



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 06:21 PM GMT

PDB ID : 4KBU
Title : 70S ribosome translocation intermediate GDPNP-II containing elongation factor EFG/GDPNP, mRNA, and tRNA bound in the pe*/E state. This entry contains 50S ribosomal subunit A. The full asymmetric unit also contains PDB entries 4KBT (30S subunit A), 4KBV (30S subunit B), and 4KBW (50S subunit B).
Authors : Zhou, J.; Lancaster, L.; Donohue, J.P.; Noller, H.F.
Deposited on : 2013-04-23
Resolution : 3.86 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>

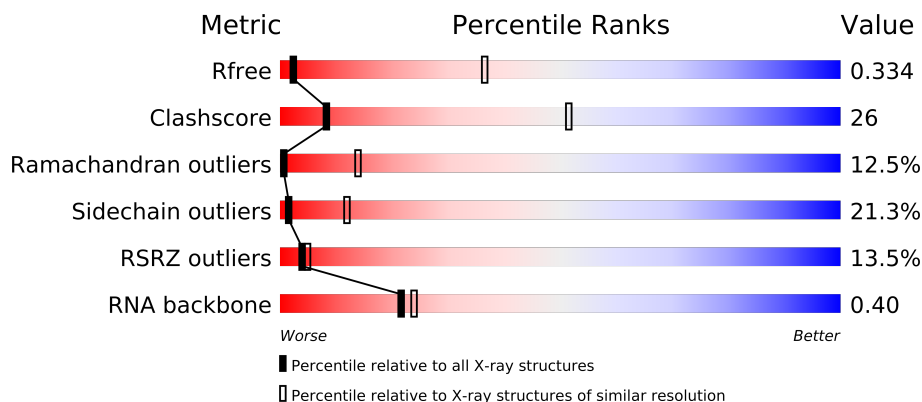
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 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 3.86 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	1013 (4.30-3.42)
Clashscore	79885	1145 (4.22-3.50)
Ramachandran outliers	78287	1091 (4.22-3.50)
Sidechain outliers	78261	1081 (4.22-3.50)
RSRZ outliers	66119	1014 (4.30-3.42)
RNA backbone	1838	1010 (4.84-2.80)

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.

Mol	Chain	Length	Quality of chain
1	C	228	
2	D	275	
3	E	205	
4	F	208	
5	G	181	
6	H	167	
7	J	170	
8	K	140	
9	O	122	
10	P	146	
11	Q	141	
12	R	117	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
13	S	99	
14	T	138	
15	U	117	
16	V	101	
17	W	113	
18	X	93	
19	Y	107	
20	Z	185	
21	0	84	
22	1	93	
23	4	35	
24	N	138	
25	2	71	
26	3	60	
27	5	59	
28	6	50	
29	7	49	
30	8	64	
31	9	37	
32	e	103	
33	f	31	
33	g	31	
34	h	30	
35	B	119	
36	A	2879	

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 95124 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 L1.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	20	VAL	ILE	CONFLICT	UNP Q72GV9
C	28	ARG	HIS	CONFLICT	UNP Q72GV9

- Molecule 2 is a protein called 50S ribosomal protein L2.

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

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	205	Total	C	N	O	S	0	0	0
			1569	991	300	272	6			

- Molecule 4 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	208	Total	C	N	O	S	0	0	0
			1628	1037	304	284	3			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	2	LYS	-	INSERTION	UNP Q72I05
F	3	GLU	-	INSERTION	UNP Q72I05

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	4	VAL	-	INSERTION	UNP Q72I05
F	5	ALA	-	INSERTION	UNP Q72I05
F	6	VAL	-	INSERTION	UNP Q72I05

- Molecule 5 is a protein called 50S ribosomal protein L5.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	5	VAL	LEU	CONFLICT	UNP Q72I16

- Molecule 6 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	167	Total	C	N	O	S	0	0	0
			1274	806	238	229	1			

- Molecule 7 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	J	170	Total	C	N	O	S	0	0	0
			851	510	170	171				

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	K	140	Total	C	N	O	S	0	0	0
			1035	659	183	188	5			

- Molecule 9 is a protein called 50S ribosomal protein L14.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	69	ILE	VAL	CONFLICT	UNP Q72I14

- Molecule 10 is a protein called 50S ribosomal protein L15.

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

- Molecule 11 is a protein called 50S ribosomal protein L16.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	32	TYR	PHE	CONFLICT	UNP Q72I11

- Molecule 12 is a protein called 50S ribosomal protein L17.

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

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	S	99	Total	C	N	O		0	0	0
			775	488	155	132				

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	138	Total	C	N	O	S	0	0	0
			1147	713	235	198	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	123	GLN	LYS	CONFLICT	UNP Q72JU9
T	135	ALA	VAL	CONFLICT	UNP Q72JU9

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 16 is a protein called 50S ribosomal protein L21.

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

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	W	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	93	Total	C	N	O	S	0	0	0
			734	477	132	125				

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Y	107	Total	C	N	O	S	0	0	0
			818	524	155	134	5			

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	Z	185	Total	C	N	O	S	0	0	0
			1473	939	262	270	2			

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	11	ARG	LYS	CONFLICT	UNP Q72HR3

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	1	93	Total	C	N	O	S	0	0	0
			732	460	145	126	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	81	LYS	ARG	CONFLICT	UNP Q72G84

- Molecule 23 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	4	35	Total	C	N	O	S	0	0	0
			271	174	44	50	3			

- Molecule 24 is a protein called 50S ribosomal protein L13.

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

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	3	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	29	THR	ILE	CONFLICT	UNP P62652

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	e	102	Total	C	N	O		0	0	0
			686	430	119	137				

- Molecule 33 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	f	31	Total	C	N	O		0	0	0
			156	93	31	32				
33	g	31	Total	C	N	O		0	0	0
			156	93	31	32				

- Molecule 34 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
34	h	30	Total	C	N	O	0	0	0
			151	90	30	31			

- Molecule 35 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 36 is a RNA chain called 23S ribosomal RNA.

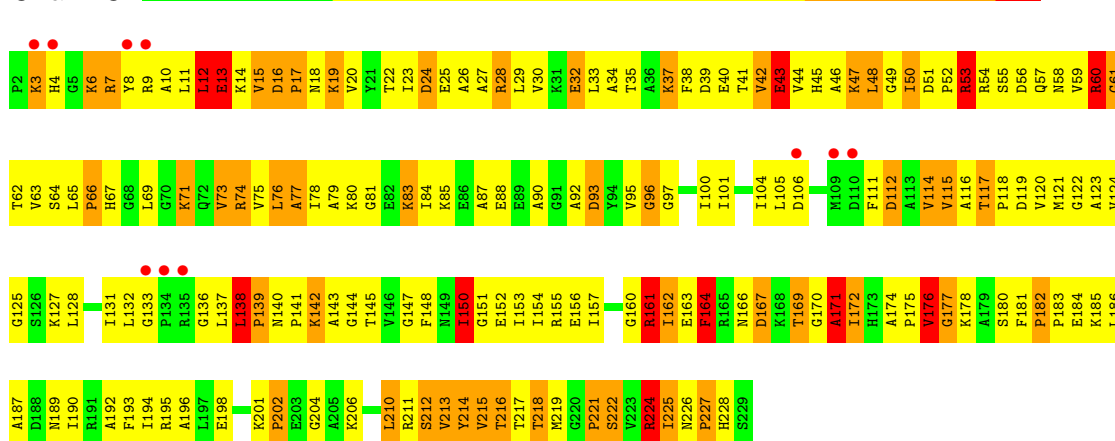
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	A	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			

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.

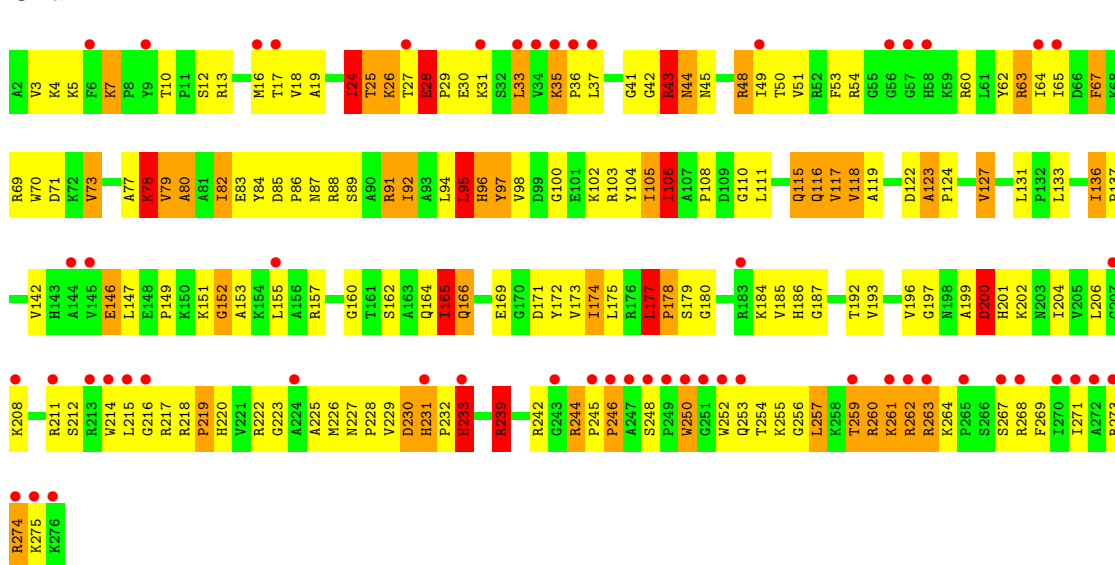
• Molecule 1: 50S ribosomal protein L1

Chain C:



• Molecule 2: 50S ribosomal protein L2

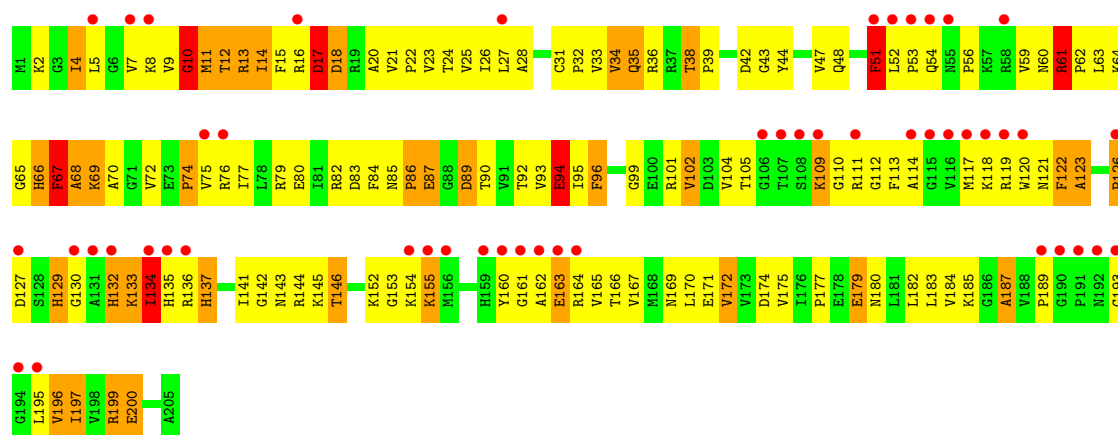
Chain D:



• Molecule 3: 50S ribosomal protein L3

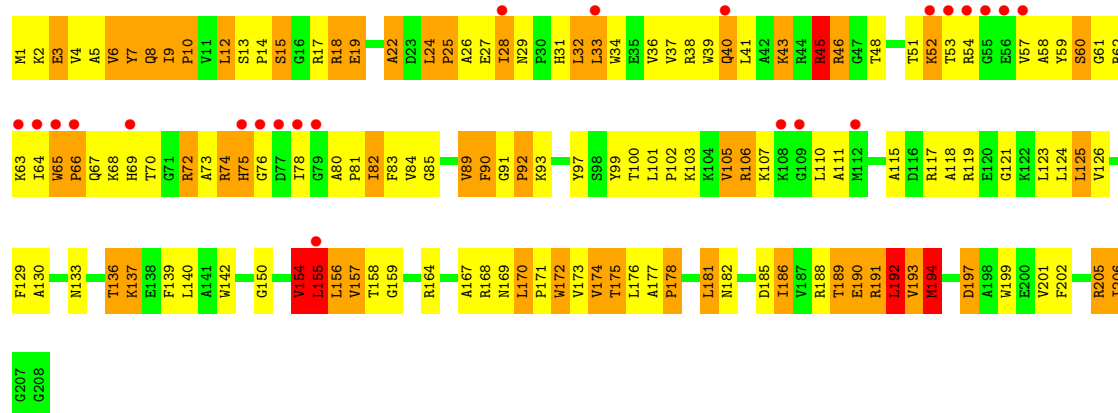
Chain E:





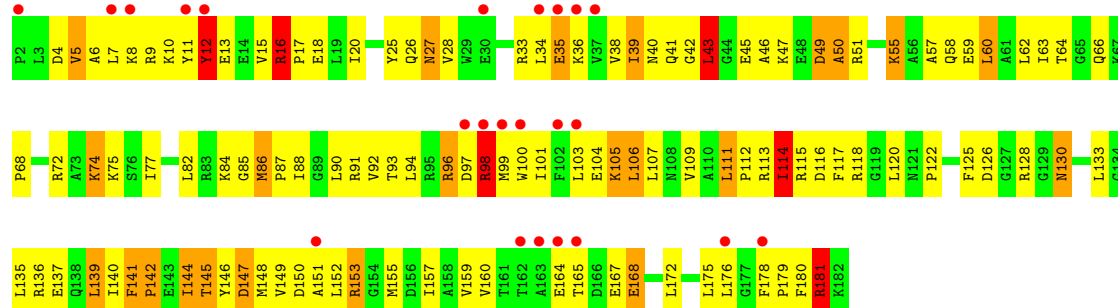
• Molecule 4: 50S ribosomal protein L4

Chain F:



• Molecule 5: 50S ribosomal protein L5

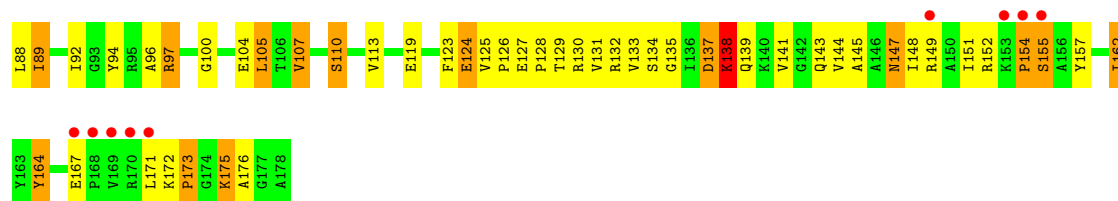
Chain G:



• Molecule 6: 50S ribosomal protein L6

Chain H:





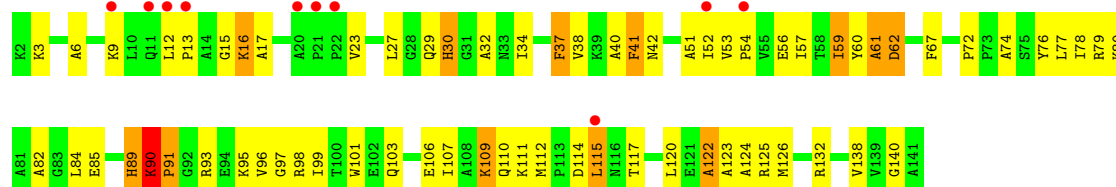
- Molecule 7: 50S ribosomal protein L10

Chain J:



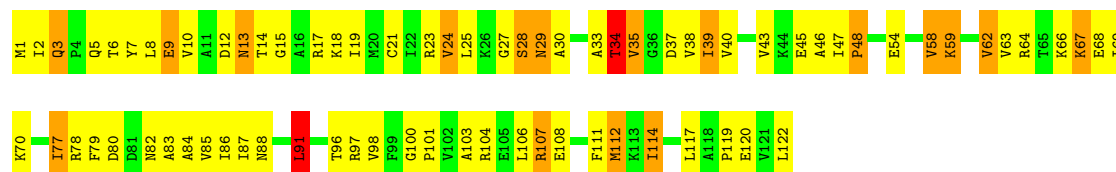
- Molecule 8: 50S ribosomal protein L11

Chain K:



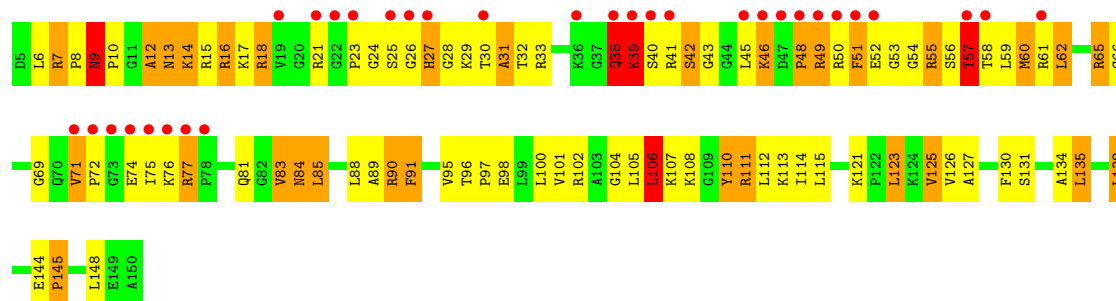
- Molecule 9: 50S ribosomal protein L14

Chain O:



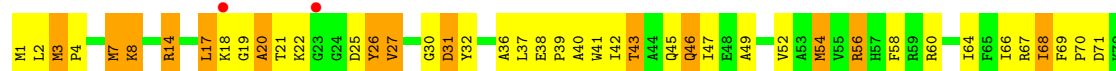
- Molecule 10: 50S ribosomal protein L15

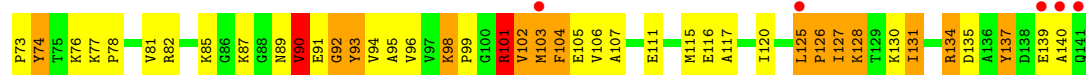
Chain P:



- Molecule 11: 50S ribosomal protein L16

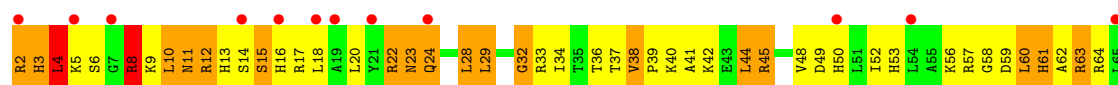
Chain Q:





• Molecule 12: 50S ribosomal protein L17

Chain R:



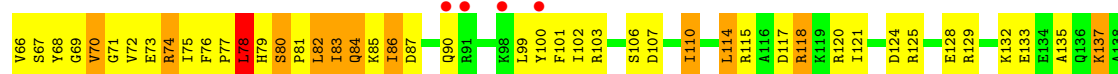
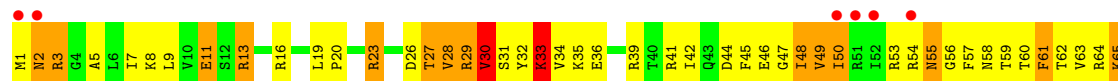
• Molecule 13: 50S ribosomal protein L18

Chain S:



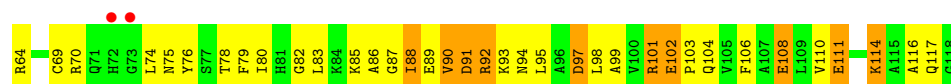
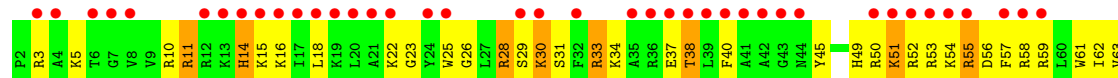
• Molecule 14: 50S ribosomal protein L19

Chain T:



• Molecule 15: 50S ribosomal protein L20

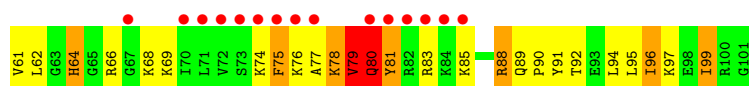
Chain U:



• Molecule 16: 50S ribosomal protein L21

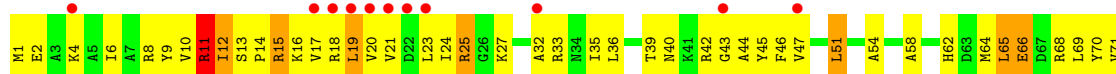
Chain V:





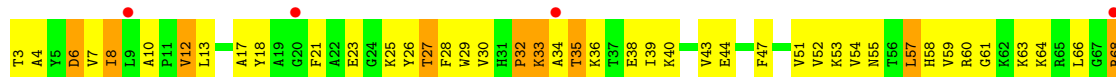
• Molecule 17: 50S ribosomal protein L22

Chain W:



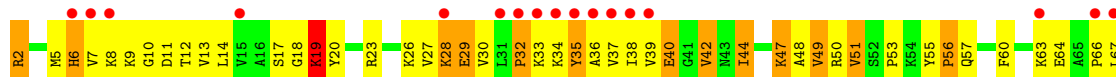
• Molecule 18: 50S ribosomal protein L23

Chain X:



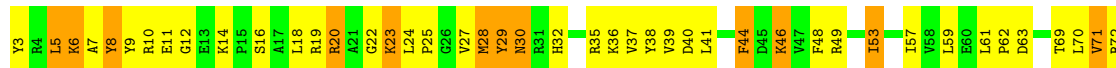
• Molecule 19: 50S ribosomal protein L24

Chain Y:



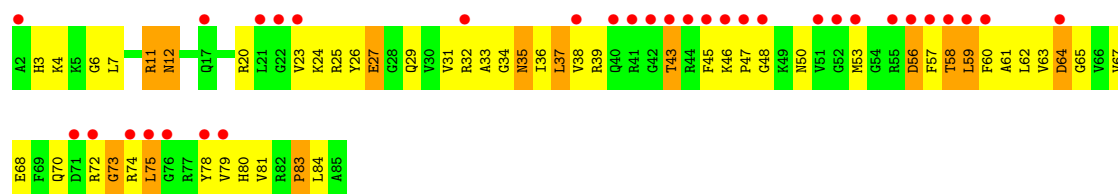
• Molecule 20: 50S ribosomal protein L25

Chain Z:



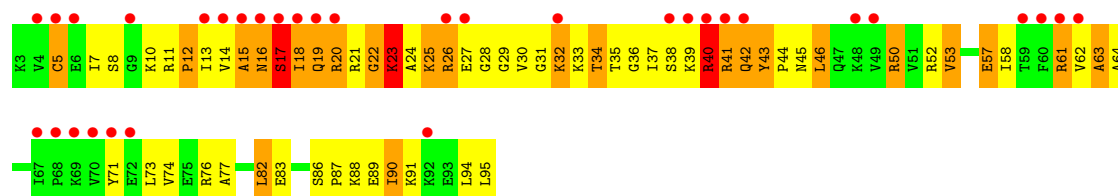
• Molecule 21: 50S ribosomal protein L27

Chain 0:



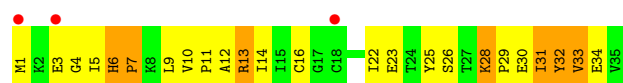
- Molecule 22: 50S ribosomal protein L28

Chain 1:



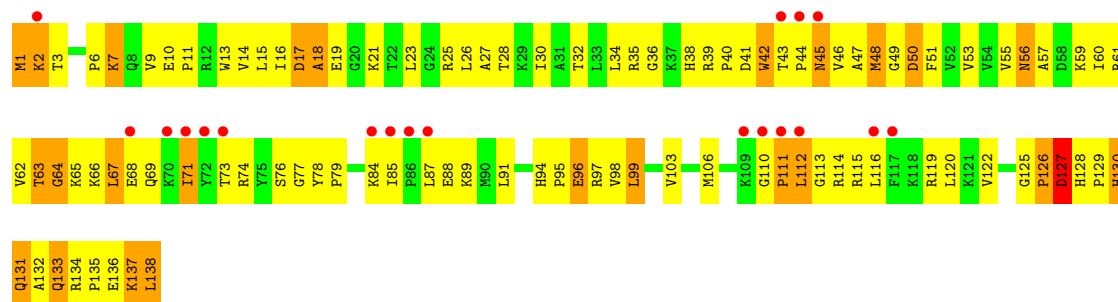
- Molecule 23: 50S ribosomal protein L31

Chain 4:



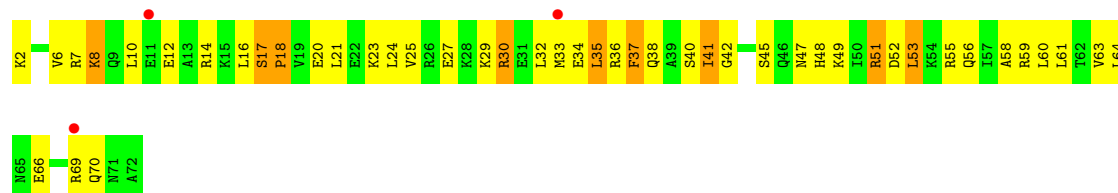
- Molecule 24: 50S ribosomal protein L13

Chain N:



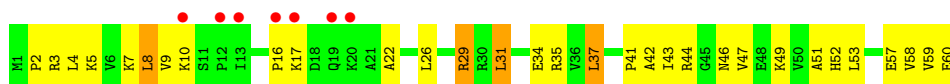
- Molecule 25: 50S ribosomal protein L29

Chain 2:



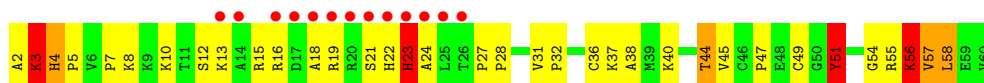
- Molecule 26: 50S ribosomal protein L30

Chain 3:



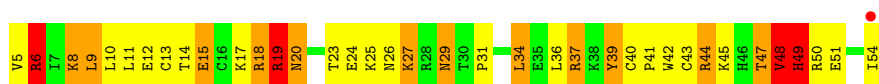
- Molecule 27: 50S ribosomal protein L32

Chain 5:



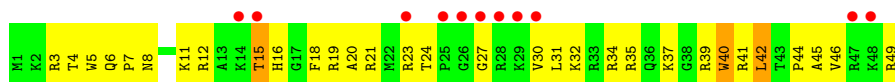
- Molecule 28: 50S ribosomal protein L33

Chain 6:



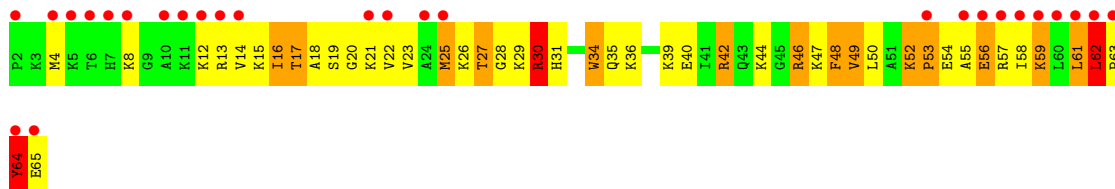
- Molecule 29: 50S ribosomal protein L34

Chain 7:



- Molecule 30: 50S ribosomal protein L35

Chain 8:



- Molecule 31: 50S ribosomal protein L36

Chain 9:



- Molecule 32: 50S ribosomal protein L7/L12

Chain e:



- Molecule 33: 50S ribosomal protein L7/L12

Chain f:

There are no outlier residues recorded for this chain.

- Molecule 33: 50S ribosomal protein L7/L12

Chain g: 

There are no outlier residues recorded for this chain.

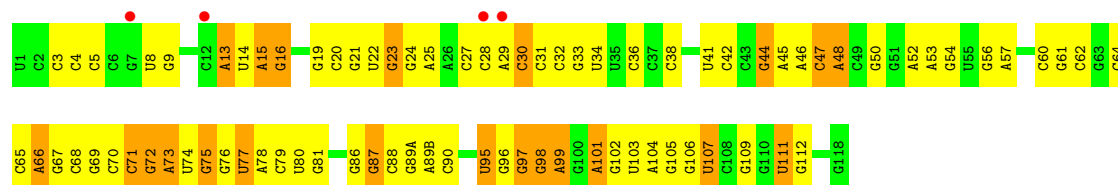
- Molecule 34: 50S ribosomal protein L7/L12

Chain h: 

There are no outlier residues recorded for this chain.

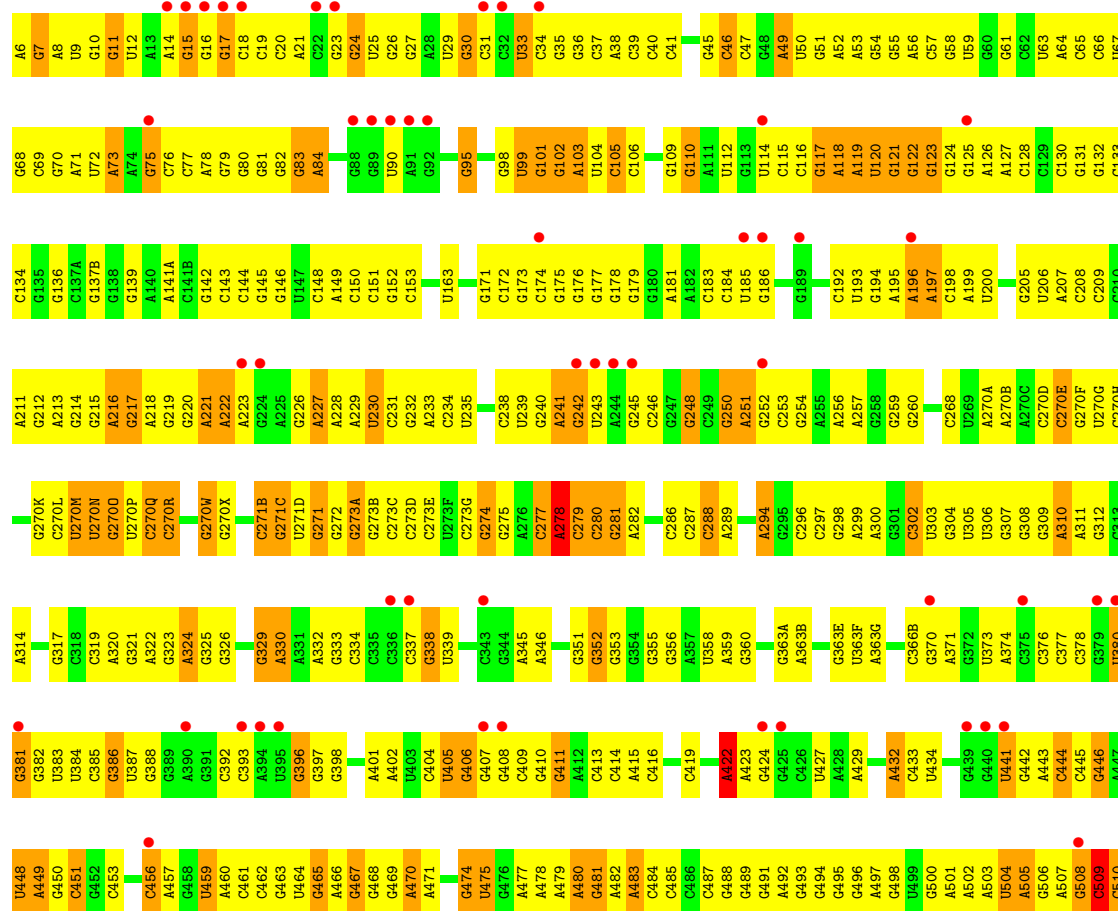
- Molecule 35: 5S ribosomal RNA

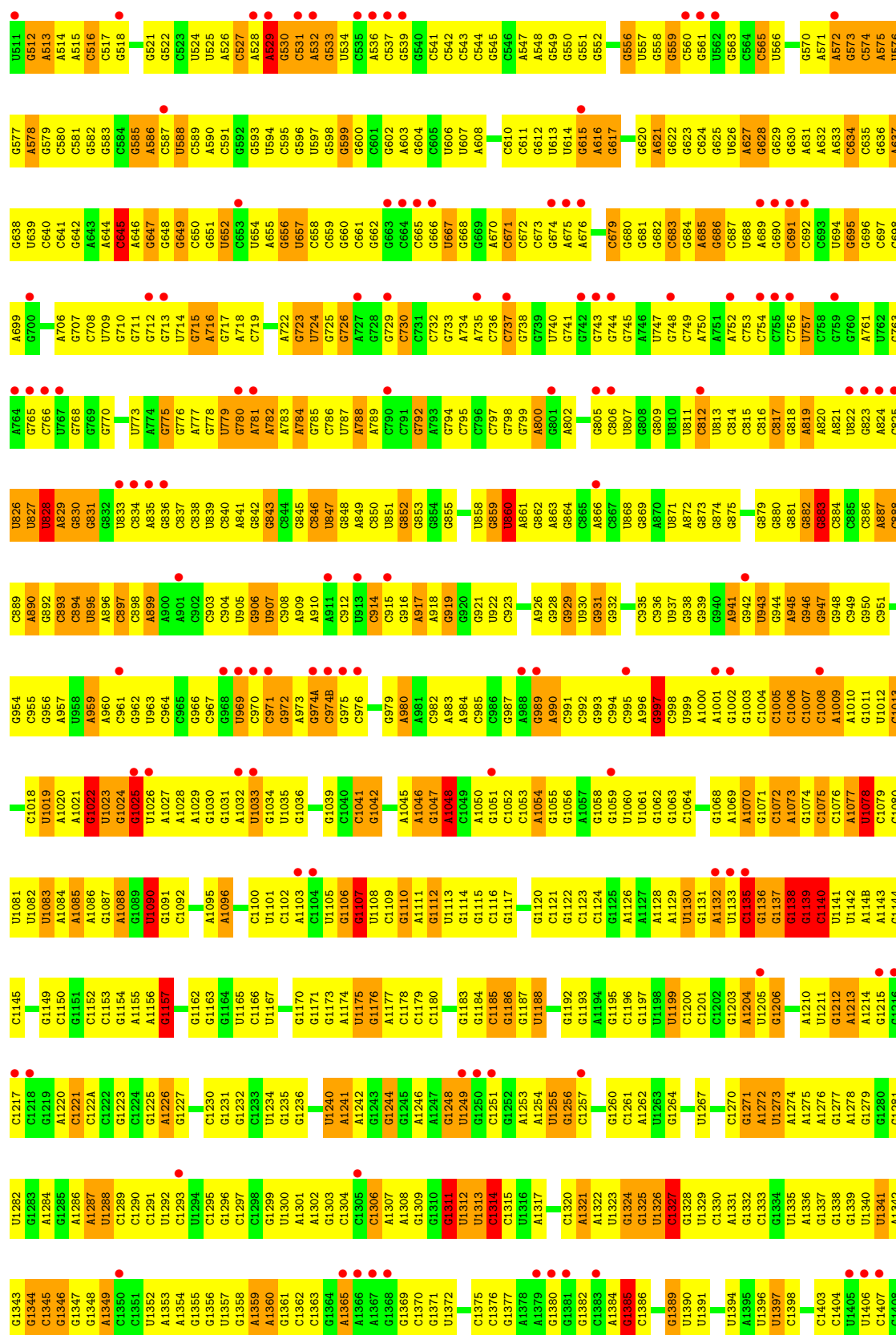
Chain B: 



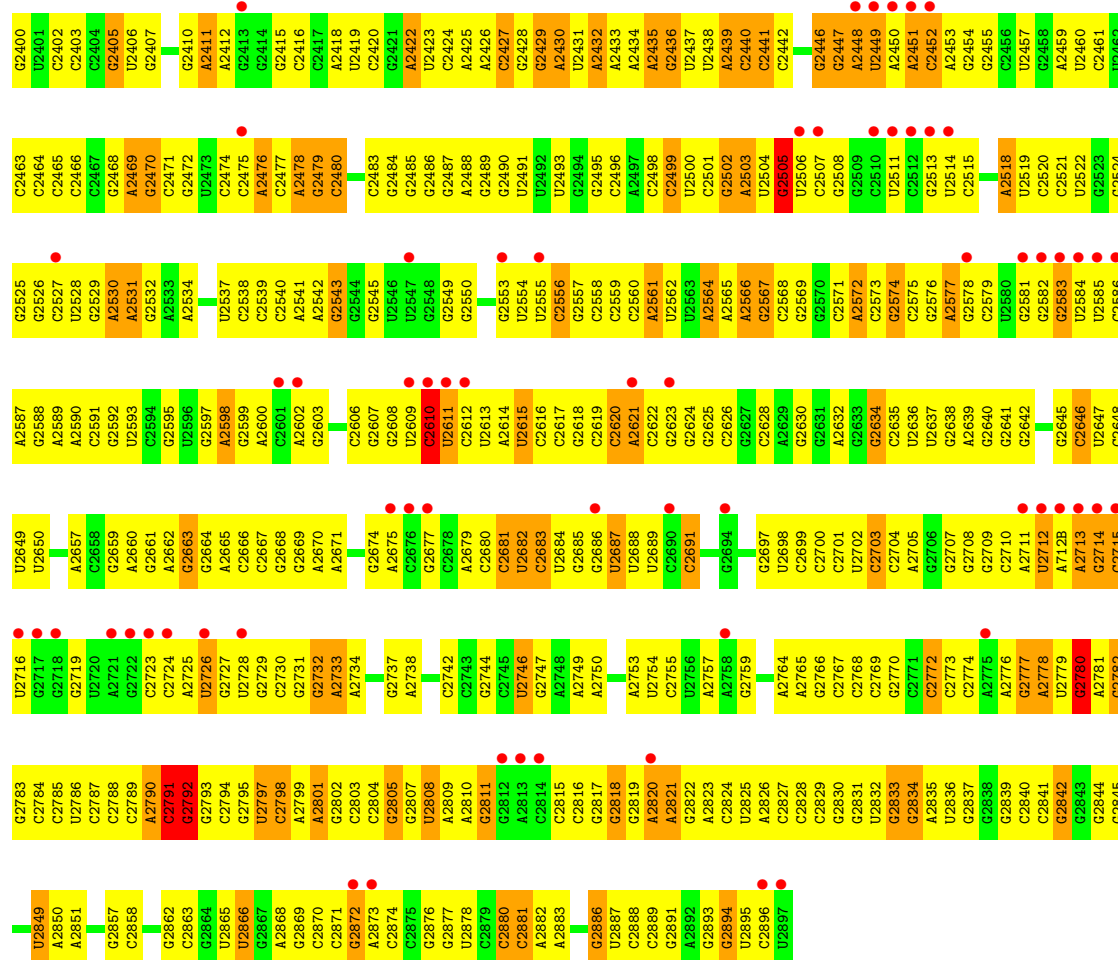
- Molecule 36: 23S ribosomal RNA

Chain A: 









4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	302.39Å 683.92Å 356.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.86 182.04 – 3.87	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.86) 64.4 (182.04-3.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.34	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 3.89Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.264 , 0.317 0.334 , 0.334	Depositor DCC
R_{free} test set	21649 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	76.3	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 459.4	EDS
Estimated twinning fraction	0.320 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.24$, $\langle L^2 \rangle = 0.09$	Xtriage
Outliers	0 of 432130 reflections	Xtriage
F_o, F_c correlation	0.59	EDS
Total number of atoms	95124	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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	C	0.52	0/1774	0.84	3/2391 (0.1%)
2	D	0.34	0/2195	0.65	2/2955 (0.1%)
3	E	0.37	0/1602	0.68	2/2160 (0.1%)
4	F	0.47	1/1663 (0.1%)	0.87	6/2249 (0.3%)
5	G	0.42	1/1499 (0.1%)	1.33	5/2016 (0.2%)
6	H	0.30	0/1298	0.56	0/1751
8	K	0.28	0/1054	0.55	0/1427
9	O	0.29	0/943	0.58	0/1269
10	P	0.32	0/1131	0.68	0/1504
11	Q	0.33	0/1143	0.60	0/1527
12	R	0.31	0/974	0.63	0/1302
13	S	0.36	0/783	0.69	0/1041
14	T	0.34	0/1161	0.67	0/1549
15	U	0.38	0/982	0.59	0/1306
16	V	0.38	0/790	0.73	0/1057
17	W	0.35	0/911	0.66	2/1220 (0.2%)
18	X	0.31	0/748	0.57	0/1004
19	Y	0.32	0/831	0.61	0/1108
20	Z	0.30	0/1505	0.60	0/2042
21	0	0.27	0/671	0.54	0/892
22	1	0.48	0/739	0.77	2/981 (0.2%)
23	4	0.40	0/276	0.62	0/372
24	N	0.34	0/1131	0.66	0/1525
25	2	0.36	0/600	0.62	0/793
26	3	0.29	0/482	0.53	0/646
27	5	0.33	0/473	0.65	0/639
28	6	0.32	0/440	0.67	0/586
29	7	0.31	0/438	0.56	0/575
30	8	0.33	0/525	0.66	0/691
31	9	0.43	0/310	0.69	0/407
32	e	0.33	0/538	0.56	0/715
35	B	0.39	0/2853	1.12	15/4451 (0.3%)
36	A	0.39	0/69437	1.09	229/108401 (0.2%)
All	All	0.38	2/101900 (0.0%)	1.01	266/152552 (0.2%)

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	C	0	5
2	D	0	2
4	F	0	1
5	G	0	2
7	J	0	1
13	S	0	3
17	W	0	1
22	1	0	2
All	All	0	17

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	114	ILE	C-N	10.70	1.58	1.34
4	F	157	VAL	CB-CG1	-5.60	1.41	1.52

The worst 5 of 266 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	114	ILE	O-C-N	-51.93	39.62	122.70
36	A	1006	C	C6-N1-C2	-15.70	114.02	120.30
36	A	1006	C	N3-C2-O2	-13.26	112.62	121.90
36	A	2505	G	N1-C6-O6	12.54	127.43	119.90
36	A	1006	C	N1-C2-O2	10.83	125.40	118.90

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	161	ARG	Peptide
1	C	171	ALA	Peptide
1	C	210	LEU	Peptide
1	C	211	ARG	Peptide
1	C	213	VAL	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	C	1742	0	1798	177	0
2	D	2145	0	2234	170	0
3	E	1569	0	1634	145	0
4	F	1628	0	1680	174	0
5	G	1474	0	1535	88	0
6	H	1274	0	1342	63	0
7	J	851	0	199	35	0
8	K	1035	0	1082	48	0
9	O	933	0	996	64	0
10	P	1114	0	1187	85	0
11	Q	1122	0	1179	67	0
12	R	960	0	1021	84	0
13	S	775	0	835	66	0
14	T	1147	0	1207	99	0
15	U	964	0	1022	86	0
16	V	779	0	852	63	0
17	W	900	0	964	57	0
18	X	734	0	789	41	0
19	Y	818	0	908	45	0
20	Z	1473	0	1497	66	0
21	0	662	0	688	44	0
22	1	732	0	808	76	0
23	4	271	0	284	17	0
24	N	1104	0	1180	201	0
25	2	598	0	653	34	0
26	3	477	0	529	20	0
27	5	459	0	477	32	0
28	6	433	0	461	37	0
29	7	430	0	480	38	0
30	8	517	0	582	46	0
31	9	307	0	336	21	0
32	e	686	0	620	0	0
33	f	156	0	37	0	0
33	g	156	0	39	0	0
34	h	151	0	39	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	B	2551	0	1295	93	0
36	A	61997	0	31250	2233	0
All	All	95124	0	63719	4122	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 26.

The worst 5 of 4122 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:U:64:ARG:CD	24:N:41:ASP:HA	1.32	1.57
15:U:64:ARG:HD2	24:N:41:ASP:CA	1.37	1.49
36:A:2681:C:N4	36:A:2725:A:H62	1.23	1.31
36:A:1311:G:N2	36:A:1603:A:H62	1.27	1.28
24:N:78:TYR:CD2	36:A:2642:G:C5'	2.17	1.27

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	C	226/228 (99%)	109 (48%)	65 (29%)	52 (23%)	0	2
2	D	273/275 (99%)	177 (65%)	66 (24%)	30 (11%)	1	17
3	E	203/205 (99%)	123 (61%)	50 (25%)	30 (15%)	0	9
4	F	206/208 (99%)	130 (63%)	47 (23%)	29 (14%)	0	10
5	G	179/181 (99%)	116 (65%)	45 (25%)	18 (10%)	1	20
6	H	165/167 (99%)	115 (70%)	35 (21%)	15 (9%)	1	25
8	K	138/140 (99%)	97 (70%)	28 (20%)	13 (9%)	1	23
9	O	120/122 (98%)	88 (73%)	25 (21%)	7 (6%)	3	39
10	P	144/146 (99%)	82 (57%)	41 (28%)	21 (15%)	0	9
11	Q	139/141 (99%)	93 (67%)	32 (23%)	14 (10%)	1	20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	R	115/117 (98%)	72 (63%)	28 (24%)	15 (13%)	0	13
13	S	97/99 (98%)	54 (56%)	22 (23%)	21 (22%)	0	3
14	T	136/138 (99%)	84 (62%)	33 (24%)	19 (14%)	0	10
15	U	115/117 (98%)	89 (77%)	21 (18%)	5 (4%)	4	48
16	V	99/101 (98%)	59 (60%)	22 (22%)	18 (18%)	0	5
17	W	111/113 (98%)	88 (79%)	16 (14%)	7 (6%)	2	37
18	X	91/93 (98%)	71 (78%)	12 (13%)	8 (9%)	1	25
19	Y	105/107 (98%)	48 (46%)	33 (31%)	24 (23%)	0	2
20	Z	183/185 (99%)	126 (69%)	42 (23%)	15 (8%)	1	27
21	0	82/84 (98%)	59 (72%)	15 (18%)	8 (10%)	1	21
22	1	91/93 (98%)	55 (60%)	19 (21%)	17 (19%)	0	4
23	4	33/35 (94%)	17 (52%)	13 (39%)	3 (9%)	1	25
24	N	136/138 (99%)	95 (70%)	25 (18%)	16 (12%)	1	15
25	2	69/71 (97%)	52 (75%)	13 (19%)	4 (6%)	3	39
26	3	58/60 (97%)	48 (83%)	7 (12%)	3 (5%)	3	42
27	5	57/59 (97%)	37 (65%)	10 (18%)	10 (18%)	0	5
28	6	48/50 (96%)	26 (54%)	11 (23%)	11 (23%)	0	2
29	7	47/49 (96%)	32 (68%)	11 (23%)	4 (8%)	1	26
30	8	62/64 (97%)	38 (61%)	18 (29%)	6 (10%)	1	21
31	9	35/37 (95%)	16 (46%)	14 (40%)	5 (14%)	0	10
32	e	70/103 (68%)	38 (54%)	25 (36%)	7 (10%)	1	20
All	All	3633/3726 (98%)	2334 (64%)	844 (23%)	455 (12%)	1	14

5 of 455 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	17	PRO
1	C	52	PRO
1	C	57	GLN
1	C	66	PRO
1	C	80	LYS

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	C	180/180 (100%)	138 (77%)	42 (23%)	1	9
2	D	217/217 (100%)	164 (76%)	53 (24%)	1	8
3	E	165/165 (100%)	131 (79%)	34 (21%)	2	13
4	F	165/165 (100%)	127 (77%)	38 (23%)	1	10
5	G	155/155 (100%)	118 (76%)	37 (24%)	1	9
6	H	136/136 (100%)	109 (80%)	27 (20%)	2	15
8	K	105/105 (100%)	94 (90%)	11 (10%)	10	49
9	O	100/100 (100%)	80 (80%)	20 (20%)	2	15
10	P	112/112 (100%)	80 (71%)	32 (29%)	0	5
11	Q	111/111 (100%)	81 (73%)	30 (27%)	1	7
12	R	100/100 (100%)	72 (72%)	28 (28%)	0	6
13	S	77/77 (100%)	55 (71%)	22 (29%)	0	5
14	T	120/120 (100%)	99 (82%)	21 (18%)	3	21
15	U	93/93 (100%)	77 (83%)	16 (17%)	3	22
16	V	82/82 (100%)	61 (74%)	21 (26%)	1	8
17	W	92/92 (100%)	73 (79%)	19 (21%)	2	13
18	X	75/75 (100%)	59 (79%)	16 (21%)	1	12
19	Y	88/88 (100%)	69 (78%)	19 (22%)	1	11
20	Z	162/162 (100%)	129 (80%)	33 (20%)	2	14
21	0	66/66 (100%)	55 (83%)	11 (17%)	3	25
22	1	78/78 (100%)	61 (78%)	17 (22%)	1	11
23	4	31/31 (100%)	23 (74%)	8 (26%)	1	7
24	N	117/117 (100%)	100 (86%)	17 (14%)	5	32
25	2	66/66 (100%)	55 (83%)	11 (17%)	3	25
26	3	52/52 (100%)	45 (86%)	7 (14%)	6	36
27	5	51/51 (100%)	42 (82%)	9 (18%)	3	21
28	6	49/49 (100%)	36 (74%)	13 (26%)	1	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
29	7	42/42 (100%)	39 (93%)	3 (7%)	21 69
30	8	54/54 (100%)	35 (65%)	19 (35%)	0 2
31	9	34/34 (100%)	29 (85%)	5 (15%)	4 31
32	e	54/54 (100%)	47 (87%)	7 (13%)	6 38
All	All	3029/3029 (100%)	2383 (79%)	646 (21%)	1 12

5 of 646 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	P	135	LEU
13	S	47	THR
27	5	56	LYS
11	Q	26	TYR
12	R	10	LEU

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

Mol	Chain	Res	Type
5	G	130	ASN
12	R	23	ASN
28	6	20	ASN
10	P	84	ASN
12	R	13	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
35	B	118/119 (99%)	26 (22%)	2 (1%)
36	A	2878/2879 (99%)	729 (25%)	26 (0%)
All	All	2996/2998 (99%)	755 (25%)	28 (0%)

5 of 755 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
35	B	13	A
35	B	15	A
35	B	16	G
35	B	25	A
35	B	30	C

5 of 28 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	A	1154	G
36	A	1542	G
36	A	2171	A
36	A	1185	C
36	A	1240	U

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, 95th 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 ²)	Q<0.9
1	C	228/228 (100%)	-0.07	10 (4%) 33 26	77, 137, 202, 235	0
2	D	275/275 (100%)	0.83	55 (20%) 2 3	12, 58, 126, 156	0
3	E	205/205 (100%)	0.93	49 (23%) 1 2	16, 58, 123, 159	0
4	F	208/208 (100%)	0.50	23 (11%) 6 8	41, 78, 145, 195	0
5	G	181/181 (100%)	0.50	23 (12%) 4 5	24, 87, 153, 191	0
6	H	167/167 (100%)	-0.03	9 (5%) 25 20	7, 68, 133, 171	0
7	J	0/170	-	-	-	-
8	K	140/140 (100%)	0.20	10 (7%) 16 14	24, 91, 182, 225	0
9	O	122/122 (100%)	-0.16	0 100 100	24, 45, 123, 162	0
10	P	146/146 (100%)	0.74	32 (21%) 1 2	22, 76, 132, 175	0
11	Q	141/141 (100%)	0.20	7 (4%) 28 22	17, 63, 130, 200	0
12	R	117/117 (100%)	0.64	16 (13%) 4 5	15, 57, 119, 178	0
13	S	99/99 (100%)	1.46	36 (36%) 1 2	22, 104, 172, 208	0
14	T	138/138 (100%)	0.07	10 (7%) 15 14	22, 71, 133, 179	0
15	U	117/117 (100%)	1.32	42 (35%) 1 2	40, 57, 131, 184	0
16	V	101/101 (100%)	0.38	15 (14%) 3 4	13, 54, 114, 146	0
17	W	113/113 (100%)	0.74	14 (12%) 5 6	16, 55, 121, 147	0
18	X	93/93 (100%)	0.69	11 (11%) 5 7	18, 60, 114, 149	0
19	Y	107/107 (100%)	1.29	34 (31%) 1 2	8, 86, 151, 180	0
20	Z	185/185 (100%)	-0.10	5 (2%) 52 38	30, 76, 142, 176	0
21	0	84/84 (100%)	1.75	33 (39%) 1 1	18, 92, 159, 181	0
22	1	93/93 (100%)	1.80	33 (35%) 1 2	26, 91, 161, 204	0
23	4	35/35 (100%)	0.05	3 (8%) 11 11	49, 106, 171, 203	0
24	N	138/138 (100%)	0.51	19 (13%) 4 5	59, 83, 108, 111	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	2	71/71 (100%)	0.43	3 (4%) 35 26	38, 79, 143, 185	0
26	3	60/60 (100%)	0.35	7 (11%) 5 7	34, 62, 117, 150	0
27	5	59/59 (100%)	0.88	13 (22%) 1 2	26, 56, 131, 149	0
28	6	50/50 (100%)	-0.25	1 (2%) 62 45	63, 99, 159, 175	0
29	7	49/49 (100%)	1.11	11 (22%) 1 2	18, 47, 122, 156	0
30	8	64/64 (100%)	1.77	27 (42%) 1 1	29, 63, 152, 160	0
31	9	37/37 (100%)	3.18	20 (54%) 0 1	71, 109, 177, 183	0
32	e	72/103 (69%)	-0.53	0 100 100	40, 109, 188, 239	0
33	f	0/31	-	-	-	-
33	g	0/31	-	-	-	-
34	h	0/30	-	-	-	-
35	B	119/119 (100%)	-0.05	4 (3%) 43 32	27, 111, 173, 187	0
36	A	2879/2879 (100%)	0.41	326 (11%) 6 7	7, 78, 171, 308	0
All	All	6693/6986 (95%)	0.50	901 (13%) 4 5	7, 79, 162, 308	0

The worst 5 of 901 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	A	2585	U	16.1
21	0	43	THR	11.6
31	9	14	CYS	11.3
31	9	27	CYS	11.3
31	9	28	GLU	10.5

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.