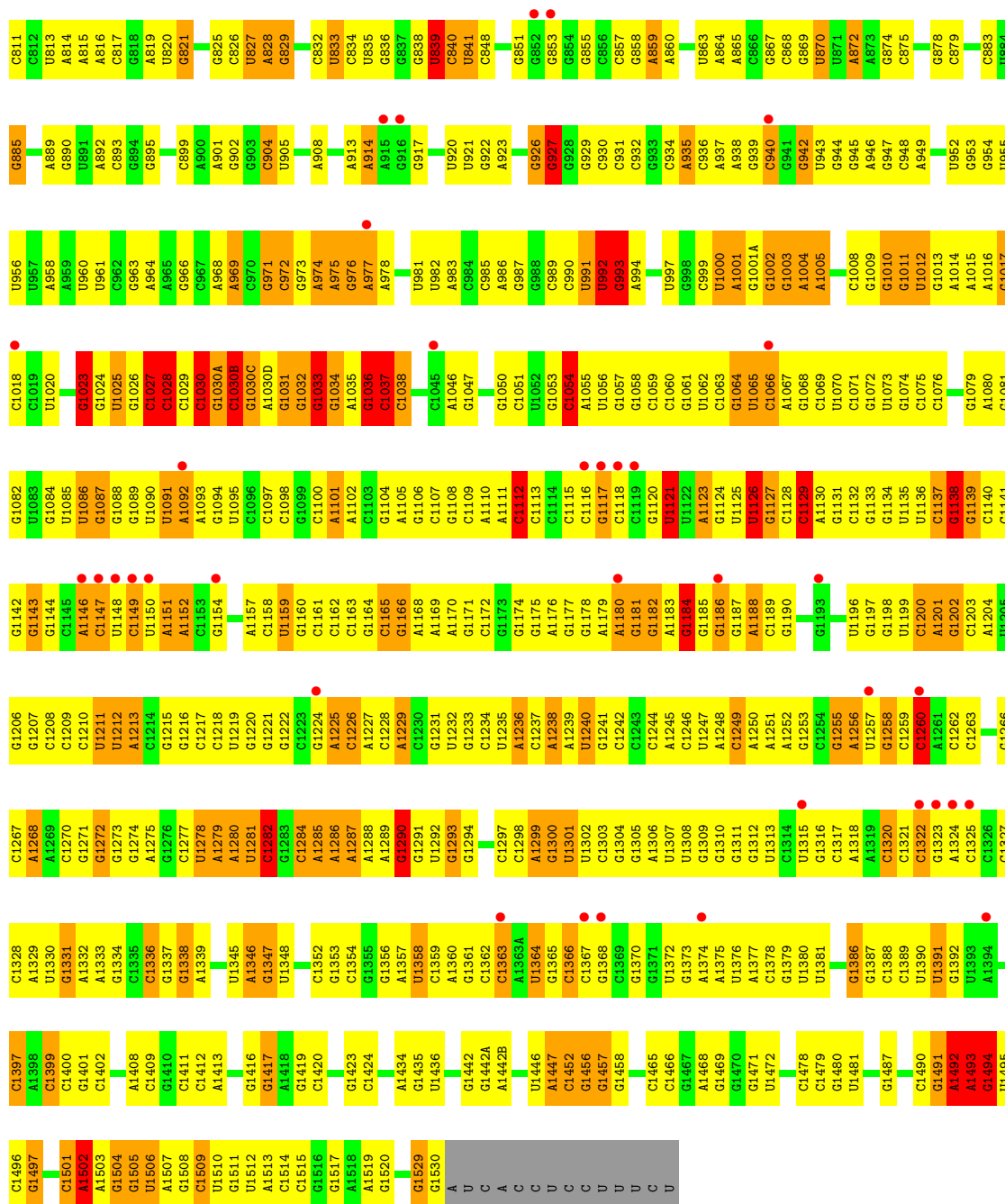
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: 16S ribosomal RNA

Chain A: 



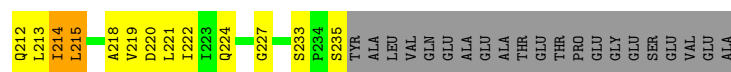




## • Molecule 2: 30S ribosomal protein S2

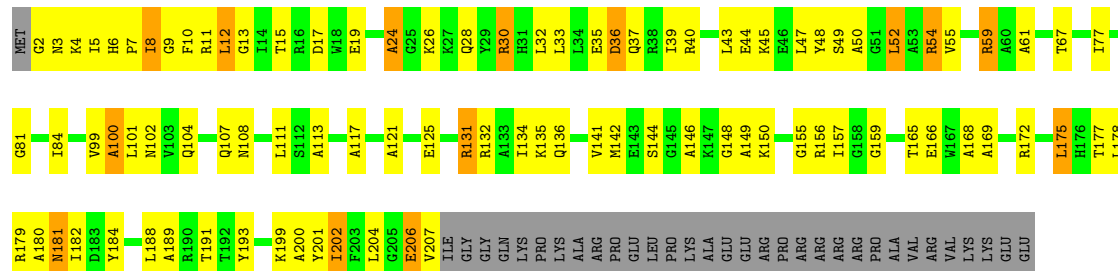
Chain B:





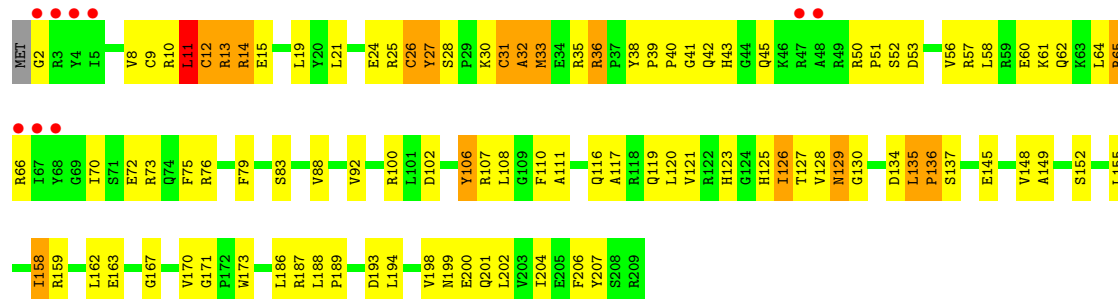
• Molecule 3: 30S ribosomal protein S3

Chain C:



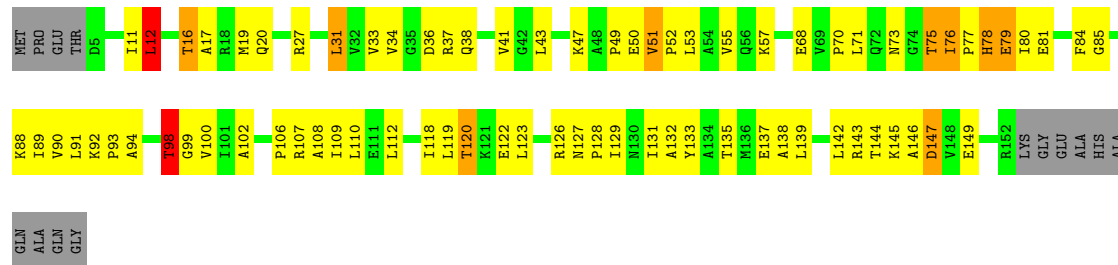
• Molecule 4: 30S ribosomal protein S4

Chain D:



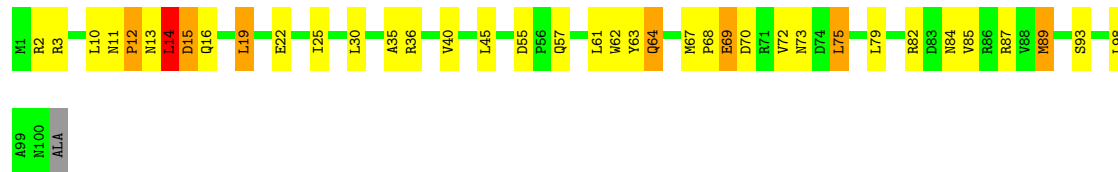
• Molecule 5: 30S ribosomal protein S5

Chain E:



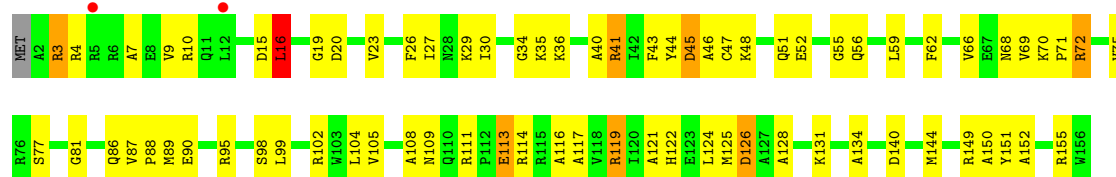
• Molecule 6: 30S ribosomal protein S6

Chain F:



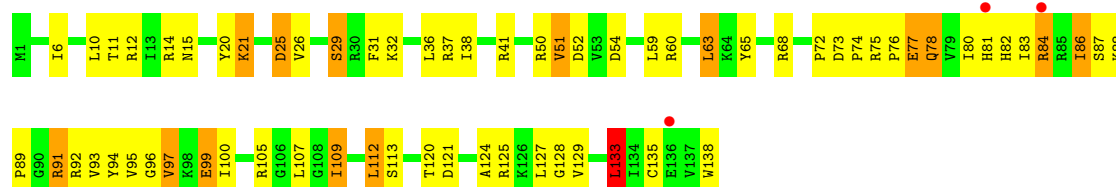
• Molecule 7: 30S ribosomal protein S7

Chain G:



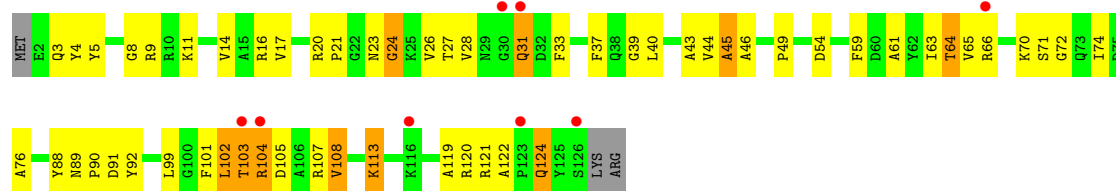
- Molecule 8: 30S ribosomal protein S8

Chain H:



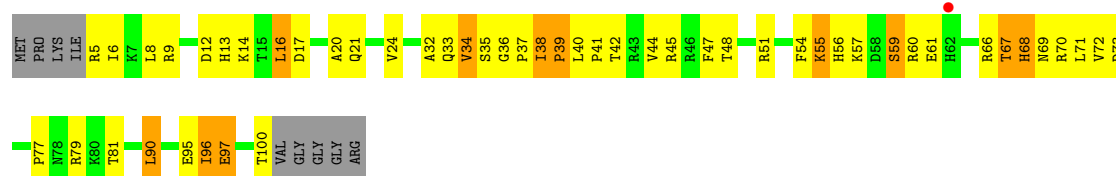
- Molecule 9: 30S ribosomal protein S9

Chain I:



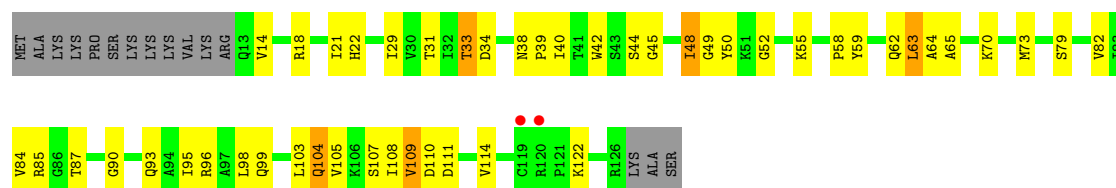
- Molecule 10: 30S ribosomal protein S10

Chain J:



- Molecule 11: 30S ribosomal protein S11

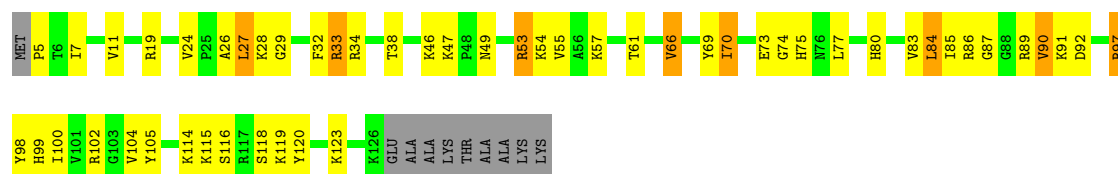
Chain K:



- Molecule 12: 30S ribosomal protein S12

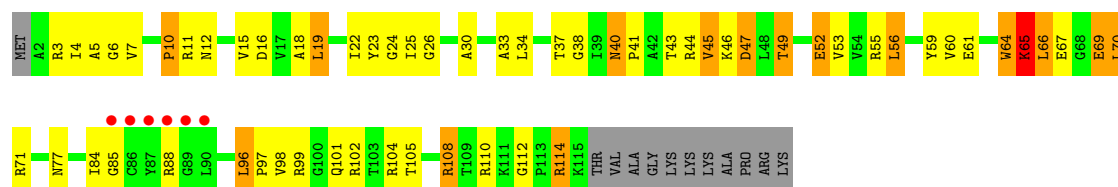
Chain L:





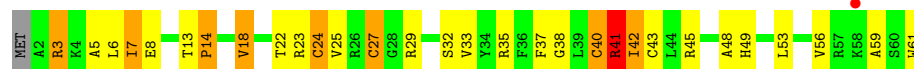
- Molecule 13: 30S ribosomal protein S13

Chain M:



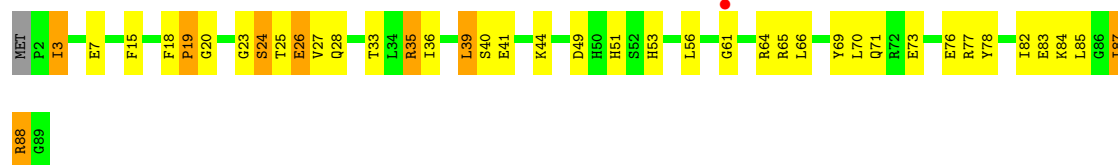
- Molecule 14: 30S ribosomal protein S14

Chain N:



- Molecule 15: 30S ribosomal protein S15

Chain O:



- Molecule 16: 30S ribosomal protein S16

Chain P:



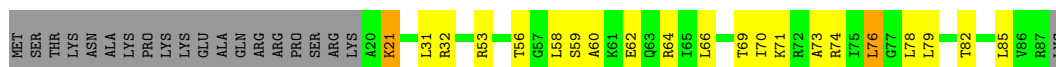
- Molecule 17: 30S ribosomal protein S17

Chain Q:



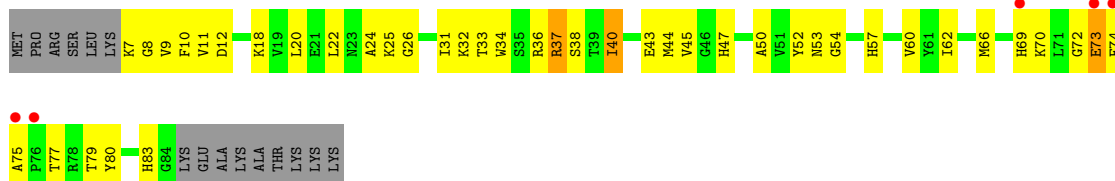
- Molecule 18: 30S ribosomal protein S18

Chain R:



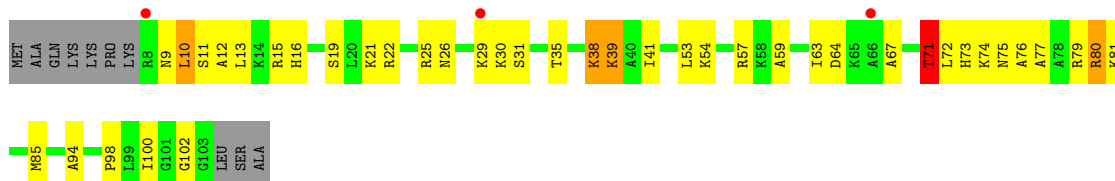
- Molecule 19: 30S ribosomal protein S19

Chain S:



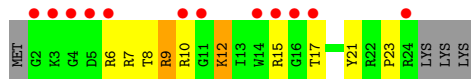
- Molecule 20: 30S ribosomal protein S20

Chain T:



- Molecule 21: 30S ribosomal protein THX

Chain U:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.37Å 445.46Å 619.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 3.20 49.43 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.29-3.20) 99.7 (49.43-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.228 , 0.273 0.515 , 0.517	Depositor DCC
$R_{free}$ test set	63137 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	75.4	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 68.0	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 1261811 reflections	Xtriage
$F_o, F_c$ correlation	0.55	EDS
Total number of atoms	49743	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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

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	0.77	7/36054 (0.0%)	1.19	211/56272 (0.4%)
2	B	0.56	0/1811	0.69	0/2452
3	C	0.58	0/1474	0.65	0/2003
4	D	0.84	2/1550 (0.1%)	0.78	4/2106 (0.2%)
5	E	0.52	0/1121	0.72	1/1517 (0.1%)
6	F	0.49	0/794	0.67	1/1082 (0.1%)
7	G	0.56	0/1186	0.62	0/1603
8	H	0.44	0/1065	0.64	0/1445
9	I	0.62	0/867	0.69	0/1180
10	J	0.60	0/672	0.70	1/919 (0.1%)
11	K	0.47	0/843	0.67	0/1144
12	L	0.46	0/925	0.69	0/1251
13	M	0.63	0/811	0.73	1/1103 (0.1%)
14	N	0.59	0/487	0.74	0/649
15	O	0.47	0/735	0.61	0/981
16	P	0.43	0/667	0.65	0/905
17	Q	0.47	0/836	0.66	0/1117
18	R	0.50	0/519	0.67	0/699
19	S	0.76	1/558 (0.2%)	0.87	3/759 (0.4%)
20	T	0.42	0/710	0.68	0/940
21	U	0.59	0/203	0.70	0/266
All	All	0.71	10/53888 (0.0%)	1.06	222/80393 (0.3%)

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
4	D	0	1
12	L	0	1
All	All	0	2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	12	CYS	CB-SG	19.94	2.16	1.82
4	D	26	CYS	CB-SG	15.79	2.09	1.82
1	A	1492	A	C6-N6	-12.21	1.24	1.33
1	A	1492	A	C2-N3	10.06	1.42	1.33
1	A	1493	A	N7-C5	8.26	1.44	1.39

The worst 5 of 222 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1492	A	C6-N1-C2	-28.45	101.53	118.60
1	A	1492	A	C5-C6-N1	26.41	130.90	117.70
1	A	1492	A	N3-C4-C5	-14.09	116.94	126.80
1	A	1492	A	C8-N9-C4	-13.58	100.37	105.80
1	A	1492	A	N1-C2-N3	13.04	135.82	129.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	11	LEU	Peptide
12	L	26	ALA	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	A	32208	0	16254	902	0
2	B	1777	0	1747	95	0
3	C	1450	0	1314	58	0
4	D	1520	0	1406	85	0
5	E	1105	0	1130	54	0
6	F	781	0	741	28	0
7	G	1167	0	1108	46	0
8	H	1045	0	1033	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	852	0	742	52	0
10	J	659	0	552	37	0
11	K	828	0	822	32	0
12	L	909	0	927	38	0
13	M	801	0	743	37	0
14	N	478	0	497	30	0
15	O	724	0	749	26	0
16	P	651	0	638	28	0
17	Q	823	0	891	22	0
18	R	514	0	530	17	0
19	S	544	0	457	26	0
20	T	708	0	764	26	0
21	U	199	0	208	6	0
All	All	49743	0	33253	1528	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 19.

The worst 5 of 1528 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:26:CYS:SG	4:D:26:CYS:CB	2.09	1.41
4:D:12:CYS:SG	4:D:12:CYS:CB	2.16	1.34
13:M:65:LYS:HA	13:M:66:LEU:HB2	1.44	0.97
1:A:1028:C:N4	1:A:1033:G:H1	1.62	0.97
1:A:1502:A:H2	1:A:1505:G:H1	1.12	0.96

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	227/256 (89%)	173 (76%)	39 (17%)	15 (7%)	2 16
3	C	204/239 (85%)	144 (71%)	42 (21%)	18 (9%)	1 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	206/209 (99%)	152 (74%)	47 (23%)	7 (3%)	6	38
5	E	146/162 (90%)	116 (80%)	25 (17%)	5 (3%)	6	38
6	F	98/101 (97%)	85 (87%)	9 (9%)	4 (4%)	4	32
7	G	153/156 (98%)	129 (84%)	18 (12%)	6 (4%)	5	33
8	H	136/138 (99%)	118 (87%)	13 (10%)	5 (4%)	5	34
9	I	123/128 (96%)	94 (76%)	21 (17%)	8 (6%)	2	17
10	J	94/105 (90%)	74 (79%)	14 (15%)	6 (6%)	2	17
11	K	112/129 (87%)	90 (80%)	19 (17%)	3 (3%)	8	46
12	L	120/132 (91%)	100 (83%)	15 (12%)	5 (4%)	4	31
13	M	112/126 (89%)	80 (71%)	20 (18%)	12 (11%)	1	5
14	N	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	3	25
15	O	86/89 (97%)	68 (79%)	16 (19%)	2 (2%)	10	52
16	P	80/88 (91%)	52 (65%)	25 (31%)	3 (4%)	5	34
17	Q	97/105 (92%)	81 (84%)	13 (13%)	3 (3%)	7	41
18	R	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
19	S	76/93 (82%)	54 (71%)	17 (22%)	5 (7%)	2	16
20	T	94/106 (89%)	72 (77%)	15 (16%)	7 (7%)	2	12
21	U	21/27 (78%)	16 (76%)	3 (14%)	2 (10%)	1	7
All	All	2309/2538 (91%)	1806 (78%)	384 (17%)	119 (5%)	3	25

5 of 119 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	15	VAL
2	B	24	TRP
2	B	26	PRO
2	B	75	LYS
2	B	120	ALA

### 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	177/220 (80%)	142 (80%)	35 (20%)	2	9
3	C	114/188 (61%)	96 (84%)	18 (16%)	4	16
4	D	139/181 (77%)	120 (86%)	19 (14%)	5	25
5	E	108/123 (88%)	88 (82%)	20 (18%)	2	11
6	F	77/90 (86%)	65 (84%)	12 (16%)	4	17
7	G	104/127 (82%)	88 (85%)	16 (15%)	4	18
8	H	103/119 (87%)	84 (82%)	19 (18%)	2	11
9	I	62/99 (63%)	54 (87%)	8 (13%)	6	28
10	J	52/92 (56%)	41 (79%)	11 (21%)	1	8
11	K	81/99 (82%)	71 (88%)	10 (12%)	7	31
12	L	92/109 (84%)	83 (90%)	9 (10%)	12	43
13	M	63/101 (62%)	49 (78%)	14 (22%)	1	6
14	N	46/50 (92%)	33 (72%)	13 (28%)	0	2
15	O	77/80 (96%)	66 (86%)	11 (14%)	5	22
16	P	63/74 (85%)	53 (84%)	10 (16%)	4	16
17	Q	94/97 (97%)	84 (89%)	10 (11%)	10	38
18	R	49/77 (64%)	46 (94%)	3 (6%)	26	71
19	S	42/80 (52%)	36 (86%)	6 (14%)	5	22
20	T	65/82 (79%)	57 (88%)	8 (12%)	7	31
21	U	18/22 (82%)	14 (78%)	4 (22%)	1	6
All	All	1626/2110 (77%)	1370 (84%)	256 (16%)	4	17

5 of 256 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	102	ARG
9	I	104	ARG
18	R	76	LEU
7	G	126	ASP
8	H	95	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	28	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
9	I	31	GLN
19	S	47	HIS
7	G	109	ASN
8	H	82	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1496/1521 (98%)	341 (22%)	27 (1%)

5 of 341 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	7	G
1	A	8	A
1	A	9	G
1	A	10	A

5 of 27 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	533	A
1	A	748	C
1	A	1300	G
1	A	560	U
1	A	115	G

## 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 ⓘ

There are no ligands in this entry.

## 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	1498/1521 (98%)	0.06	49 (3%) 44 9	65, 99, 120, 128	0
2	B	229/256 (89%)	-0.25	1 (0%) 90 51	95, 105, 112, 115	0
3	C	206/239 (86%)	-0.21	0 100 100	97, 108, 115, 120	0
4	D	208/209 (99%)	-0.04	9 (4%) 34 7	87, 97, 107, 123	0
5	E	148/162 (91%)	-0.28	0 100 100	84, 96, 104, 110	0
6	F	100/101 (99%)	-0.35	0 100 100	84, 93, 103, 110	0
7	G	155/156 (99%)	-0.13	2 (1%) 74 24	97, 109, 115, 119	0
8	H	138/138 (100%)	0.05	3 (2%) 59 14	86, 96, 102, 106	0
9	I	125/128 (97%)	0.15	8 (6%) 19 4	100, 112, 118, 120	0
10	J	96/105 (91%)	-0.16	1 (1%) 79 29	97, 110, 115, 119	0
11	K	114/129 (88%)	-0.09	2 (1%) 65 18	75, 95, 103, 107	0
12	L	122/132 (92%)	-0.16	0 100 100	77, 87, 96, 105	0
13	M	114/126 (90%)	0.08	6 (5%) 25 5	101, 109, 115, 117	0
14	N	60/61 (98%)	0.22	1 (1%) 67 19	103, 111, 116, 122	0
15	O	88/89 (98%)	-0.04	1 (1%) 77 27	81, 93, 103, 107	0
16	P	82/88 (93%)	0.02	3 (3%) 39 8	86, 94, 103, 111	0
17	Q	99/105 (94%)	-0.13	1 (1%) 79 29	79, 92, 100, 103	0
18	R	68/88 (77%)	-0.21	0 100 100	85, 93, 104, 106	0
19	S	78/93 (83%)	0.16	5 (6%) 19 4	91, 112, 117, 119	0
20	T	96/106 (90%)	0.11	3 (3%) 47 10	82, 92, 100, 101	0
21	U	23/27 (85%)	2.27	12 (52%) 0 0	104, 109, 112, 113	0
All	All	3847/4059 (94%)	-0.02	107 (2%) 50 11	65, 101, 117, 128	0

The worst 5 of 107 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1149	C	9.5
1	A	1148	U	7.5
1	A	1363	C	6.0
21	U	2	GLY	6.0
13	M	86	CYS	5.9

## 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 ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.