



wwPDB X-ray Structure Validation Summary Report

Jul 11, 2014 – 11:43 PM EDT

PDB ID : 4L6K
Title : Crystal Structure of Blasticidin S Bound to Thermus Thermophilus 70S Ribosome. This file contains the 30S subunit, tRNA and mRNA molecules from the first 70S ribosome.
Authors : Svidritskiy, E.; Ling, C.; Ermolenko, D.N.; Korostelev, A.A.
Deposited on : 2013-06-12
Resolution : 3.40 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

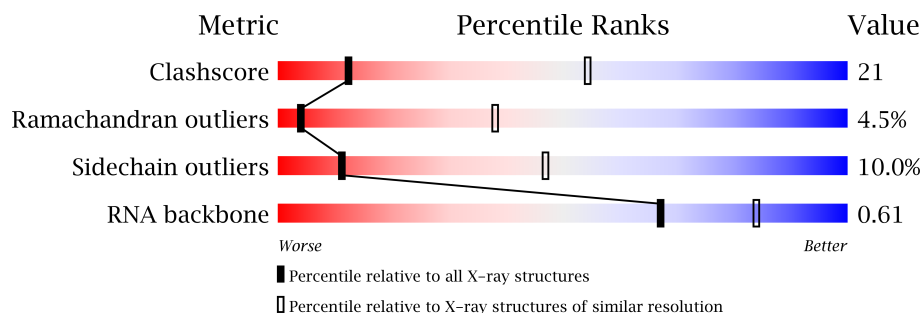
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : **FAILED**
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23161

1 Overall quality at a glance

The reported resolution of this entry is 3.40 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))
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RNA backbone	1838	1002 (4.02-2.76)

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 ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1504	
2	B	234	
3	C	206	
4	D	208	
5	E	151	
6	F	101	
7	G	155	
8	H	138	
9	I	127	
10	J	98	
11	K	114	
12	L	122	
13	M	117	
14	N	60	

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Mol	Chain	Length	Quality of chain
15	O	88	
16	P	83	
17	Q	99	
18	R	70	
19	S	78	
20	T	99	
21	U	24	
22	V	77	
22	W	77	
23	X	5	

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 54782 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	1504	Total	C	N	O	P	0	0	0
			32336	14391	5994	10447	1504			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	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
			1613	1016	314	282	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	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	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
			795	499	156	139	1			

- 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
			843	522	159	159	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
			957	603	193	160	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	117	Total	C	N	O	S	0	0	0
			934	577	192	163	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	118	ALA	-	EXPRESSION TAG	UNP P62655

- 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
			701	443	139	118	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
			824	528	152	142	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	70	Total	C	N	O	0	0	0
			574	367	112	95			

- 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
			630	403	114	111	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			

- 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
			209	128	50	31			

- Molecule 22 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	W	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	X	5	Total	C	N	O	P	0	0	0
			109	49	22	33	5			

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

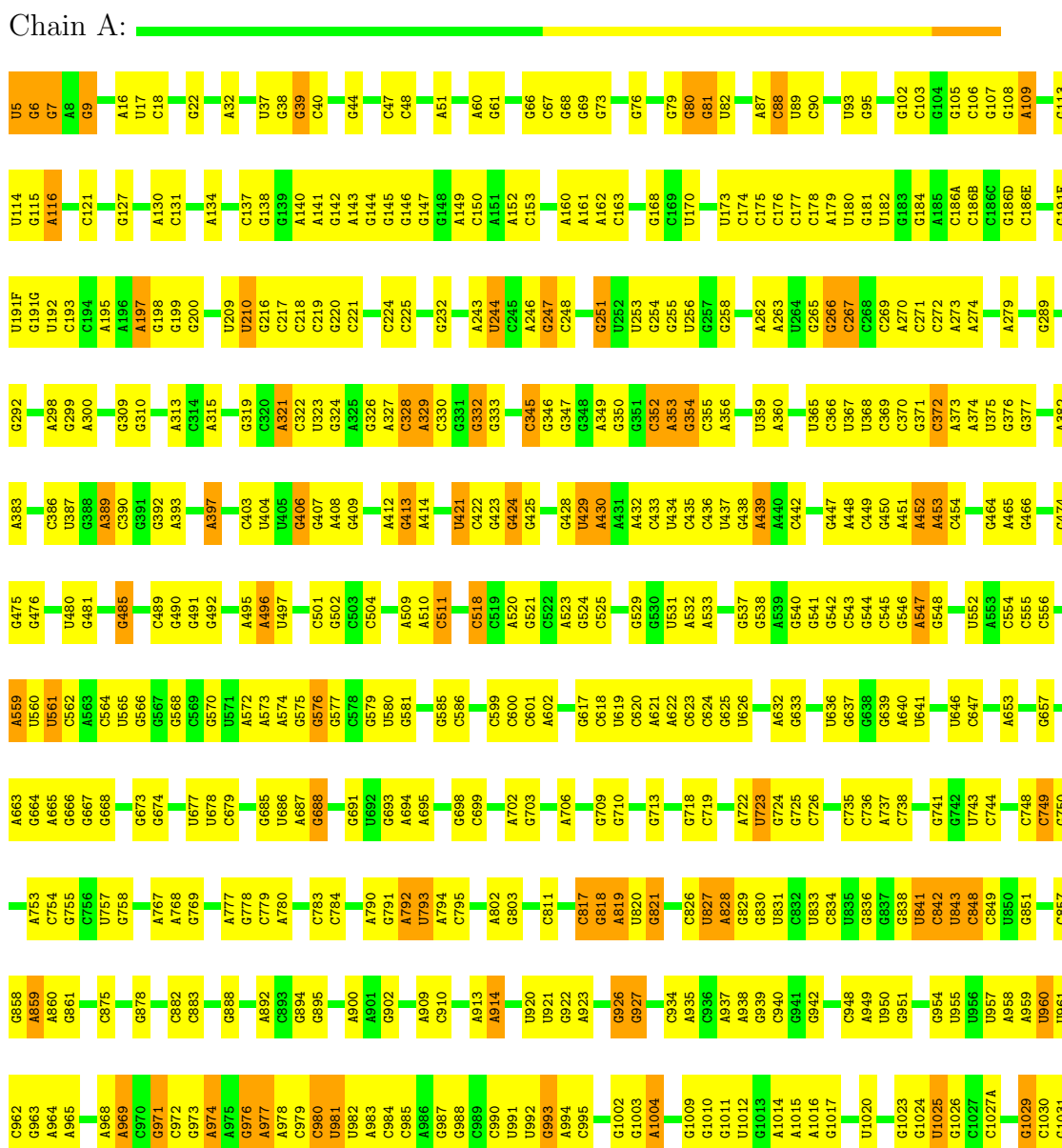
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	D	1	Total	Zn	0	0
			1	1		
24	N	1	Total	Zn	0	0
			1	1		

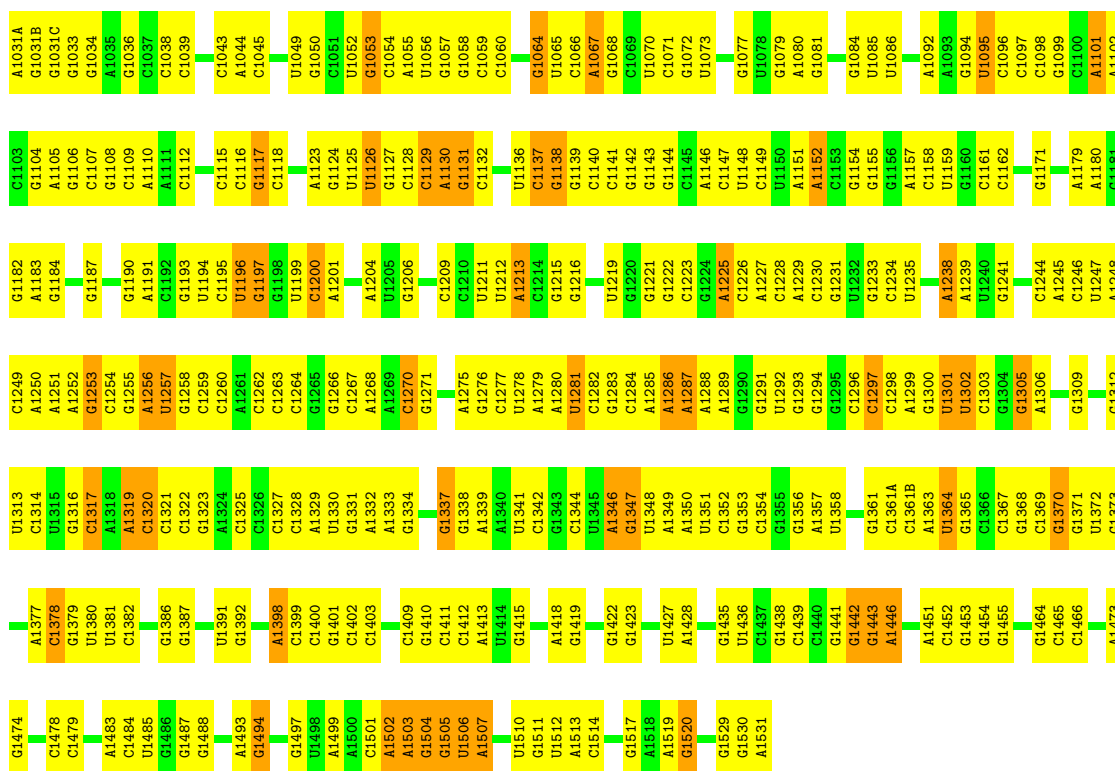
3 Residue-property plots

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 ($RSRZ > 2$). 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.

Note EDS was not executed.

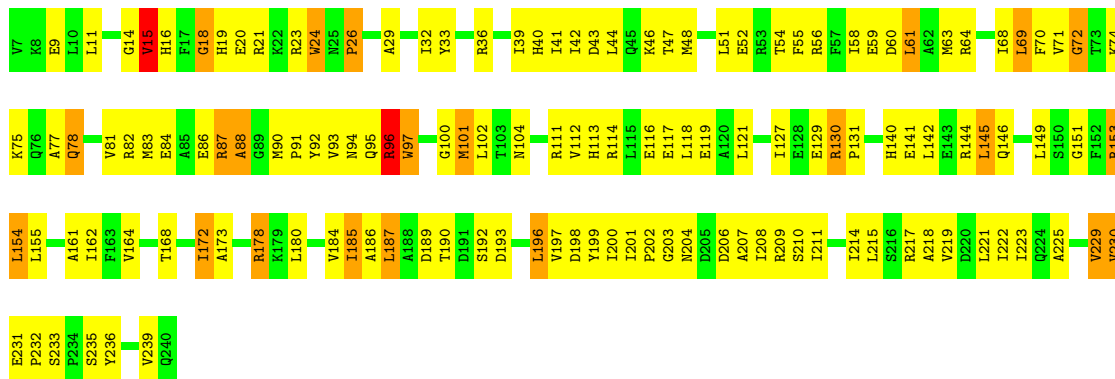
• Molecule 1: 16S ribosomal RNA





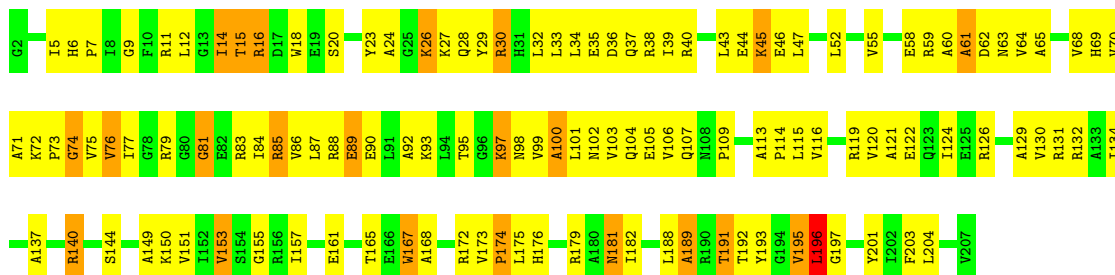
• Molecule 2: 30S ribosomal protein S2

Chain B:



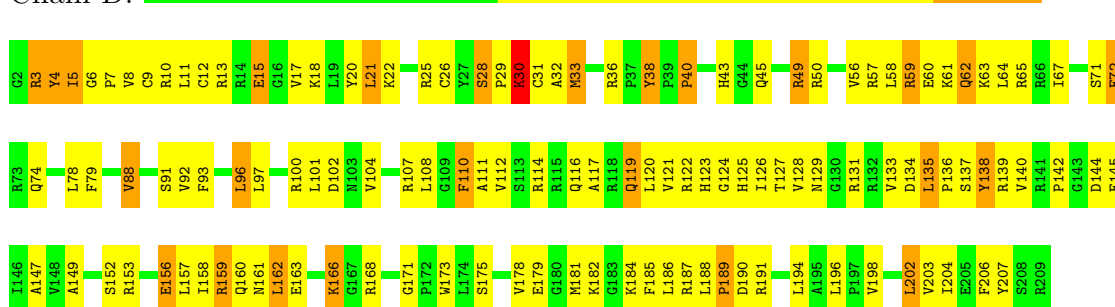
• Molecule 3: 30S ribosomal protein S3

Chain C:



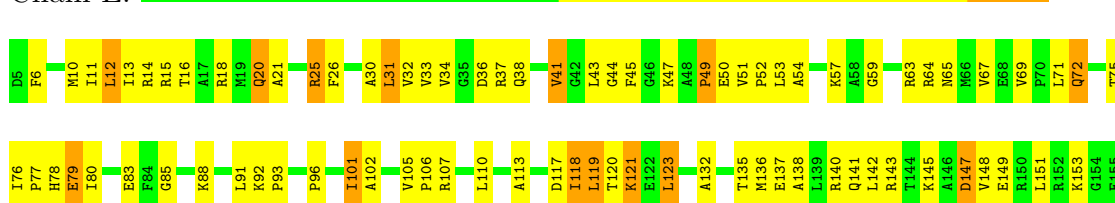
• Molecule 4: 30S ribosomal protein S4

Chain D:



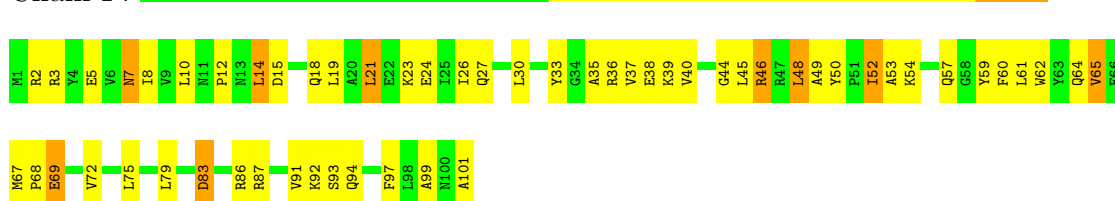
• Molecule 5: 30S ribosomal protein S5

Chain E:



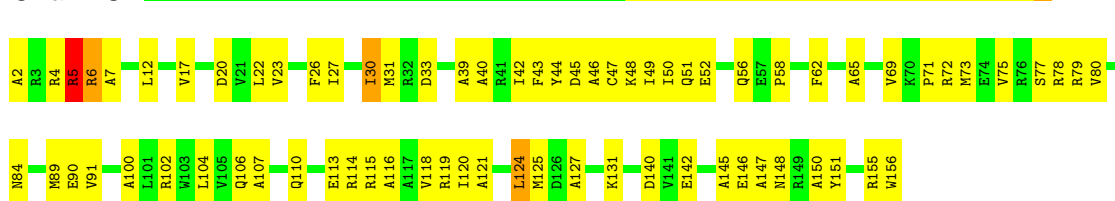
• Molecule 6: 30S ribosomal protein S6

Chain F:



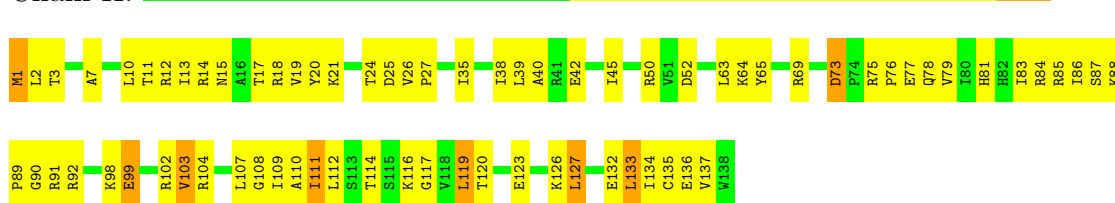
• Molecule 7: 30S ribosomal protein S7

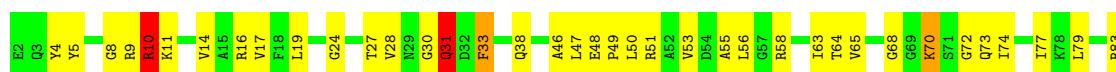
Chain G:



• Molecule 8: 30S ribosomal protein S8

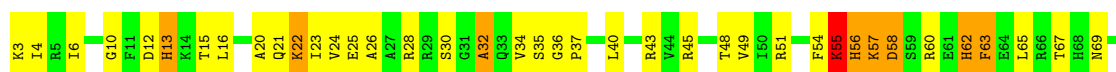
Chain H:





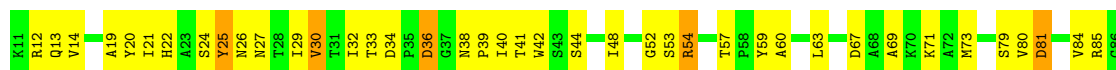
• Molecule 10: 30S ribosomal protein S10

Chain J:



• Molecule 11: 30S ribosomal protein S11

Chain K:



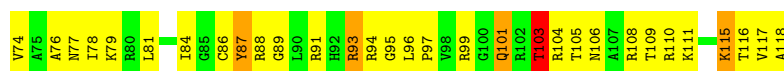
• Molecule 12: 30S ribosomal protein S12

Chain L:



• Molecule 13: 30S ribosomal protein S13

Chain M:



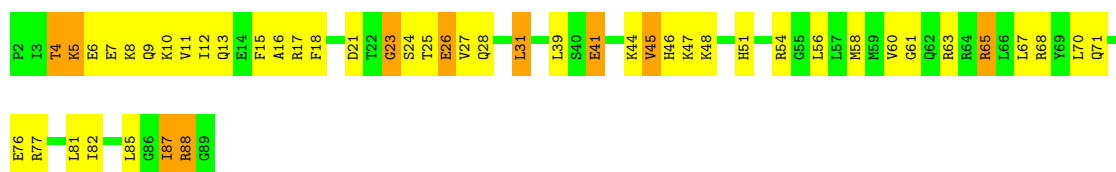
• Molecule 14: 30S ribosomal protein S14

Chain N:



• Molecule 15: 30S ribosomal protein S15

Chain O:



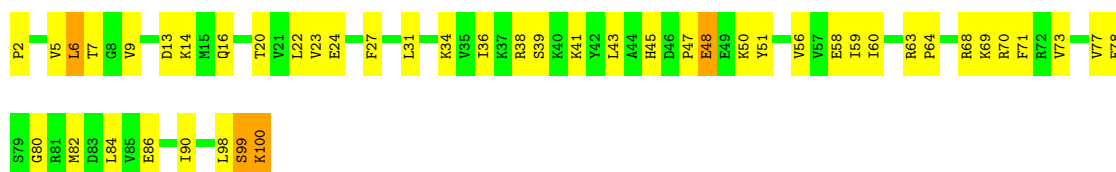
• Molecule 16: 30S ribosomal protein S16

Chain P:



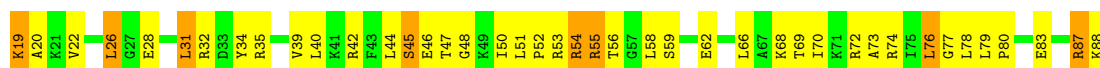
• Molecule 17: 30S ribosomal protein S17

Chain Q:



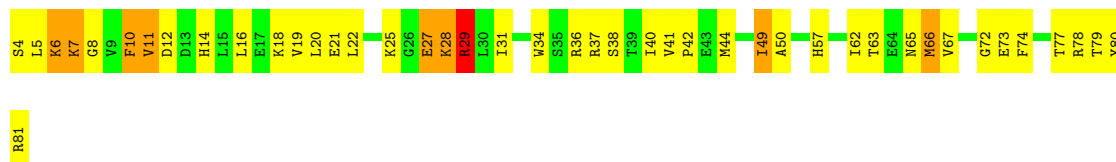
• Molecule 18: 30S ribosomal protein S18

Chain R:



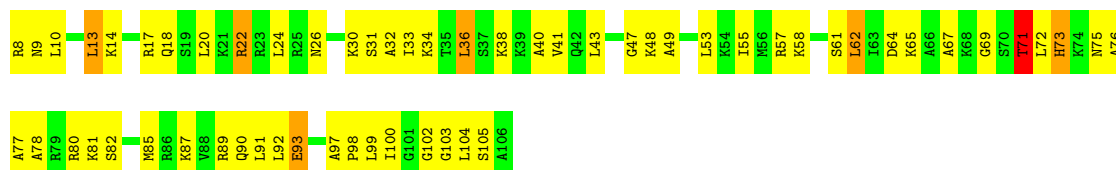
• Molecule 19: 30S ribosomal protein S19

Chain S:



• Molecule 20: 30S ribosomal protein S20

Chain T:



• Molecule 21: 30S ribosomal protein Thx

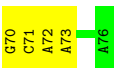
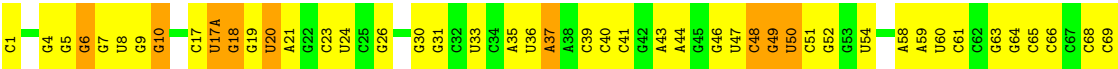
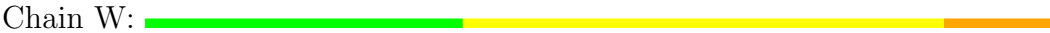
Chain U:



• Molecule 22: tRNA



• Molecule 22: tRNA



• Molecule 23: mRNA



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.53Å 454.44Å 620.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 3.40	Depositor
% Data completeness (in resolution range)	99.8 (49.98-3.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.231 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	54782	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.28	1/36198 (0.0%)	0.55	0/56497
2	B	0.22	0/1936	0.40	0/2609
3	C	0.22	0/1637	0.40	0/2205
4	D	0.27	0/1733	0.45	0/2318
5	E	0.24	0/1172	0.43	0/1576
6	F	0.24	0/856	0.43	0/1154
7	G	0.22	0/1276	0.36	0/1709
8	H	0.23	0/1136	0.44	0/1527
9	I	0.22	0/1029	0.39	0/1378
10	J	0.21	0/808	0.41	0/1085
11	K	0.23	0/857	0.44	0/1157
12	L	0.25	0/973	0.46	0/1301
13	M	0.21	0/944	0.41	0/1265
14	N	0.24	0/501	0.39	0/664
15	O	0.25	0/745	0.40	0/992
16	P	0.26	0/717	0.45	0/963
17	Q	0.25	0/837	0.42	0/1117
18	R	0.24	0/579	0.44	0/768
19	S	0.20	0/643	0.40	0/865
20	T	0.24	0/764	0.42	0/1006
21	U	0.20	0/213	0.37	0/277
22	V	0.21	0/1832	0.48	0/2855
22	W	0.17	0/1832	0.44	0/2855
23	X	0.26	0/122	0.47	0/188
All	All	0.26	1/59340 (0.0%)	0.51	0/88331

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	U	OP3-P	-10.80	1.48	1.61

There are no bond angle outliers.

There are no chirality outliers.

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	32336	0	16317	769	0
2	B	1901	0	1951	125	0
3	C	1613	0	1677	116	0
4	D	1703	0	1764	134	0
5	E	1156	0	1213	73	0
6	F	843	0	857	62	0
7	G	1257	0	1296	52	0
8	H	1116	0	1177	67	0
9	I	1011	0	1043	95	0
10	J	795	0	840	62	0
11	K	843	0	859	54	0
12	L	957	0	1046	68	0
13	M	934	0	992	74	0
14	N	492	0	531	46	0
15	O	734	0	771	44	0
16	P	701	0	720	51	0
17	Q	824	0	893	42	0
18	R	574	0	644	47	0
19	S	630	0	652	57	0
20	T	762	0	859	45	0
21	U	209	0	221	19	0
22	V	1640	0	837	33	0
22	W	1640	0	837	50	0
23	X	109	0	55	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
All	All	54782	0	38052	1965	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 21.

The worst 5 of 1965 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:V:74:C:H5"	22:V:75:C:H5"	1.43	1.01
1:A:979:C:H3'	1:A:980:C:H5"	1.40	0.99
1:A:545:C:H5'	4:D:72:GLU:HG3	1.42	0.98
3:C:33:LEU:HD21	14:N:53:LEU:HD22	1.46	0.97
9:I:28:VAL:HG22	9:I:63:ILE:HB	1.42	0.97

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	232/234 (99%)	183 (79%)	36 (16%)	13 (6%)	3	30
3	C	204/206 (99%)	159 (78%)	28 (14%)	17 (8%)	1	18
4	D	206/208 (99%)	161 (78%)	34 (16%)	11 (5%)	3	32
5	E	149/151 (99%)	120 (80%)	26 (17%)	3 (2%)	11	62
6	F	99/101 (98%)	88 (89%)	10 (10%)	1 (1%)	22	78
7	G	153/155 (99%)	131 (86%)	17 (11%)	5 (3%)	6	50
8	H	136/138 (99%)	114 (84%)	20 (15%)	2 (2%)	15	68
9	I	125/127 (98%)	92 (74%)	25 (20%)	8 (6%)	2	26
10	J	96/98 (98%)	80 (83%)	11 (12%)	5 (5%)	3	32
11	K	112/114 (98%)	93 (83%)	15 (13%)	4 (4%)	5	47
12	L	120/122 (98%)	94 (78%)	22 (18%)	4 (3%)	6	50
13	M	115/117 (98%)	97 (84%)	15 (13%)	3 (3%)	8	56
14	N	58/60 (97%)	47 (81%)	8 (14%)	3 (5%)	3	32
15	O	86/88 (98%)	75 (87%)	9 (10%)	2 (2%)	10	59
16	P	81/83 (98%)	65 (80%)	13 (16%)	3 (4%)	5	46
17	Q	97/99 (98%)	82 (84%)	12 (12%)	3 (3%)	7	52
18	R	68/70 (97%)	55 (81%)	8 (12%)	5 (7%)	2	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	76/78 (97%)	57 (75%)	12 (16%)	7 (9%)	1	15
20	T	97/99 (98%)	75 (77%)	16 (16%)	6 (6%)	2	27
21	U	22/24 (92%)	16 (73%)	5 (23%)	1 (4%)	4	38
All	All	2332/2372 (98%)	1884 (81%)	342 (15%)	106 (4%)	4	38

5 of 106 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	15	VAL
3	C	14	ILE
3	C	79	ARG
3	C	100	ALA
4	D	28	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/202 (100%)	184 (91%)	18 (9%)	14	55
3	C	160/160 (100%)	144 (90%)	16 (10%)	11	47
4	D	180/180 (100%)	156 (87%)	24 (13%)	6	30
5	E	116/116 (100%)	103 (89%)	13 (11%)	9	39
6	F	90/90 (100%)	78 (87%)	12 (13%)	6	30
7	G	126/126 (100%)	120 (95%)	6 (5%)	35	80
8	H	119/119 (100%)	105 (88%)	14 (12%)	8	36
9	I	98/98 (100%)	87 (89%)	11 (11%)	9	39
10	J	88/88 (100%)	79 (90%)	9 (10%)	11	46
11	K	86/86 (100%)	77 (90%)	9 (10%)	10	44
12	L	103/103 (100%)	93 (90%)	10 (10%)	12	49
13	M	94/94 (100%)	83 (88%)	11 (12%)	8	37
14	N	49/49 (100%)	46 (94%)	3 (6%)	26	73
15	O	79/79 (100%)	69 (87%)	10 (13%)	6	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	72/72 (100%)	65 (90%)	7 (10%)	12	49
17	Q	94/94 (100%)	90 (96%)	4 (4%)	40	83
18	R	61/61 (100%)	56 (92%)	5 (8%)	17	60
19	S	69/69 (100%)	61 (88%)	8 (12%)	8	37
20	T	76/76 (100%)	68 (90%)	8 (10%)	10	44
21	U	19/19 (100%)	19 (100%)	0	100	100
All	All	1981/1981 (100%)	1783 (90%)	198 (10%)	11	47

5 of 198 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	1	MET
9	I	114	TYR
19	S	6	LYS
8	H	52	ASP
8	H	133	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
8	H	82	HIS
12	L	7	ASN
19	S	23	ASN
10	J	56	HIS
11	K	26	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1503/1504 (99%)	204 (13%)	0
22	V	76/77 (98%)	11 (14%)	0
22	W	76/77 (98%)	12 (15%)	0
23	X	4/5 (80%)	1 (25%)	0
All	All	1659/1663 (99%)	228 (13%)	0

5 of 228 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	G
1	A	22	G
1	A	32	A

There are no RNA pucker outliers to report.

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

Mogul failed to run properly - this section will therefore be empty.

5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.