wwPDB X-ray Structure Validation Summary Report (i)

May 17, 2020 – 12:33 pm BST

PDB ID	:	2D3O
Title	:	Structure of Ribosome Binding Domain of the Trigger Factor on the 50S ribosomal subunit from D. radiodurans
Authors	:	Schluenzen, F.; Wilson, D.N.; Hansen, H.A.; Tian, P.; Harms, J.M.; McInnes, S.J.; Albrecht, R.; Buerger, J.; Wilbanks, S.M.; Fucini, P.
Deposited on	:	2005-09-30
Resolution	:	3.35 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

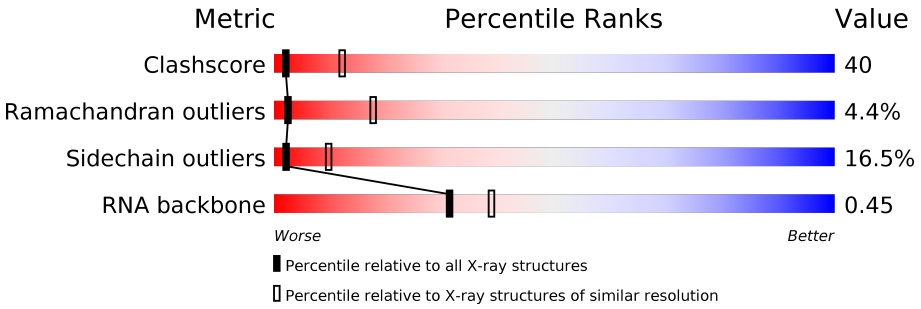
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RNA backbone	3102	1023 (3.80-2.92)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	2880	17% 59% 18%
2	R	95	28% 52% 17%
3	S	115	41% 42% 13%
4	W	67	30% 54% 13%
5	1	112	41% 39% 9% 11%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 63004 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	0	2802	60132	26824	11089	19418	2801	0	0	0

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	R	93	726	458	136	130	2	0	0	0

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	S	110	825	513	160	151	1	0	0	0

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	W	66	533	327	107	96	3	0	0	0

- Molecule 5 is a protein called Trigger Factor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	1	100	788	494	146	148	0	0	0

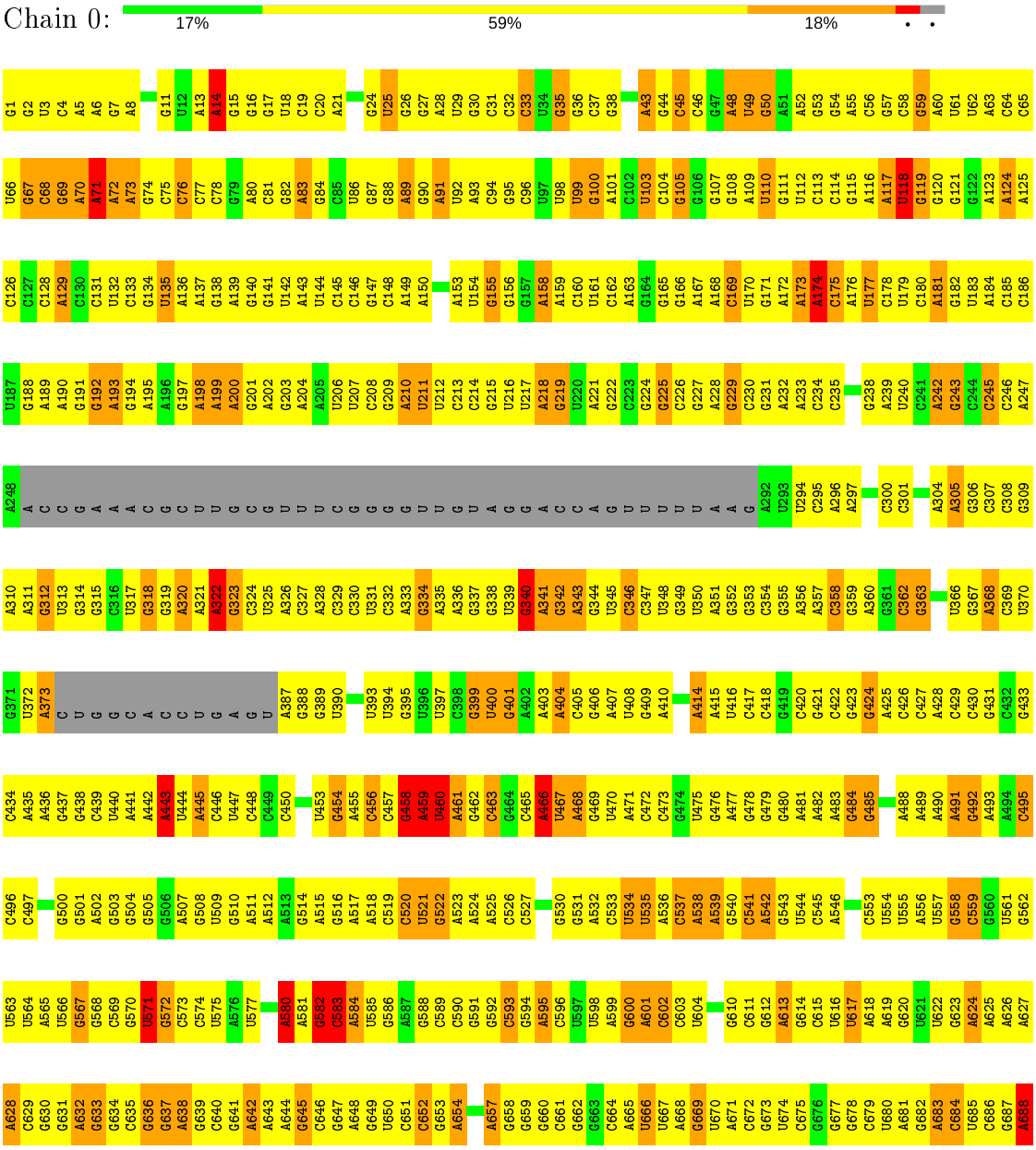
3 Residue-property plots (i)

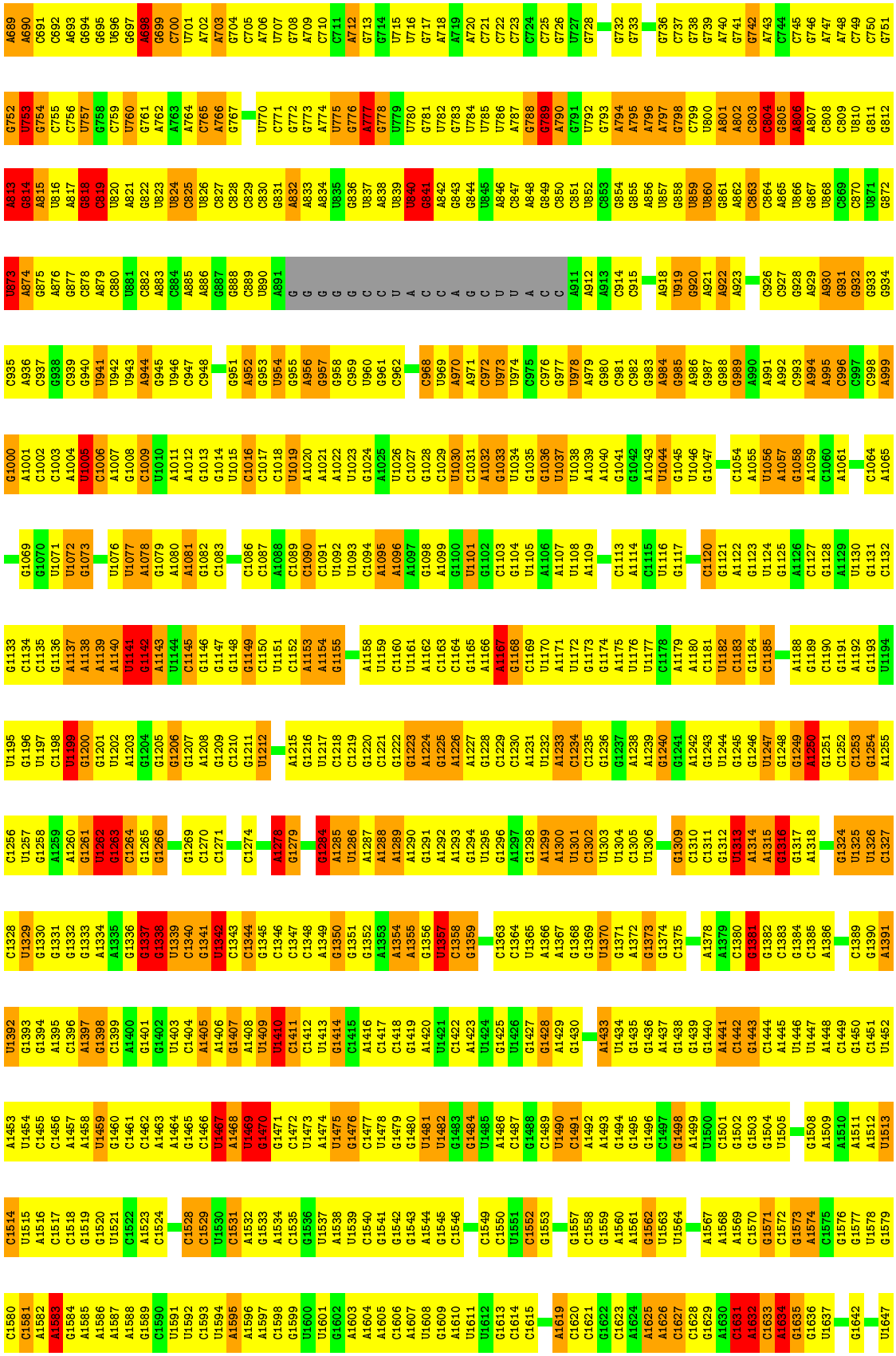
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

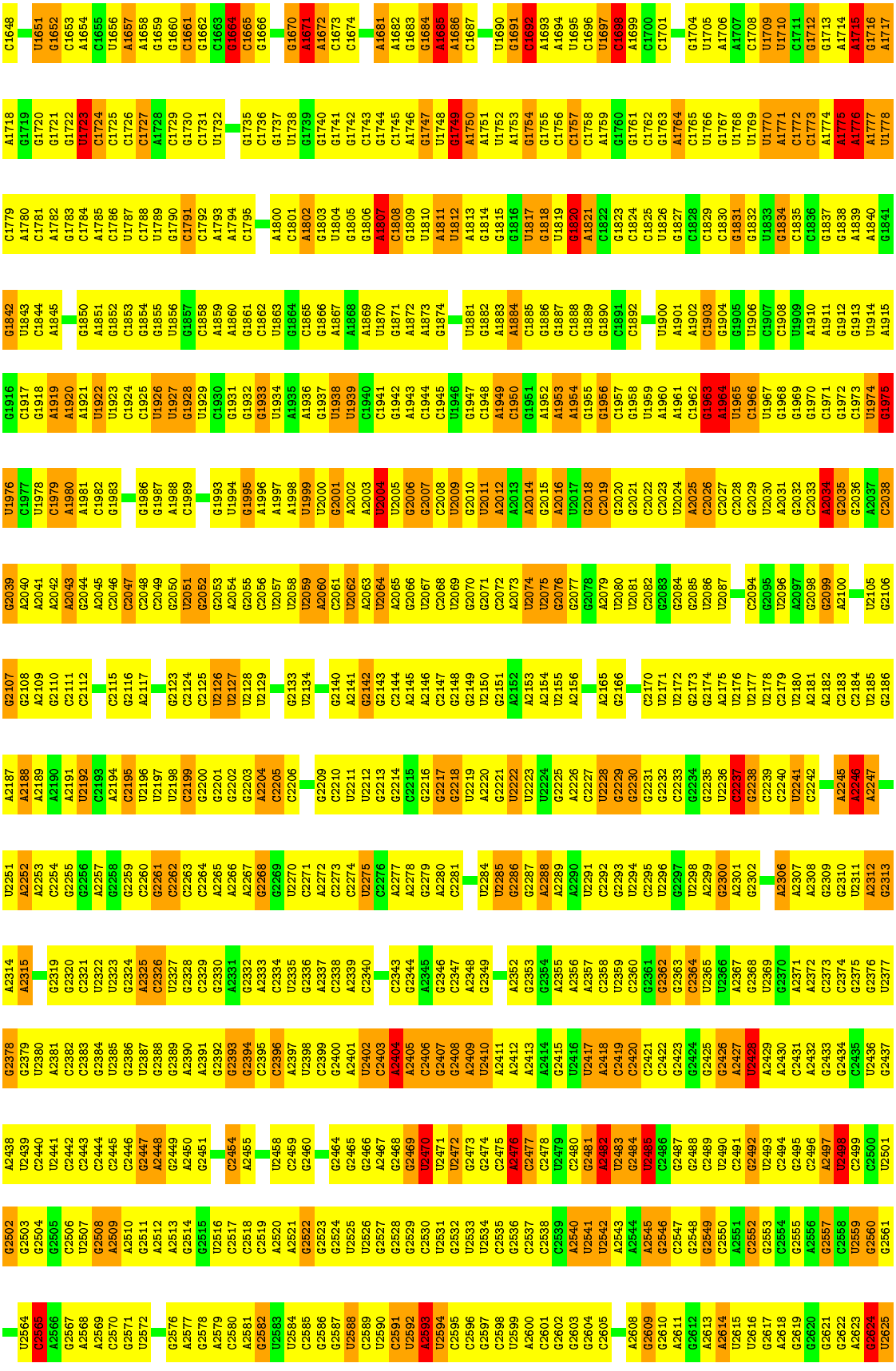
Note EDS was not executed.

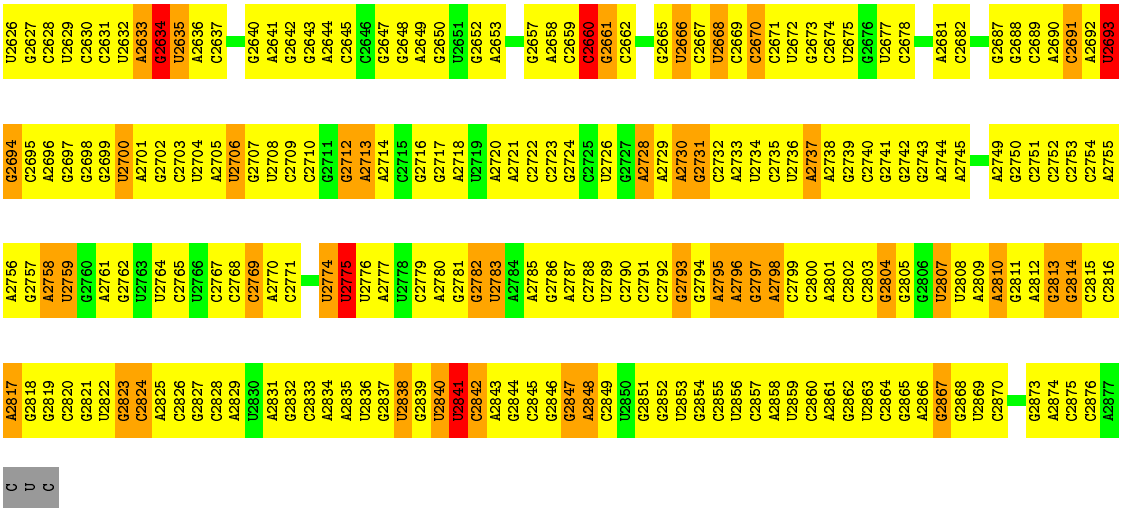
- Molecule 1: 23S RIBOSOMAL RNA

Chain 0:



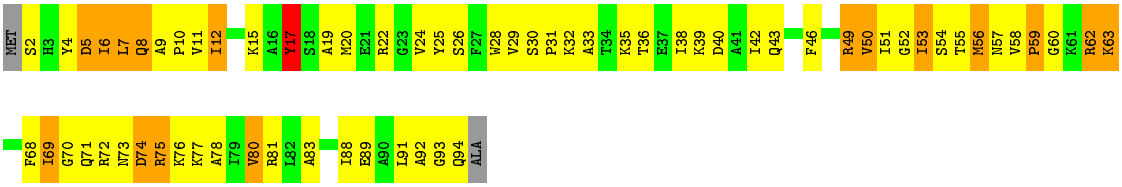






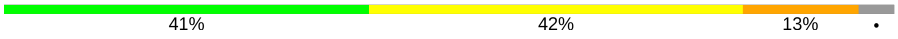
- Molecule 2: 50S RIBOSOMAL PROTEIN L23

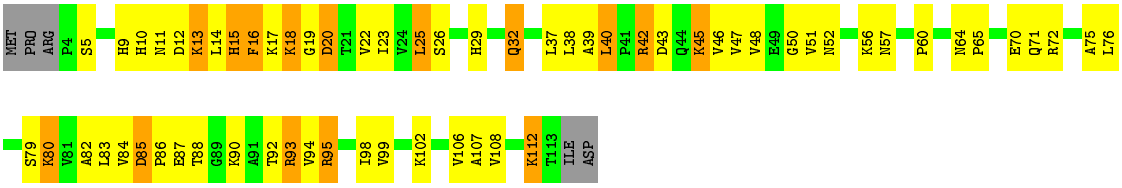
Chain R:



- Molecule 3: 50S RIBOSOMAL PROTEIN L24

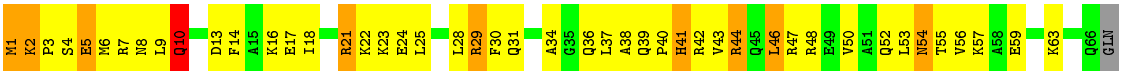
Chain S:





- Molecule 4: 50S RIBOSOMAL PROTEIN L29

Chain W:



- Molecule 5: Trigger Factor

Chain 1:


Y75
S76
Q77
R80
E81
V87
D88
A89
T90
V91
V96
Q97
S98
G99
Q100
A101
F102
E103
F104
T105
V106
K107
G108
E109
THR
TYR
PRO

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	169.50Å 410.50Å 695.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 3.35	Depositor
% Data completeness (in resolution range)	(Not available) (29.84-3.35)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.299 , 0.322	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	63004	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

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	0	0.67	3/67338 (0.0%)	0.82	72/105044 (0.1%)
2	R	0.48	0/737	0.80	0/988
3	S	0.42	0/835	0.73	1/1121 (0.1%)
4	W	0.44	0/537	0.58	0/714
5	1	0.48	0/802	0.68	0/1084
All	All	0.66	3/70249 (0.0%)	0.82	73/108951 (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
1	0	0	169
2	R	0	1
All	All	0	170

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2776	U	C1'-N1	6.38	1.58	1.48
1	0	2775	U	C1'-N1	6.21	1.58	1.48
1	0	567	G	C5-C6	-5.13	1.37	1.42

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	2034	A	N9-C1'-C2'	10.22	127.28	114.00
1	0	1342	U	N1-C1'-C2'	9.78	126.71	114.00
1	0	1467	U	N1-C1'-C2'	8.63	125.23	114.00
1	0	2775	U	C2-N1-C1'	-8.26	107.78	117.70
1	0	1631	C	N1-C1'-C2'	8.21	124.68	114.00

There are no chirality outliers.

5 of 170 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	118	U	Sidechain
1	0	14	A	Sidechain
1	0	25	U	Sidechain
1	0	43	A	Sidechain
1	0	71	A	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	60132	0	30298	3519	0
2	R	726	0	753	126	0
3	S	825	0	881	117	0
4	W	533	0	558	81	0
5	1	788	0	784	74	0
All	All	63004	0	33274	3848	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 40.

The worst 5 of 3848 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:69:ILE:CG2	2:R:70:GLY:H	1.26	1.38
1:0:1325:U:H1'	1:0:1619:A:N1	1.50	1.25
2:R:69:ILE:HG22	2:R:70:GLY:N	1.30	1.19
3:S:92:THR:HB	3:S:95:ARG:HH22	1.05	1.18
1:0:67:G:H21	1:0:72:A:H2'	1.09	1.16

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	R	91/95 (96%)	70 (77%)	16 (18%)	5 (6%)	2 13
3	S	108/115 (94%)	79 (73%)	24 (22%)	5 (5%)	2 16
4	W	64/67 (96%)	54 (84%)	8 (12%)	2 (3%)	4 25
5	1	98/112 (88%)	81 (83%)	13 (13%)	4 (4%)	3 19
All	All	361/389 (93%)	284 (79%)	61 (17%)	16 (4%)	2 18

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	S	42	ARG
3	S	65	PRO
4	W	2	LYS
5	1	49	PRO
2	R	69	ILE

5.3.2 Protein sidechains (i)

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	R	75/76 (99%)	61 (81%)	14 (19%)	1 6
3	S	91/96 (95%)	77 (85%)	14 (15%)	2 12
4	W	54/55 (98%)	43 (80%)	11 (20%)	1 4
5	1	83/93 (89%)	72 (87%)	11 (13%)	4 16
All	All	303/320 (95%)	253 (84%)	50 (16%)	2 10

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	S	40	LEU
3	S	112	LYS
5	1	88	ASP
3	S	43	ASP
3	S	80	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
3	S	64	ASN
3	S	71	GLN
5	1	55	ASN
3	S	57	ASN
5	1	24	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2798/2880 (97%)	580 (20%)	88 (3%)

5 of 580 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	14	A
1	0	25	U
1	0	33	C
1	0	35	G
1	0	45	C

5 of 88 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1342	U
1	0	1664	G
1	0	2660	C
1	0	1355	A
1	0	1626	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

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.