



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 04:59 PM GMT

PDB ID : 2Y0Z  
Title : THE CRYSTAL STRUCTURE OF EF-TU AND G24A-TRNA-TRP BOUND  
TO A NEAR-COGNATE CODON ON THE 70S RIBOSOME  
Authors : Schmeing, T.M.; Voorhees, R.M.; Ramakrishnan, V.  
Deposited on : 2010-12-07  
Resolution : 3.10 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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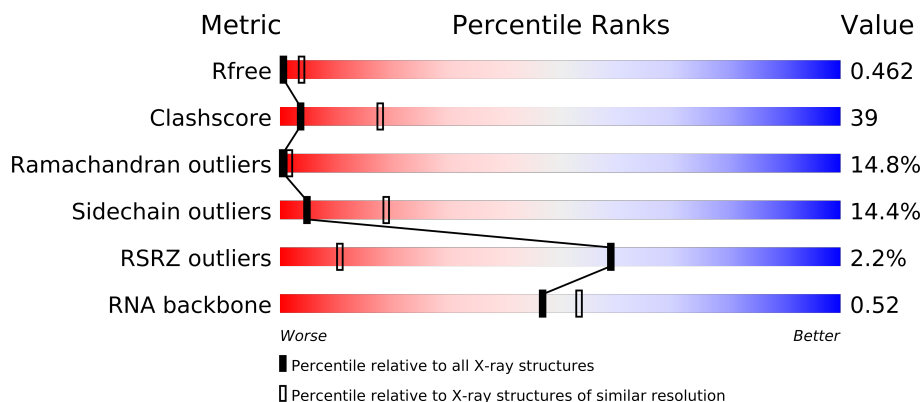
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.10 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.



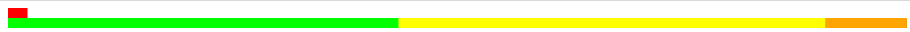
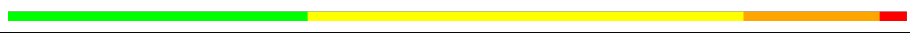
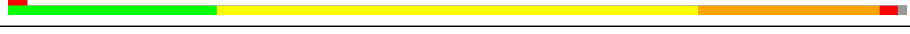

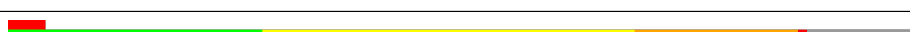


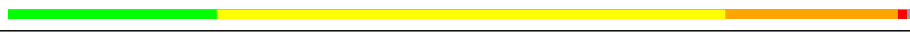
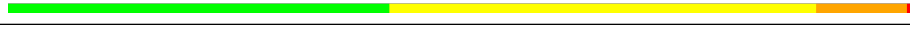

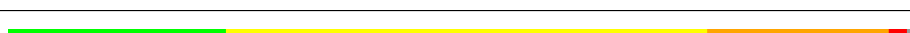
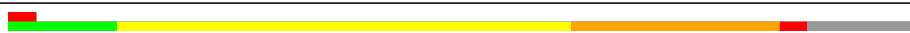
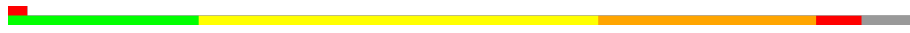
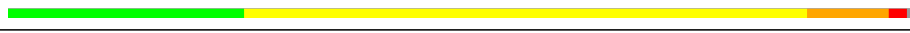
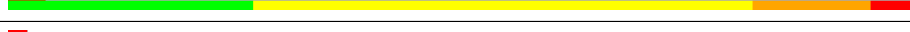

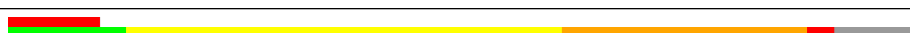
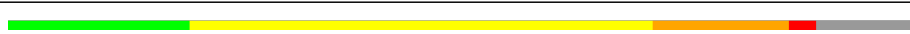



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)
RNA backbone	1838	1047 (3.60-2.60)

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	0	85	
2	1	98	
3	2	72	
4	3	60	
5	4	71	
6	5	60	
7	6	54	
8	7	49	
9	8	65	
10	9	37	
11	A	2915	
12	B	122	

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Mol	Chain	Length	Quality of chain
13	C	229	
14	D	276	
15	E	206	
16	F	210	
17	G	182	
18	H	180	
19	J	173	
20	K	147	
21	N	140	
22	O	122	
23	P	150	
24	Q	141	
25	R	118	
26	S	112	
27	T	146	
28	U	118	
29	V	101	
30	W	113	
31	X	96	
32	Y	110	
33	Z	206	

## 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 93806 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 protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	93	Total	C	N	O	S	0	0	0
			731	460	145	125	1			

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			

- Molecule 5 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4	44	Total	C	N	O	S	0	0	0
			340	218	57	61	4			

- Molecule 6 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 7 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 11 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	A	2901	Total	C	N	O	P	0	0	0
			62477	27807	11683	20087	2900			

- Molecule 12 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	B	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	C	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	D	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	E	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	F	207	Total	C	N	O	S	0	0	0
			1623	1035	303	282	3			

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	G	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	H	159	Total	C	N	O	S	0	0	0
			1222	773	228	220	1			

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	J	130	Total	C	N	O		0	0	0
			651	391	130	130				

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	K	140	Total	C	N	O		0	0	0
			700	420	140	140				

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	N	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	P	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	R	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	S	98	Total	C	N	O	0	0	0
			770	486	154	130			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	T	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	U	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	V	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	W	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	X	92	Total	C	N	O	S	0	0	0
			725	471	131	123				

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	Y	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	Z	183	Total	C	N	O	S	0	0	0
			1459	932	260	265	2			

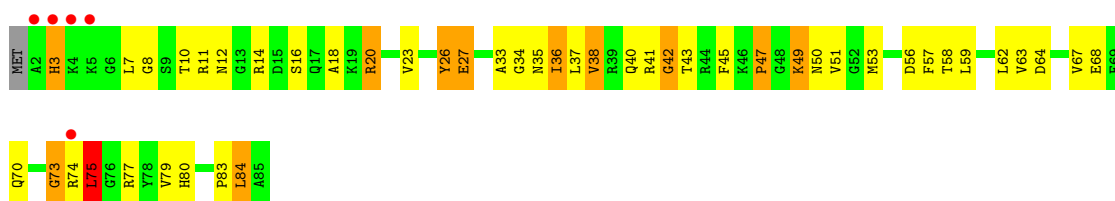


### 3 Residue-property plots

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.

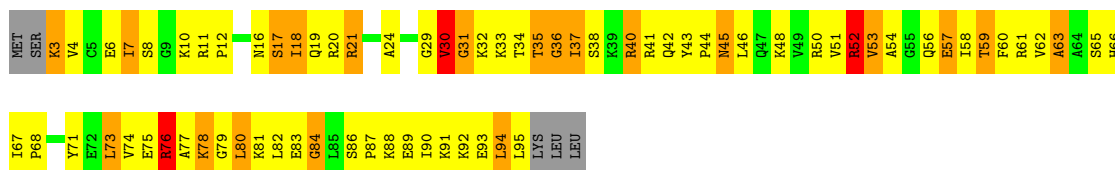
- Molecule 1: 50S RIBOSOMAL PROTEIN L27

Chain 0: 



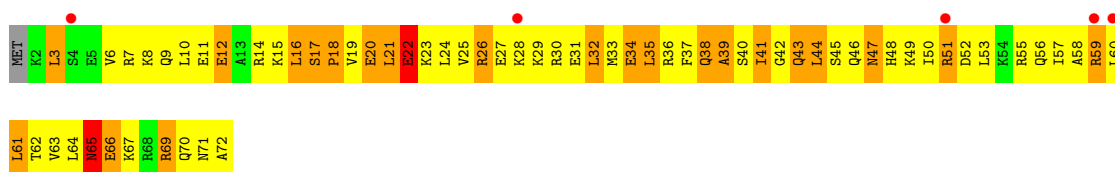
- Molecule 2: 50S RIBOSOMAL PROTEIN L28

Chain 1: 



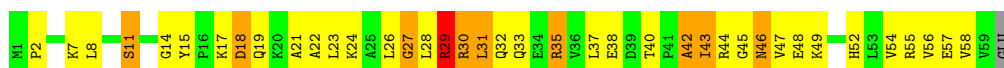
- Molecule 3: 50S RIBOSOMAL PROTEIN L29

Chain 2: 



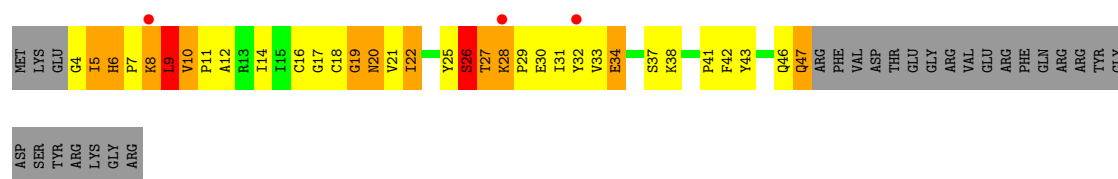
- Molecule 4: 50S RIBOSOMAL PROTEIN L30

Chain 3: 



- Molecule 5: 50S RIBOSOMAL PROTEIN L31

Chain 4: 



• Molecule 6: 50S RIBOSOMAL PROTEIN L32

Chain 5:



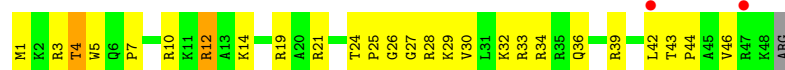
• Molecule 7: 50S RIBOSOMAL PROTEIN L33

Chain 6:



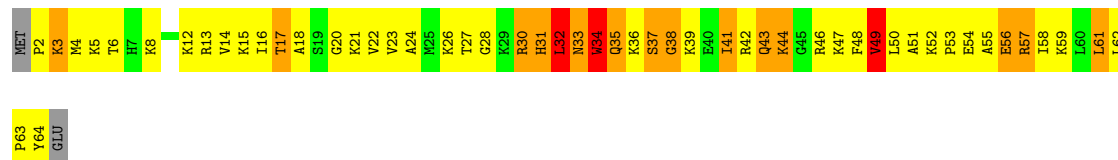
• Molecule 8: 50S RIBOSOMAL PROTEIN L34

Chain 7:



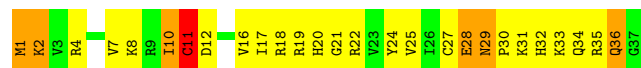
• Molecule 9: 50S RIBOSOMAL PROTEIN L35

Chain 8:



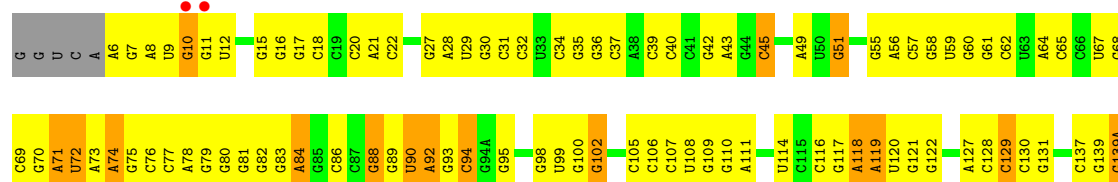
• Molecule 10: 50S RIBOSOMAL PROTEIN L36

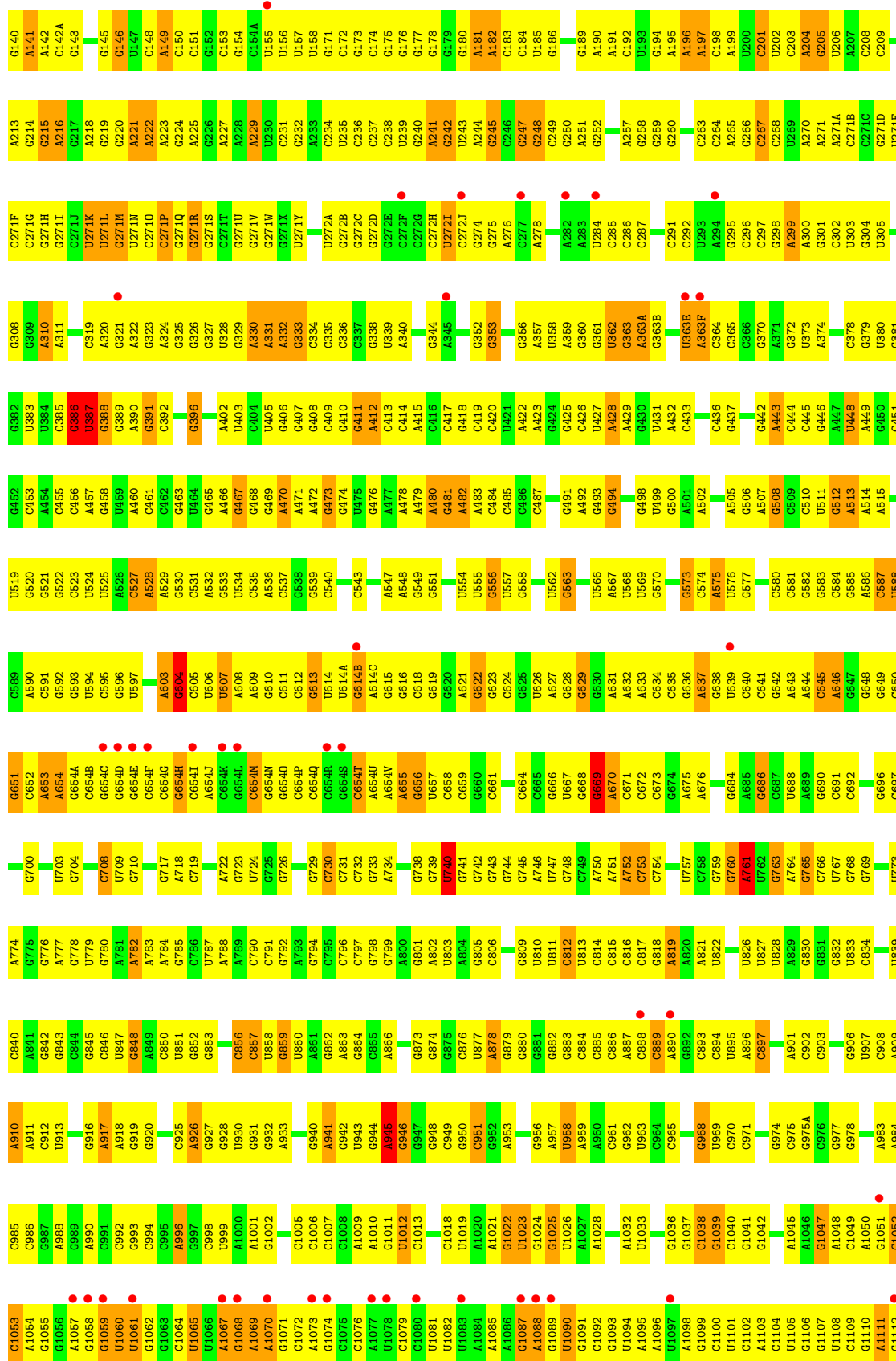
Chain 9:



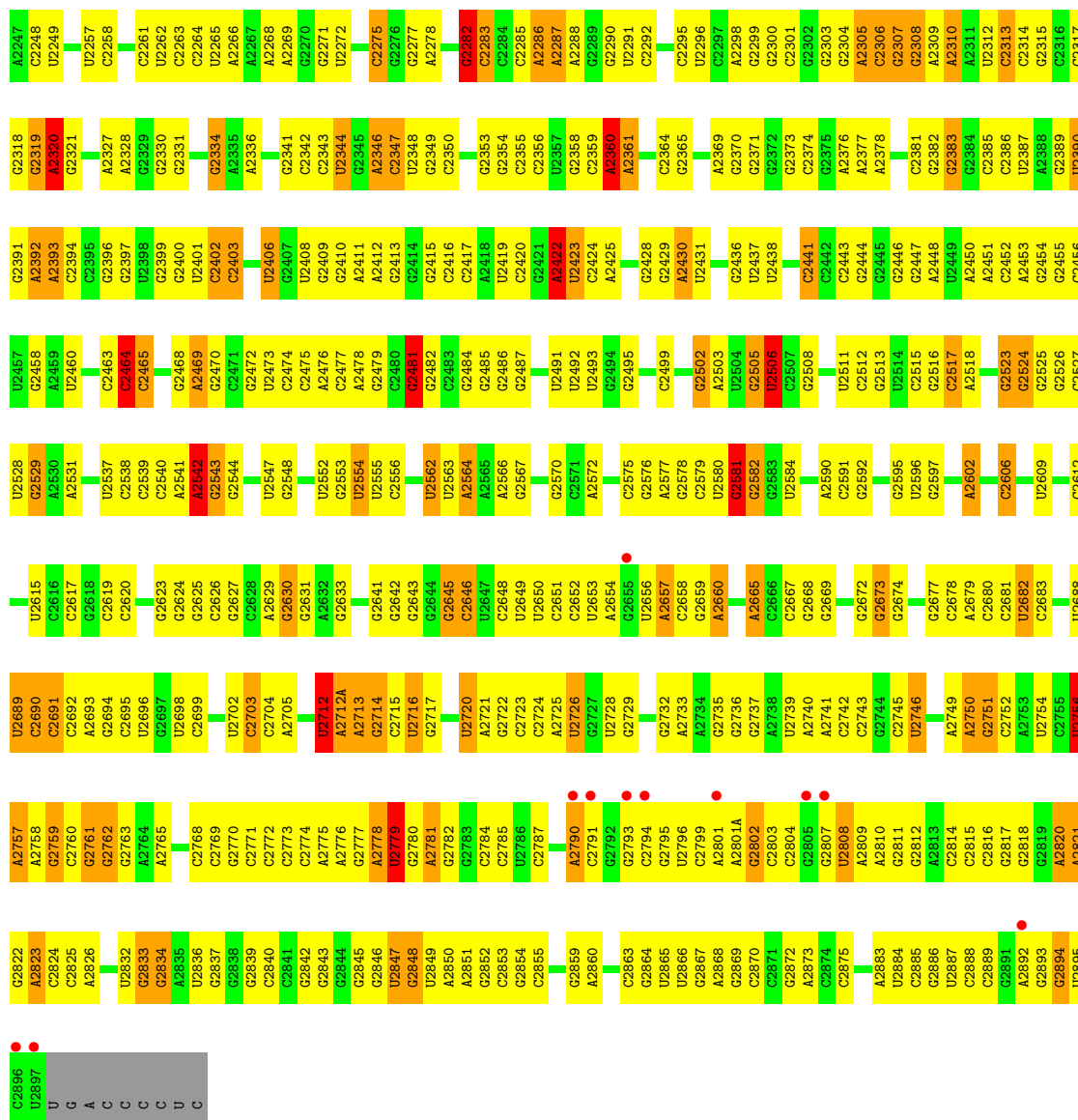
• Molecule 11: 23S RIBOSOMAL RNA

Chain A:



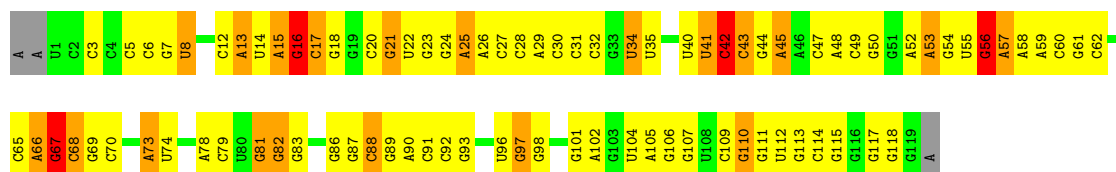
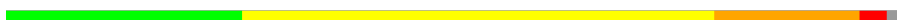






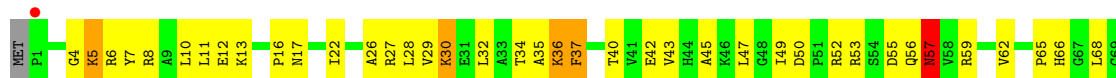
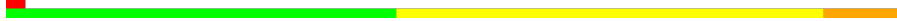
• Molecule 12: 5S RIBOSOMAL RNA

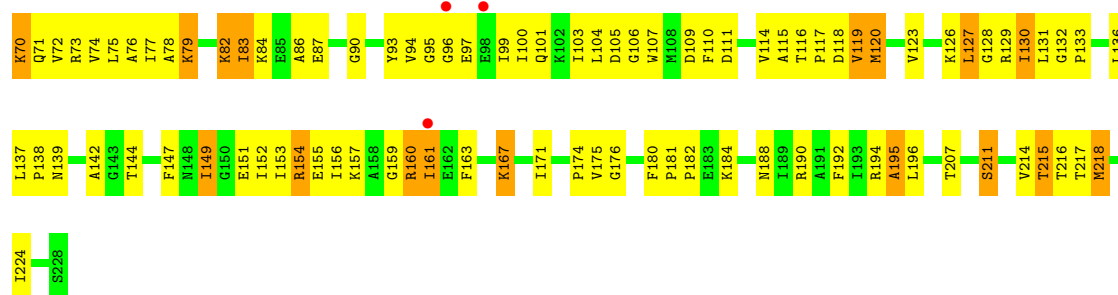
Chain B:



• Molecule 13: 50S RIBOSOMAL PROTEIN L1

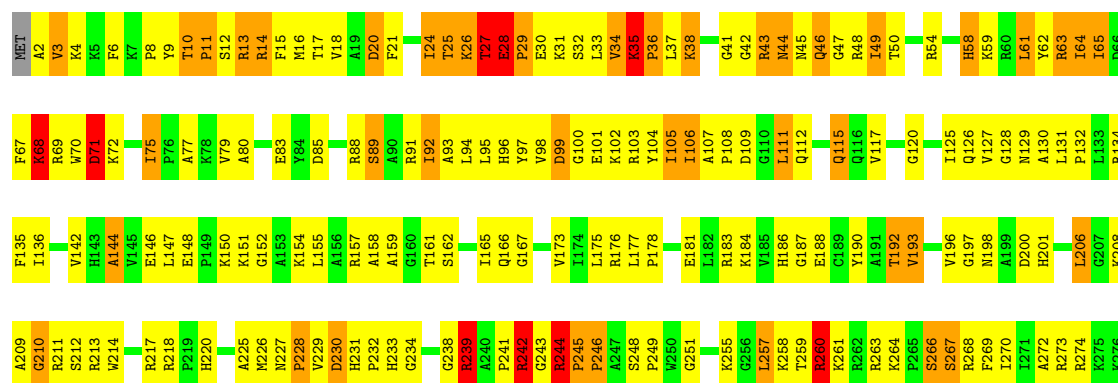
Chain C:





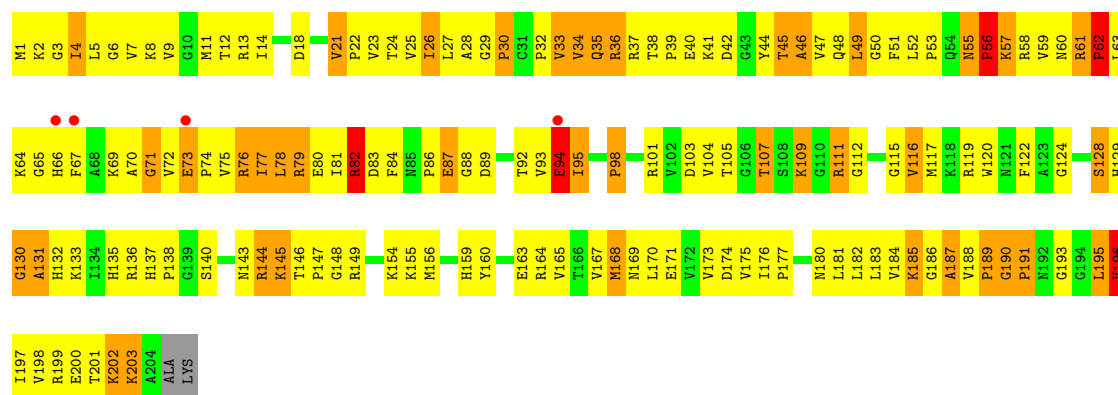
• Molecule 14: 50S RIBOSOMAL PROTEIN L2

Chain D:



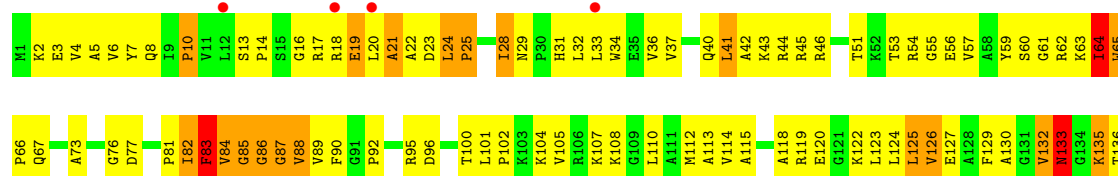
• Molecule 15: 50S RIBOSOMAL PROTEIN L3

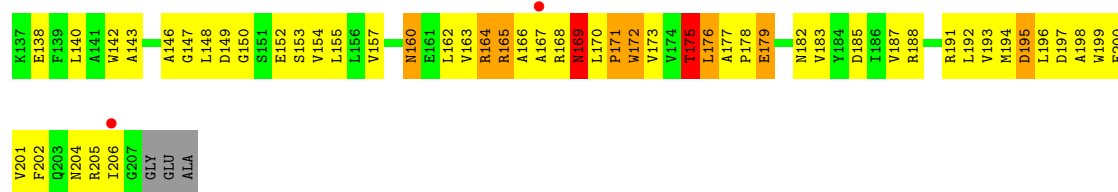
Chain E:



• Molecule 16: 50S RIBOSOMAL PROTEIN L4

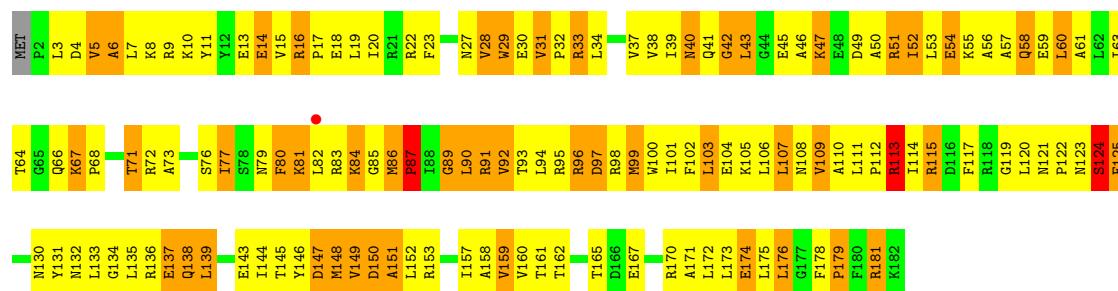
Chain F:





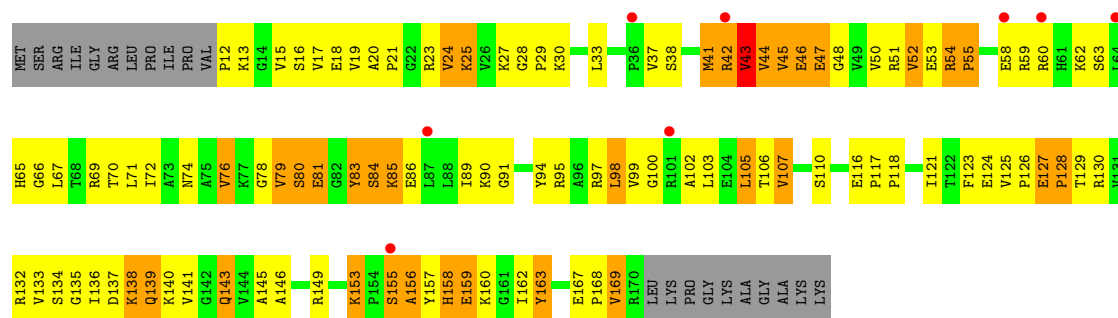
• Molecule 17: 50S RIBOSOMAL PROTEIN L5

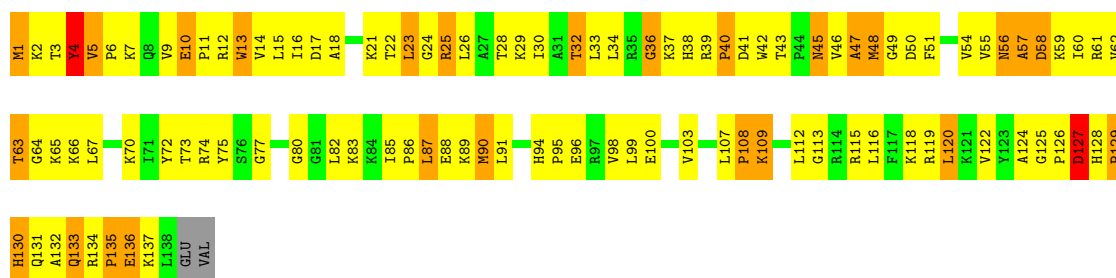
Chain G:



• Molecule 18: 50S RIBOSOMAL PROTEIN L6

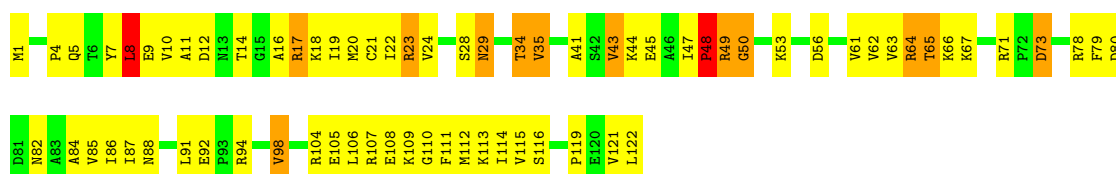
Chain H:





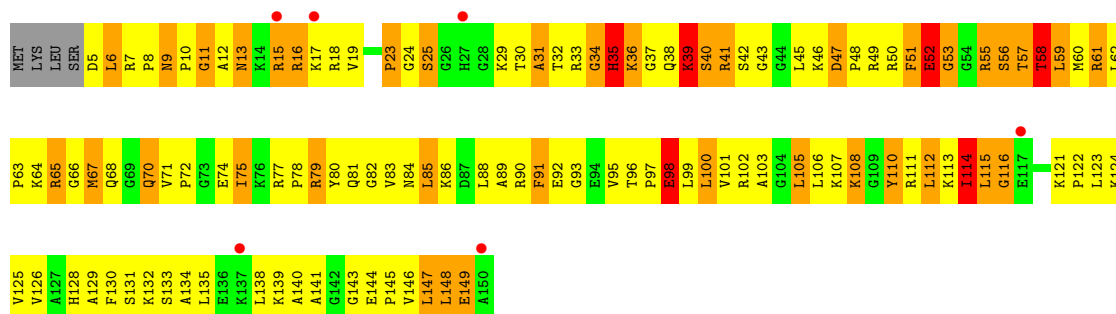
• Molecule 22: 50S RIBOSOMAL PROTEIN L14

Chain O:



• Molecule 23: 50S RIBOSOMAL PROTEIN L15

Chain P:



• Molecule 24: 50S RIBOSOMAL PROTEIN L16

Chain Q:



• Molecule 25: 50S RIBOSOMAL PROTEIN L17

Chain R:







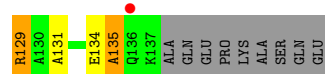
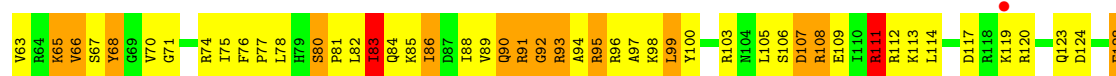
• Molecule 26: 50S RIBOSOMAL PROTEIN L18

Chain S:



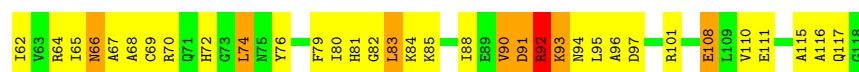
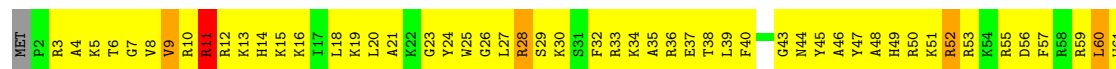
• Molecule 27: 50S RIBOSOMAL PROTEIN L19

Chain T:



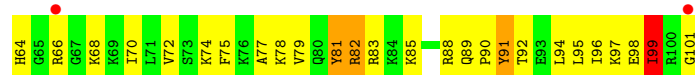
• Molecule 28: 50S RIBOSOMAL PROTEIN L20

Chain U:



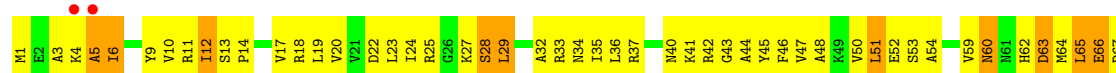
• Molecule 29: 50S RIBOSOMAL PROTEIN L21

Chain V:



• Molecule 30: 50S RIBOSOMAL PROTEIN L22

Chain W:



• Molecule 31: 50S RIBOSOMAL PROTEIN L23

Chain X:

• Molecule 32: 50S RIBOSOMAL PROTEIN L24

Chain Y:

• Molecule 33: 50S RIBOSOMAL PROTEIN L25

Chain Z:

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	289.90Å 269.40Å 404.50Å 90.00° 91.51° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.22 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-3.10) 91.8 (49.22-2.80)	Depositor EDS
$R_{merge}$	0.02	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 2.81Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.238 , 0.275 0.456 , 0.462	Depositor DCC
$R_{free}$ test set	69565 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.1	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 59.9	EDS
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	2 of 1394902 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.62	EDS
Total number of atoms	93806	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.01% 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	0	0.47	0/671	0.78	0/892
2	1	0.51	0/738	0.81	1/981 (0.1%)
3	2	0.38	0/600	0.73	0/793
4	3	0.40	0/472	0.67	0/634
5	4	0.46	0/349	0.66	0/474
6	5	0.44	0/473	0.73	0/639
7	6	0.70	0/440	0.94	0/586
8	7	0.49	0/426	0.73	0/561
9	8	0.58	0/515	0.89	1/679 (0.1%)
10	9	0.56	0/310	0.73	0/407
11	A	0.56	7/69976 (0.0%)	0.74	36/109244 (0.0%)
12	B	0.51	0/2853	0.77	3/4451 (0.1%)
13	C	0.46	2/1774 (0.1%)	0.65	0/2391
14	D	0.62	0/2195	0.93	3/2955 (0.1%)
15	E	0.46	0/1596	0.77	1/2153 (0.0%)
16	F	0.40	0/1658	0.65	0/2244
17	G	0.48	0/1499	0.78	0/2016
18	H	0.37	0/1245	0.66	0/1682
21	N	0.39	0/1131	0.72	0/1525
22	O	0.53	0/943	0.74	1/1269 (0.1%)
23	P	0.46	0/1131	0.96	4/1504 (0.3%)
24	Q	0.52	0/1143	0.73	0/1527
25	R	0.41	0/974	0.81	2/1302 (0.2%)
26	S	0.45	0/778	0.79	0/1036
27	T	0.48	0/1155	0.78	1/1542 (0.1%)
28	U	0.42	0/975	0.69	0/1297
29	V	0.38	0/790	0.68	0/1057
30	W	0.39	0/907	0.76	0/1216
31	X	0.45	0/739	0.70	0/993
32	Y	0.36	0/788	0.69	0/1051
33	Z	0.50	0/1491	0.75	0/2024
All	All	0.53	9/100735 (0.0%)	0.75	53/151125 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying

if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	A	2	87
12	B	0	4
14	D	0	1
21	N	0	1
All	All	2	93

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	761	A	C5-C6	-9.78	1.32	1.41
11	A	945	A	C5-C6	8.28	1.48	1.41
11	A	2506	U	N1-C2	6.57	1.44	1.38
11	A	2180	U	N1-C2	5.43	1.43	1.38
11	A	761	A	C6-N6	-5.41	1.29	1.33

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1992	G	C2'-C3'-O3'	9.07	129.45	109.50
11	A	1820	U	C2'-C3'-O3'	8.51	128.23	109.50
11	A	1786	A	N9-C1'-C2'	8.39	124.91	114.00
11	A	1300	U	C2'-C3'-O3'	8.10	127.32	109.50
11	A	1970	A	C5'-C4'-O4'	8.09	118.81	109.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	A	1300	U	C3'
11	A	1820	U	C3'

5 of 93 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	A	114	U	Sidechain
11	A	201	C	Sidechain
11	A	247	G	Sidechain
11	A	383	U	Sidechain
11	A	463	G	Sidechain

## 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	0	662	0	688	75	0
2	1	731	0	808	88	0
3	2	598	0	653	179	0
4	3	467	0	523	57	0
5	4	340	0	339	51	0
6	5	459	0	480	82	0
7	6	433	0	461	139	0
8	7	418	0	467	35	0
9	8	507	0	576	118	0
10	9	307	0	338	35	0
11	A	62477	0	31497	2260	0
12	B	2551	0	1295	108	0
13	C	1742	0	1800	151	0
14	D	2145	0	2234	297	0
15	E	1563	0	1629	227	0
16	F	1623	0	1677	197	0
17	G	1474	0	1535	240	0
18	H	1222	0	1282	171	0
19	J	651	0	170	19	0
20	K	700	0	175	15	0
21	N	1104	0	1180	160	0
22	O	933	0	996	90	0
23	P	1114	0	1187	291	0
24	Q	1122	0	1179	141	0
25	R	960	0	1021	131	0
26	S	770	0	832	166	0
27	T	1141	0	1202	224	0
28	U	958	0	1015	141	0
29	V	779	0	852	135	0
30	W	896	0	953	100	0
31	X	725	0	778	98	0
32	Y	775	0	870	176	0
33	Z	1459	0	1488	216	0
All	All	93806	0	62180	6018	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 39.

The worst 5 of 6018 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:5:4:HIS:HB3	6:5:5:PRO:HD3	1.26	1.17
13:C:119:VAL:HG13	13:C:120:MET:HE3	1.27	1.17
11:A:2101:G:H2'	11:A:2102:U:H5''	1.24	1.16
11:A:11:G:H22	11:A:2627:G:H5''	1.11	1.15
18:H:149:ARG:HA	18:H:162:ILE:HD11	1.25	1.14

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	
1	0	82/85 (96%)	65 (79%)	10 (12%)	7 (8%)	1	9
2	1	91/98 (93%)	58 (64%)	18 (20%)	15 (16%)	0	0
3	2	69/72 (96%)	34 (49%)	20 (29%)	15 (22%)	0	0
4	3	57/60 (95%)	42 (74%)	9 (16%)	6 (10%)	1	5
5	4	42/71 (59%)	25 (60%)	10 (24%)	7 (17%)	0	0
6	5	57/60 (95%)	40 (70%)	7 (12%)	10 (18%)	0	0
7	6	48/54 (89%)	20 (42%)	10 (21%)	18 (38%)	0	0
8	7	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
9	8	61/65 (94%)	31 (51%)	18 (30%)	12 (20%)	0	0
10	9	35/37 (95%)	19 (54%)	11 (31%)	5 (14%)	0	2
13	C	226/229 (99%)	176 (78%)	33 (15%)	17 (8%)	2	11
14	D	273/276 (99%)	199 (73%)	46 (17%)	28 (10%)	1	6
15	E	202/206 (98%)	125 (62%)	45 (22%)	32 (16%)	0	1
16	F	205/210 (98%)	145 (71%)	34 (17%)	26 (13%)	0	3
17	G	179/182 (98%)	110 (62%)	33 (18%)	36 (20%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	H	157/180 (87%)	97 (62%)	31 (20%)	29 (18%)	0	0
21	N	136/140 (97%)	91 (67%)	27 (20%)	18 (13%)	0	2
22	O	120/122 (98%)	97 (81%)	15 (12%)	8 (7%)	2	14
23	P	144/150 (96%)	77 (54%)	36 (25%)	31 (22%)	0	0
24	Q	139/141 (99%)	112 (81%)	20 (14%)	7 (5%)	3	22
25	R	115/118 (98%)	81 (70%)	15 (13%)	19 (16%)	0	0
26	S	96/112 (86%)	44 (46%)	29 (30%)	23 (24%)	0	0
27	T	135/146 (92%)	76 (56%)	28 (21%)	31 (23%)	0	0
28	U	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	11
29	V	99/101 (98%)	65 (66%)	21 (21%)	13 (13%)	0	3
30	W	111/113 (98%)	78 (70%)	17 (15%)	16 (14%)	0	2
31	X	90/96 (94%)	63 (70%)	15 (17%)	12 (13%)	0	2
32	Y	98/110 (89%)	43 (44%)	28 (29%)	27 (28%)	0	0
33	Z	181/206 (88%)	117 (65%)	38 (21%)	26 (14%)	0	2
All	All	3409/3607 (94%)	2260 (66%)	646 (19%)	503 (15%)	0	2

5 of 503 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	42	GLY
1	0	47	PRO
2	1	17	SER
2	1	30	VAL
2	1	53	VAL

### 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	
1	0	66/67 (98%)	53 (80%)	13 (20%)	2	8
2	1	78/83 (94%)	68 (87%)	10 (13%)	6	24
3	2	66/67 (98%)	55 (83%)	11 (17%)	3	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	3	51/52 (98%)	44 (86%)	7 (14%)	5	21
5	4	39/63 (62%)	28 (72%)	11 (28%)	0	1
6	5	51/52 (98%)	44 (86%)	7 (14%)	5	21
7	6	49/52 (94%)	32 (65%)	17 (35%)	0	0
8	7	41/42 (98%)	37 (90%)	4 (10%)	12	40
9	8	53/55 (96%)	43 (81%)	10 (19%)	2	9
10	9	34/34 (100%)	28 (82%)	6 (18%)	3	10
13	C	180/181 (99%)	168 (93%)	12 (7%)	23	63
14	D	217/218 (100%)	176 (81%)	41 (19%)	2	9
15	E	165/166 (99%)	137 (83%)	28 (17%)	3	11
16	F	165/166 (99%)	147 (89%)	18 (11%)	9	34
17	G	155/156 (99%)	130 (84%)	25 (16%)	3	13
18	H	132/148 (89%)	122 (92%)	10 (8%)	19	58
21	N	117/119 (98%)	102 (87%)	15 (13%)	6	24
22	O	100/100 (100%)	92 (92%)	8 (8%)	17	55
23	P	112/116 (97%)	89 (80%)	23 (20%)	2	8
24	Q	111/111 (100%)	94 (85%)	17 (15%)	4	15
25	R	100/101 (99%)	88 (88%)	12 (12%)	7	27
26	S	77/88 (88%)	65 (84%)	12 (16%)	4	14
27	T	120/127 (94%)	101 (84%)	19 (16%)	4	14
28	U	92/94 (98%)	84 (91%)	8 (9%)	15	49
29	V	82/82 (100%)	69 (84%)	13 (16%)	4	13
30	W	91/92 (99%)	85 (93%)	6 (7%)	24	64
31	X	74/78 (95%)	65 (88%)	9 (12%)	7	26
32	Y	84/91 (92%)	72 (86%)	12 (14%)	5	19
33	Z	161/179 (90%)	134 (83%)	27 (17%)	3	11
All	All	2863/2980 (96%)	2452 (86%)	411 (14%)	5	19

5 of 411 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	F	125	LEU
21	N	1	MET

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Mol	Chain	Res	Type
32	Y	50	ARG
16	F	169	ASN
17	G	107	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
15	E	169	ASN
17	G	132	ASN
31	X	55	ASN
15	E	192	ASN
16	F	133	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	2900/2915 (99%)	511 (17%)	48 (1%)
12	B	118/122 (96%)	26 (22%)	4 (3%)
All	All	3018/3037 (99%)	537 (17%)	52 (1%)

5 of 537 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	10	G
11	A	45	C
11	A	51	G
11	A	69	C
11	A	71	A

5 of 52 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	1378	A
11	A	1819	A
12	B	16	G
11	A	1427	A
11	A	1558	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 ⓘ

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	0	84/85 (98%)	0.17	5 (5%) 21 3	58, 73, 107, 122	0
2	1	93/98 (94%)	0.05	0 100 100	45, 69, 129, 134	0
3	2	71/72 (98%)	0.55	5 (7%) 16 3	130, 143, 155, 158	0
4	3	59/60 (98%)	0.06	0 100 100	65, 81, 106, 122	0
5	4	44/71 (61%)	0.44	3 (6%) 17 3	111, 140, 167, 173	0
6	5	59/60 (98%)	0.11	1 (1%) 67 15	62, 87, 148, 163	0
7	6	50/54 (92%)	0.26	3 (6%) 21 3	57, 84, 103, 110	0
8	7	48/49 (97%)	0.31	2 (4%) 35 5	51, 64, 101, 121	0
9	8	63/65 (96%)	0.08	0 100 100	56, 73, 91, 115	0
10	9	37/37 (100%)	0.16	0 100 100	73, 85, 103, 104	0
11	A	2901/2915 (99%)	-0.01	65 (2%) 59 11	26, 77, 181, 200	0
12	B	119/122 (97%)	-0.23	0 100 100	59, 85, 112, 132	0
13	C	228/229 (99%)	0.12	4 (1%) 65 14	50, 79, 160, 173	0
14	D	275/276 (99%)	-0.20	0 100 100	30, 49, 83, 105	0
15	E	204/206 (99%)	0.08	4 (1%) 62 12	50, 79, 128, 140	0
16	F	207/210 (98%)	0.30	6 (2%) 49 7	53, 112, 162, 170	0
17	G	181/182 (99%)	-0.06	1 (0%) 86 36	63, 86, 117, 130	0
18	H	159/180 (88%)	0.39	8 (5%) 28 4	93, 134, 152, 156	0
19	J	0/173	-	-	-	-
20	K	0/147	-	-	-	-
21	N	138/140 (98%)	0.13	0 100 100	63, 89, 125, 134	0
22	O	122/122 (100%)	-0.29	0 100 100	46, 63, 77, 85	0
23	P	146/150 (97%)	0.47	6 (4%) 35 5	55, 103, 133, 150	0
24	Q	141/141 (100%)	-0.10	2 (1%) 72 17	46, 64, 86, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	R	117/118 (99%)	0.08	0 100 100	60, 85, 107, 126	0
26	S	98/112 (87%)	0.19	3 (3%) 47 7	63, 90, 116, 126	0
27	T	137/146 (93%)	-0.03	3 (2%) 59 11	58, 84, 142, 167	0
28	U	117/118 (99%)	0.07	0 100 100	64, 79, 111, 128	0
29	V	101/101 (100%)	0.32	4 (3%) 36 5	62, 116, 129, 136	0
30	W	113/113 (100%)	0.15	2 (1%) 65 14	65, 90, 116, 141	0
31	X	92/96 (95%)	0.25	2 (2%) 59 11	75, 95, 110, 118	0
32	Y	100/110 (90%)	0.70	11 (11%) 6 1	108, 134, 162, 168	0
33	Z	183/206 (88%)	-0.01	0 100 100	56, 83, 120, 132	0
All	All	6487/6964 (93%)	0.06	140 (2%) 59 11	26, 82, 154, 200	0

The worst 5 of 140 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	A	654(D)	G	5.6
11	A	654(S)	G	5.5
26	S	59	LYS	4.7
11	A	1089	G	4.7
11	A	654(K)	C	4.6

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.