



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 06:21 PM GMT

PDB ID : 4KBW
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 B. The full asymmetric unit also contains PDB entries 4KBV (30S subunit B), 4KBT (30S subunit A), and 4KBU (50S subunit A).
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>

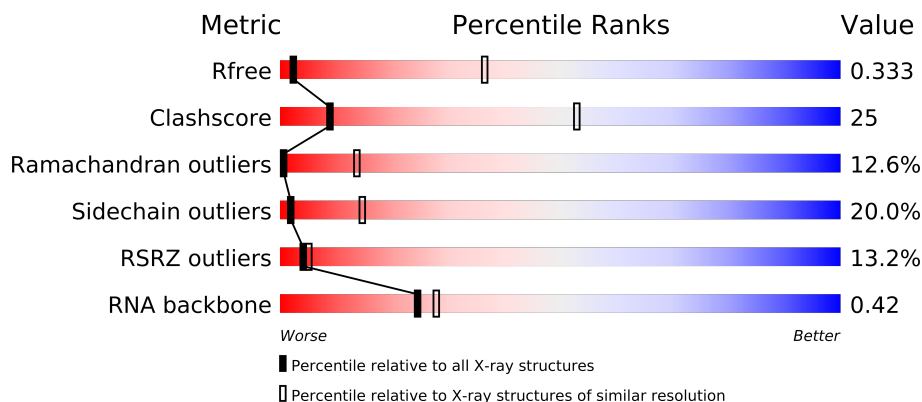
The following versions of software and data (see [references](#)) were used in the production of this report:

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	

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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

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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		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			

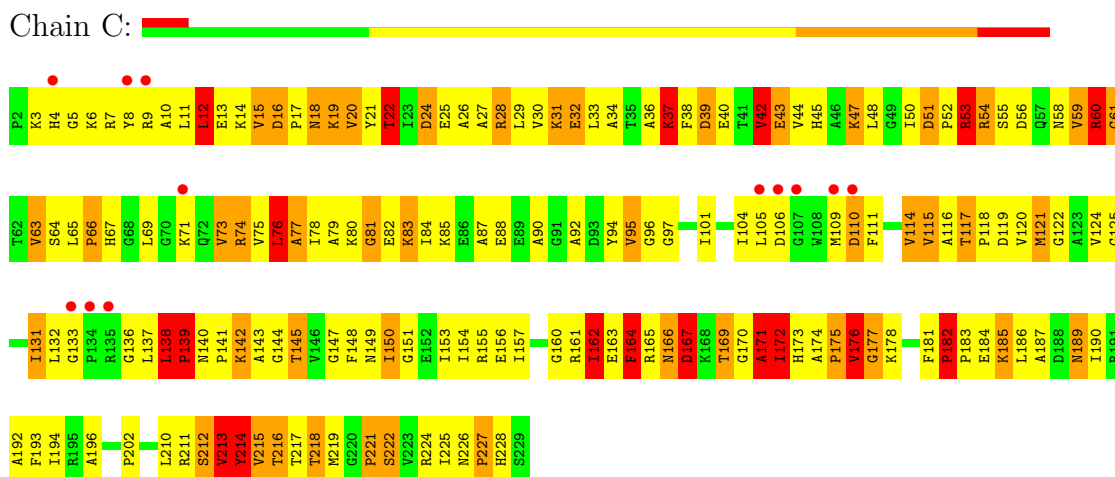
- Molecule 36 is a RNA chain called 23S ribosomal RNA.

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

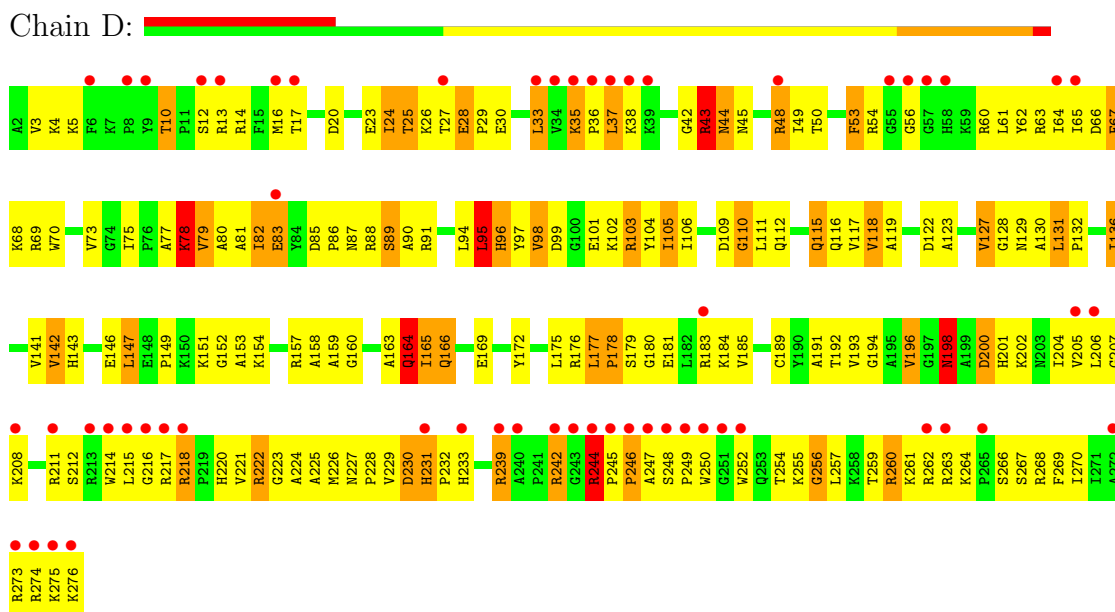
3 Residue-property plots

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

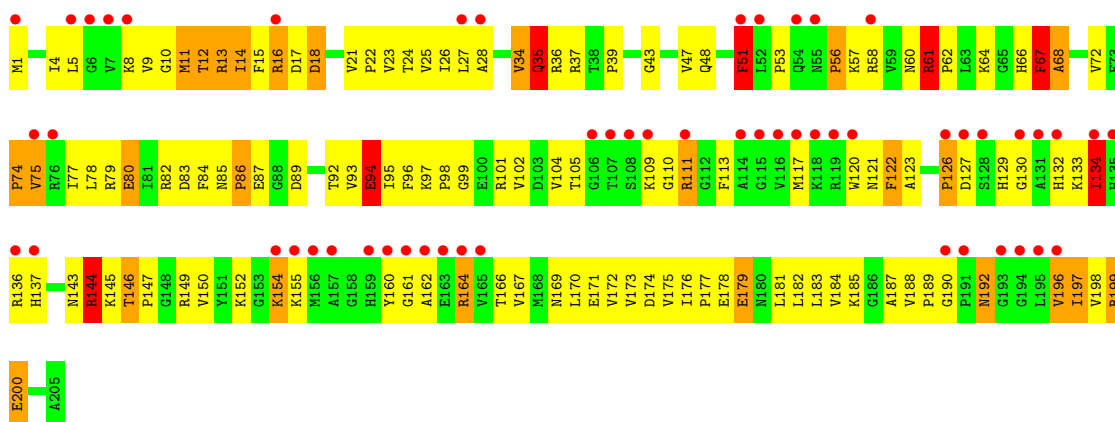


• Molecule 2: 50S ribosomal protein L2



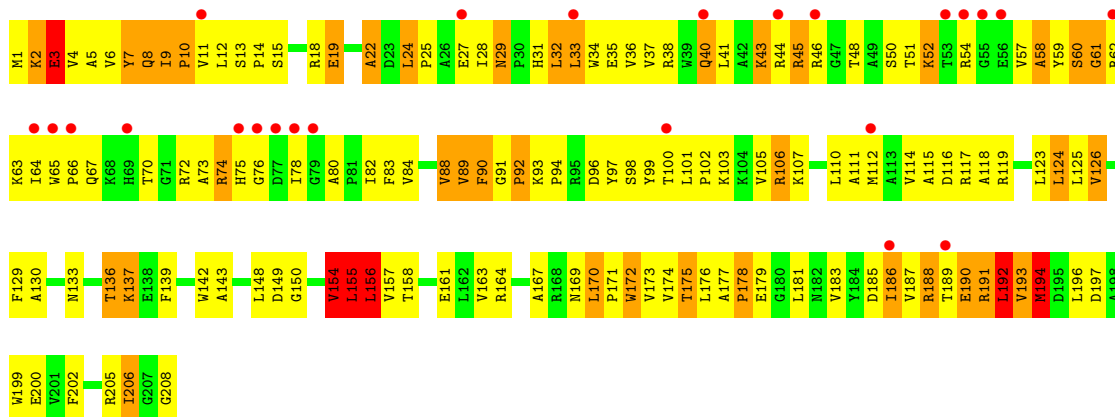
• Molecule 3: 50S ribosomal protein L3





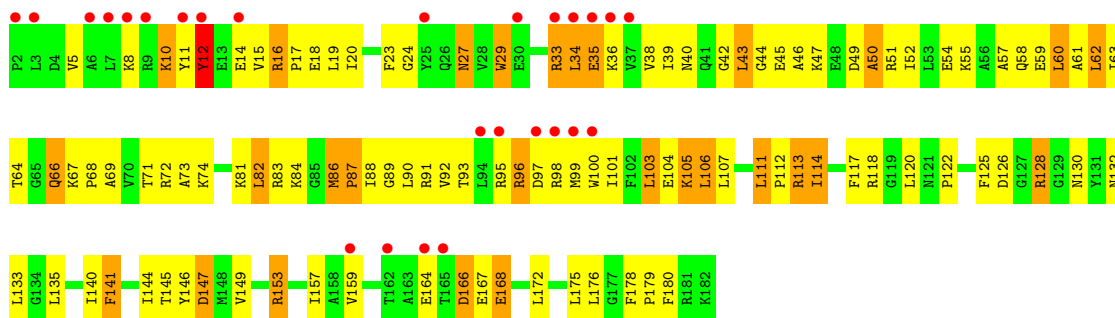
• Molecule 4: 50S ribosomal protein L4

Chain F:



• Molecule 5: 50S ribosomal protein L5

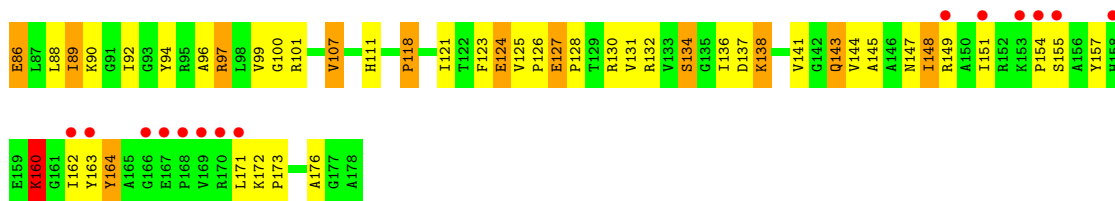
Chain G:



• Molecule 6: 50S ribosomal protein L6

Chain H:





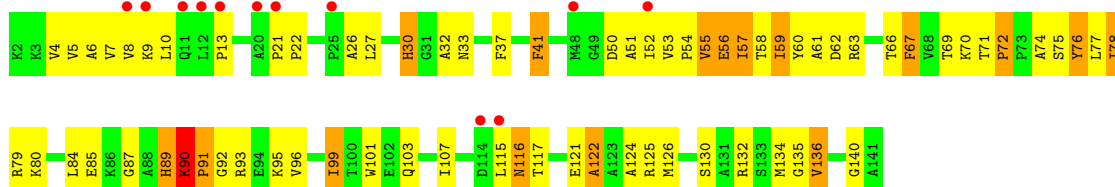
• Molecule 7: 50S ribosomal protein L10

Chain J:



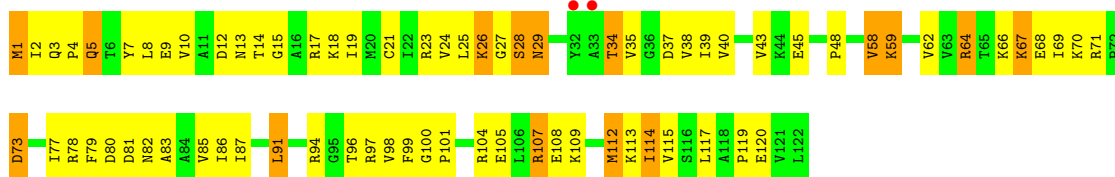
• Molecule 8: 50S ribosomal protein L11

Chain K:



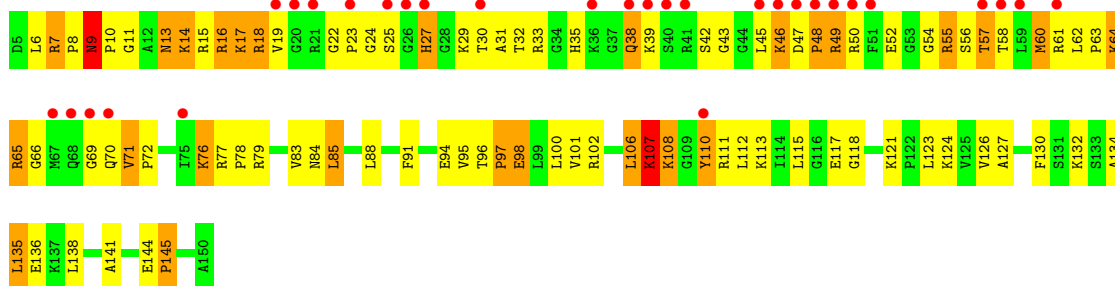
• Molecule 9: 50S ribosomal protein L14

Chain O:



• Molecule 10: 50S ribosomal protein L15

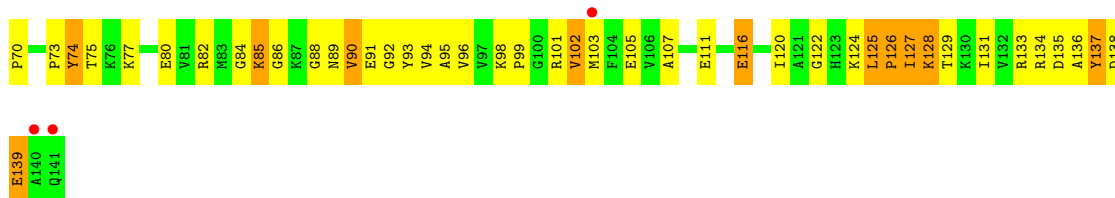
Chain P:



• Molecule 11: 50S ribosomal protein L16

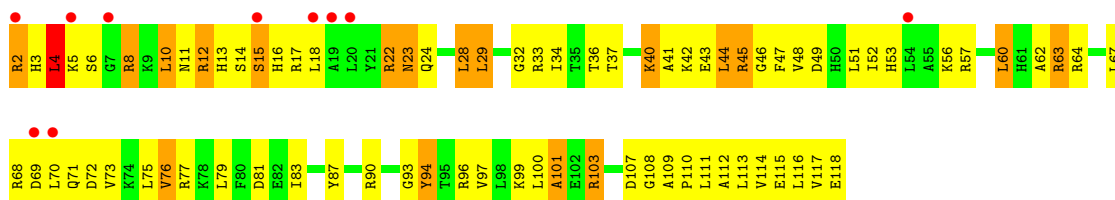
Chain Q:





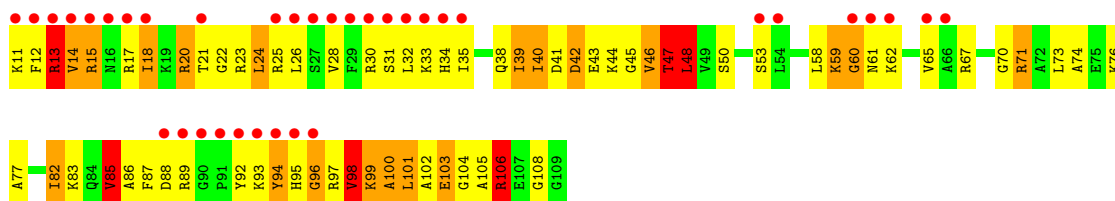
• Molecule 12: 50S ribosomal protein L17

Chain R:



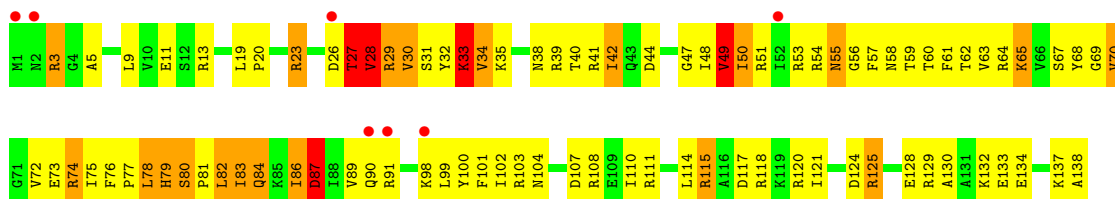
• Molecule 13: 50S ribosomal protein L18

Chain S:



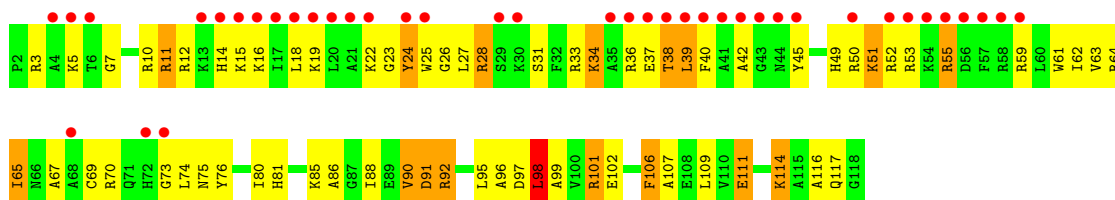
• Molecule 14: 50S ribosomal protein L19

Chain T:



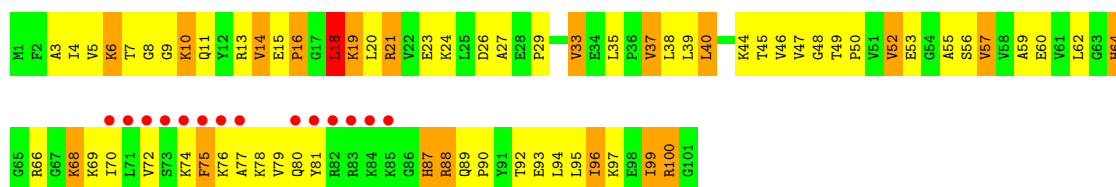
• Molecule 15: 50S ribosomal protein L20

Chain U:



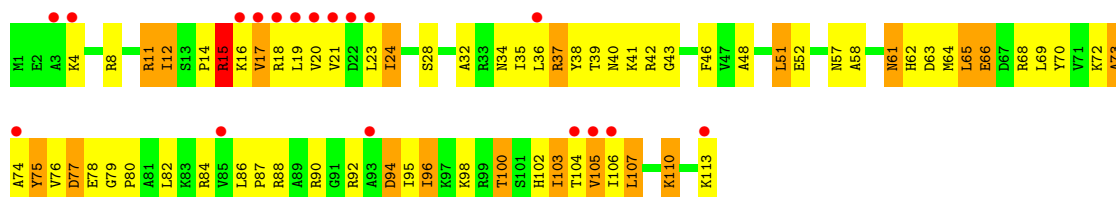
• Molecule 16: 50S ribosomal protein L21

Chain V:



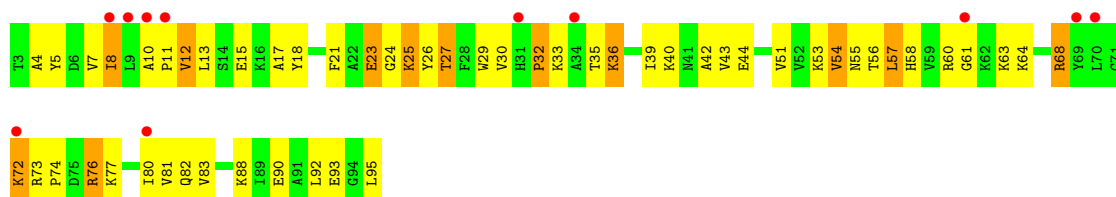
• Molecule 17: 50S ribosomal protein L22

Chain W:



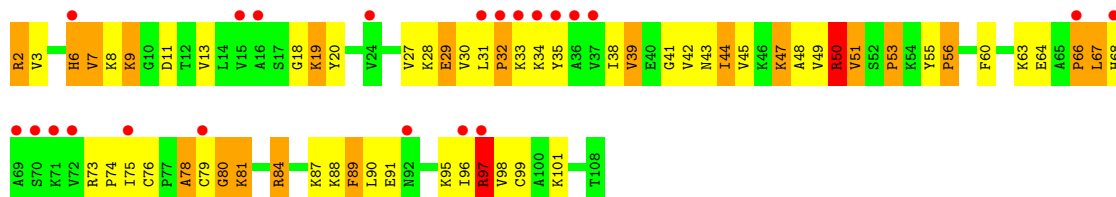
• Molecule 18: 50S ribosomal protein L23

Chain X:



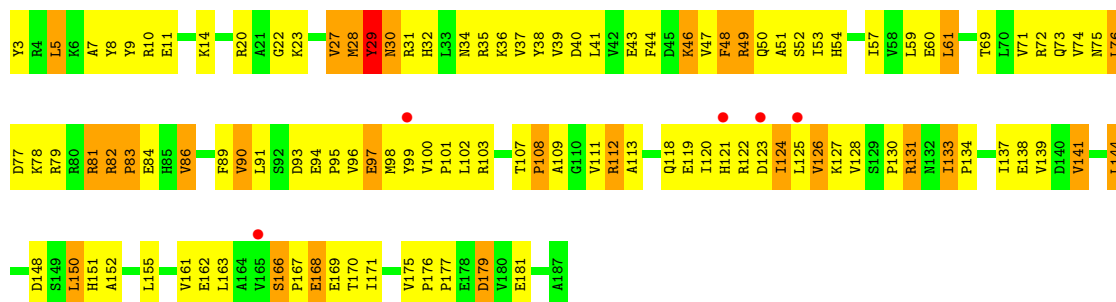
• Molecule 19: 50S ribosomal protein L24

Chain Y:



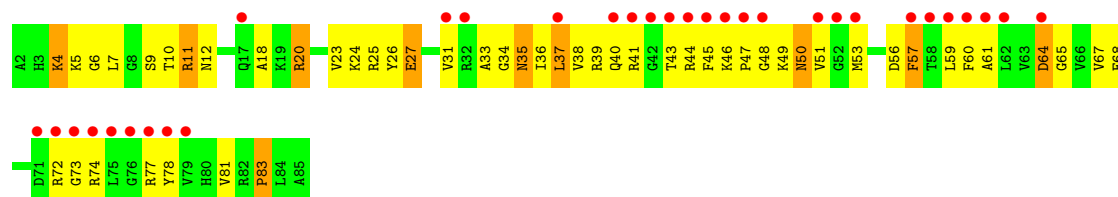
• Molecule 20: 50S ribosomal protein L25

Chain Z:



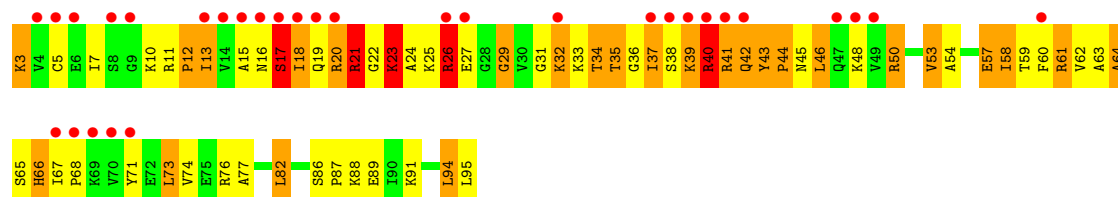
• Molecule 21: 50S ribosomal protein L27

Chain 0:



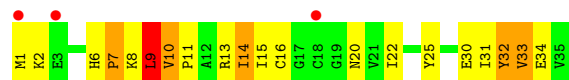
- Molecule 22: 50S ribosomal protein L28

Chain 1:



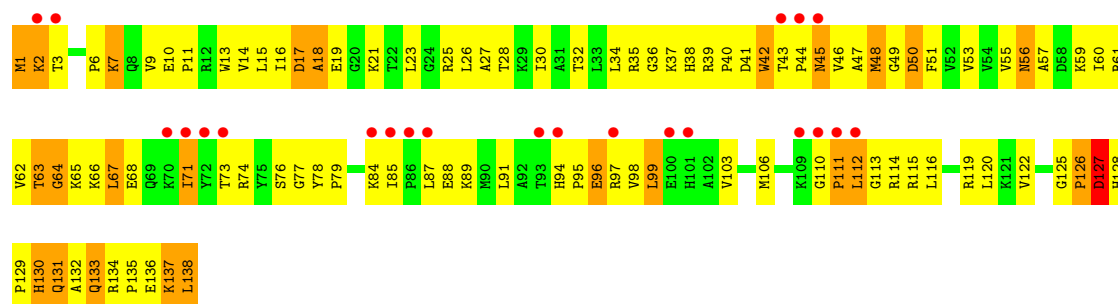
- Molecule 23: 50S ribosomal protein L31

Chain 4:



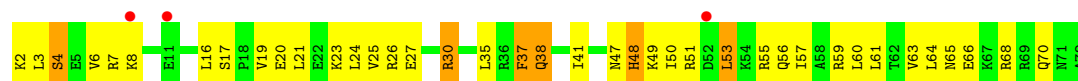
- Molecule 24: 50S ribosomal protein L13

Chain N:



- Molecule 25: 50S ribosomal protein L29

Chain 2:



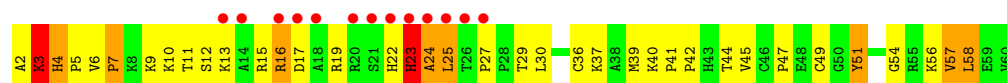
- Molecule 26: 50S ribosomal protein L30

Chain 3:



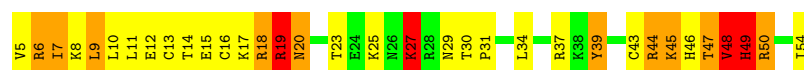
- Molecule 27: 50S ribosomal protein L32

Chain 5: 



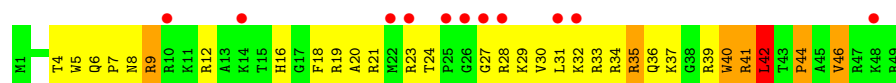
- Molecule 28: 50S ribosomal protein L33

Chain 6: 



- Molecule 29: 50S ribosomal protein L34

Chain 7: 



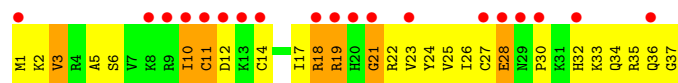
- Molecule 30: 50S ribosomal protein L35

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

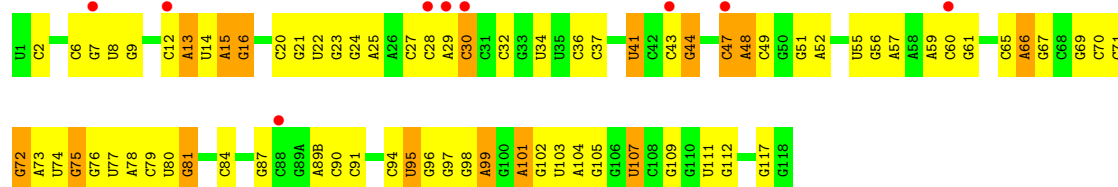
Chain h:



There are no outlier residues recorded for this chain.

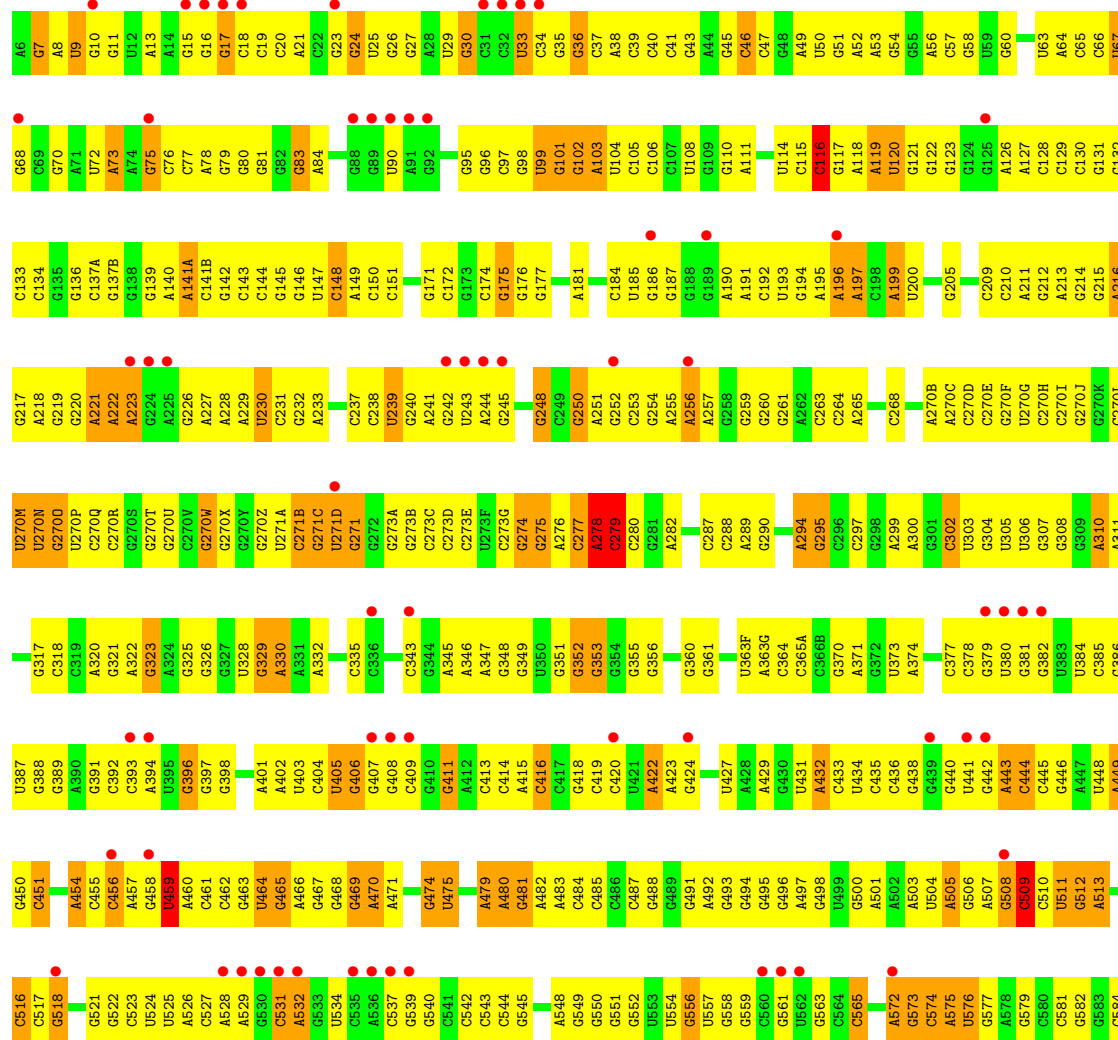
- Molecule 35: 5S ribosomal RNA

Chain B:



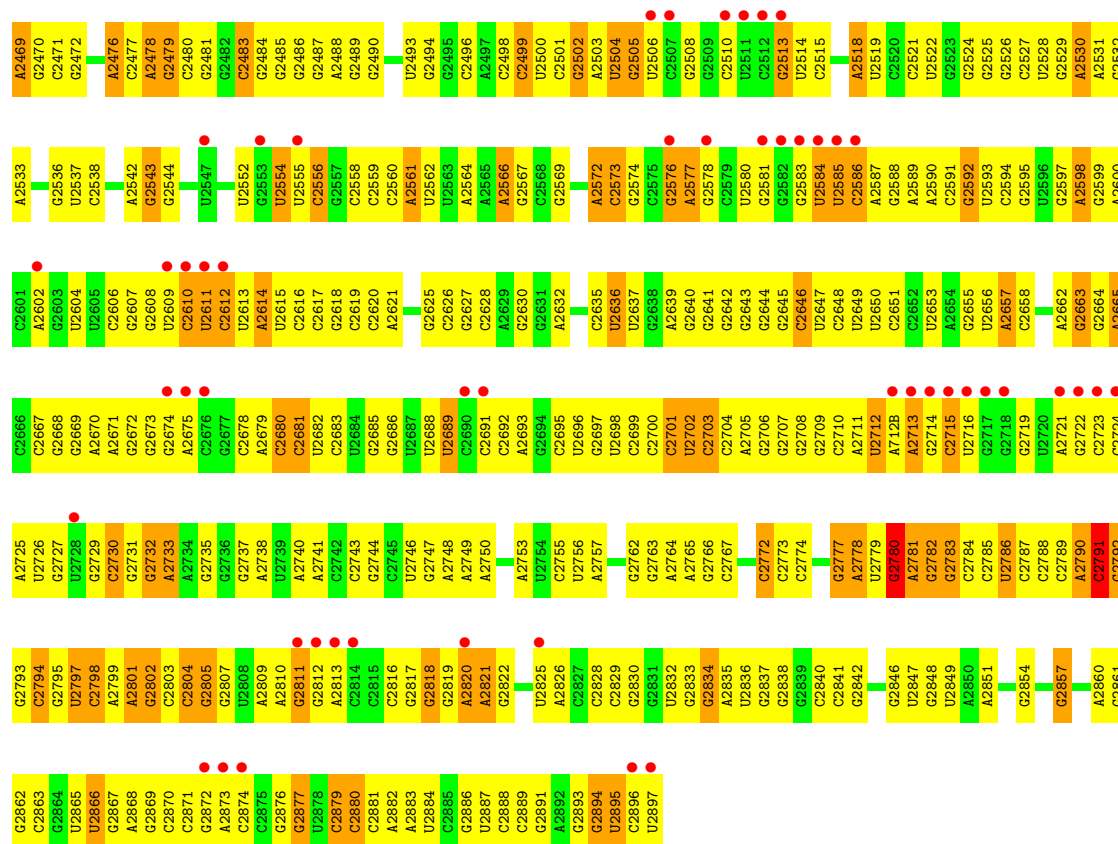
- Molecule 36: 23S ribosomal RNA

Chain A:



U1420	A1353	G1291	A1095	G1031	C970	G906	C838	G776	G710	G647	G585
G1421	A1354	U1292	A1096	A1032	C971	U907	U839	A777	G711	G648	A586
G1422	G1355	C1293	U1097	U1033	G974A	A909	C840	G779	G712	G649	C587
G1423	G1356	U1294	C1100	G1034	C974B	A908	A841	U779	G713	G650	U588
G1424	U1357	G1295	G1101	G1035	G975	A911	G843	G780	U714	U652	C589
G1425	G1358	G1232	G1102	U1036	C976	C912	C844	A781	A716	G653	A590
G1426	A1359	G1233	A1103	G1039	G977	U913	G845	A782	G717	G654	C591
A1427	A1360	U1234	U1104	U1040	G978	C914	C846	A783	G718	U594	
C1428	G1361	U1235	U1105	C1041	G979	C915	A847	A784	G719	A655	U595
G1429	G1364	A1301	U1106	G1042	A980	G916	G848	G785	C720	G656	C596
C1430	A1365	A1302	G1107	G1043	A981	A917	A849	U787		G658	U597
U1431	A1366	G1303	U1108	C1044	C982	A918	C850	A788	U724	C659	G598
A1434	A1367	C1304	C1109	A1045	A983	G919	U851	G660	G725	G660	G599
G1435	G1371	C1305	G1110	U1046	A984	U922	G852	G790	A726	G662	G600
G1436	U1372	A1306	A1111	G1047	C985	C923	G853	G791	G727	G663	C601
G1437	A1373	A1307	G1112	A1048	A988	C924	G854	G792	G728	G664	A603
G1438	G1374	G1309	U1113	C1049	G989	C925	G855	G793	G729	G665	G604
U1439	G1375	G1310	G1114	A1050	A990	A926	C856	G794	C730	G666	C605
G1440	C1376	C1311	G1115	G1051	C991	U928	U858	G795		G667	U606
G1441	U1377	U1312	C1116	A1052	A996	A933	A861	G800	G733	G672	A609A
G1442	A1378	U1313	C1117	C1052	G997	G934	G862	G796	G734	C673	G612
G1443	A1379	C1314	U1118	C1053	C998	C935	A863	G797	A734	G674	U613
G1444	G1380	G1315	G1119	A1054	G999	U930	G865	G798	A735	A675	G615
A1445	A1448	U1316	C1120	G1055	C994	G931	G866	G799	C736	G676	A616
C1446	G1381	A1254	C1121	G1056	C995	G932	G867	G800	C737	A677	G617
G1447	G1382	U1255	G1122	A1057	A996	A933	A868	G801	G738	G678	G618A
A1448	C1383	G1256	C1123	U1058	G997	G934	G869	A802	G739	G679	
A1498	A1384	C1257	U1124	G1059	C998	C935	A870	G805	G740	G674	
	G1385	U1258	G1125	U1060	U999	U936	U871	U807	G741	A676	
	G1389	G1259	A1126	U1061	A1000	G938	G872	G806	G742		
A1453	U1390	C1260	A1127	G1062	A1001	G939	A873	G807	G743		
U1454	U1391	G1261	A1128	C1063	G1002	C940	G874	U810	G744		
G1455	A1392	A1262	A1129	U1064	G1003	A941	G875	U811	G745		
	G1393	U1263	G1130	C1065	C1004	U943	G876	G882	G746		
G1459	A1394	G1328	G1131	U1066	U1005	G944	C877	G883	G747		
A1460	A1395	A1265	A1132	A1070	C1006	G944	U877	G884	G748		
G1461	U1396	G1266	U1133	G1071	C1007	A945	G880	G885	C749		
C1462	U1397	A1269	C1136	C1072	U1008	G946	G881	G886	A750		
C1463	C1398	C1270	G1137	G1073	A1009	G947	G882	G887	A751		
C1464	C1399	G1271	U1138	A1074	A1010	G948	G883	U888	A752		
G1465	G1400	A1272	G1139	C1075	G1011	C949	G884	G889	C753		
G1466	G1401	A1273	C1140	U1076	U1012	G950	G885	G890	G754		
C1467	C1402	A1274	U1141	A1077	G1013	C951	C884	G891	G755		
C1468	C1403	U1274	U1142	U1078	U1014		A821	C692	C756		
A1469	C1404	A1275	U1143	C1079	G1015	G954	U822	C893	U757		
	U1405	G1276	A1144	U1080	G1016	C955	G823	C888	G758		
A1472	U1406	G1277	U1145	U1081	G1017	G956	A824	G889	C759		
G1473	G1407	A1278	G1146	C1082	C1018	A957	C825	G890	G760		
C1474	C1408	G1280	C1147	U1083	U1019	U958	U826	G892	G761		
	C1409	U1281	C1148	A1084	A1020	A959	U827	C893	U762		
	G1410	G1282	A1149	A1085	A1021	A960	U828	C894	G763		
G1477	G1478	C1344	U1148	U1086	G1022	C961	A829	U895	G764		
G1479	G1479	C1345	G1149	G1087	U1023	G962	G830	G896	G765		
G1480	G1480	G1283	C1150	A1088	G1024	U963	G831	C897	G766		
U1481	U1481	G1285	G1151	U1089	G1025	C964	G832	C898	U767		
G1483	G1415	A1286	C1152	U1090	G1026	C965	U833	A899	G768		
	G1416	A1287	C1153	G1091	A1027	G966	C834	C835	A705		
	C1417	U1288	A1028	G1092	A1028	C967	A835	G836	A706		
A1486	G1418	C1351	A1029	G1093	A1029	U969	C904	G708	G707		
G1487		U1352	G1157	U1094	G1030		C837	U773	G774		
								G775			





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 0.332 , 0.333	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)	0.25 , 432.4	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)	88.0	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	0.55	1/1774 (0.1%)	0.93	7/2391 (0.3%)
2	D	0.34	0/2195	0.64	2/2955 (0.1%)
3	E	0.34	0/1602	0.65	1/2160 (0.0%)
4	F	0.43	0/1663	0.87	6/2249 (0.3%)
5	G	0.39	1/1499 (0.1%)	0.63	0/2016
6	H	0.30	0/1298	0.56	0/1751
8	K	0.27	0/1054	0.52	0/1427
9	O	0.29	0/943	0.55	0/1269
10	P	0.30	0/1131	0.62	0/1504
11	Q	0.32	0/1143	0.63	0/1527
12	R	0.32	0/974	0.63	0/1302
13	S	0.36	0/783	0.68	0/1041
14	T	0.32	0/1161	0.65	0/1549
15	U	0.38	0/982	0.61	0/1306
16	V	0.34	0/790	0.66	1/1057 (0.1%)
17	W	0.34	0/911	0.63	0/1220
18	X	0.29	0/748	0.55	1/1004 (0.1%)
19	Y	0.31	0/831	0.58	0/1108
20	Z	0.31	0/1505	0.60	0/2042
21	0	0.27	0/671	0.53	0/892
22	1	0.50	0/739	0.82	3/981 (0.3%)
23	4	0.36	0/276	0.59	0/372
24	N	0.34	0/1131	0.66	0/1525
25	2	0.34	0/600	0.58	0/793
26	3	0.29	0/482	0.53	0/646
27	5	0.31	0/473	0.58	0/639
28	6	0.34	0/440	0.66	0/586
29	7	0.32	0/438	0.55	0/575
30	8	0.32	0/525	0.63	0/691
31	9	0.30	0/310	0.63	0/407
32	e	0.31	0/538	0.56	0/715
35	B	0.38	0/2853	1.07	10/4451 (0.2%)
36	A	0.38	3/69437 (0.0%)	1.06	187/108401 (0.2%)
All	All	0.37	5/101900 (0.0%)	0.97	218/152552 (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	C	0	3
2	D	0	2
4	F	0	1
5	G	0	2
7	J	0	1
13	S	0	3
14	T	0	1
17	W	0	2
22	1	0	2
All	All	0	17

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	114	ILE	N-CA	-7.54	1.31	1.46
1	C	214	TYR	CD1-CE1	6.83	1.49	1.39
36	A	1020	A	N9-C8	-5.47	1.33	1.37
36	A	1137	G	N9-C4	5.46	1.42	1.38
36	A	1006	C	N1-C2	5.06	1.45	1.40

The worst 5 of 218 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A	1006	C	N1-C2-O2	12.16	126.20	118.90
36	A	1006	C	N3-C2-O2	-11.85	113.61	121.90
36	A	1137	G	N3-C4-C5	-10.22	123.49	128.60
36	A	1006	C	C6-N1-C2	-9.95	116.32	120.30
36	A	2040	C	C6-N1-C2	-9.65	116.44	120.30

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	171	ALA	Peptide
1	C	211	ARG	Peptide
1	C	60	ARG	Peptide
2	D	164	GLN	Peptide
2	D	78	LYS	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	182	0
2	D	2145	0	2234	162	0
3	E	1569	0	1634	129	0
4	F	1628	0	1680	164	0
5	G	1474	0	1535	79	0
6	H	1274	0	1342	51	0
7	J	851	0	203	34	0
8	K	1035	0	1082	62	0
9	O	933	0	996	57	0
10	P	1114	0	1187	76	0
11	Q	1122	0	1179	71	0
12	R	960	0	1021	71	0
13	S	775	0	835	67	0
14	T	1147	0	1207	81	0
15	U	964	0	1022	83	0
16	V	779	0	852	63	0
17	W	900	0	964	60	0
18	X	734	0	789	48	0
19	Y	818	0	908	42	0
20	Z	1473	0	1497	70	0
21	0	662	0	688	44	0
22	1	732	0	808	75	0
23	4	271	0	284	16	0
24	N	1104	0	1180	211	0
25	2	598	0	653	29	0
26	3	477	0	529	25	0
27	5	459	0	477	40	0
28	6	433	0	461	30	0
29	7	430	0	480	37	0
30	8	517	0	582	38	0
31	9	307	0	338	29	0
32	e	686	0	620	0	0
33	f	156	0	38	0	0
33	g	156	0	40	0	0
34	h	151	0	40	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	B	2551	0	1295	84	0
36	A	61997	0	31250	2172	0
All	All	95124	0	63728	3961	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 25.

The worst 5 of 3961 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:N:78:TYR:CD2	36:A:2642:G:C5'	1.74	1.62
15:U:64:ARG:CD	24:N:41:ASP:HA	1.14	1.60
15:U:64:ARG:HD2	24:N:41:ASP:CA	1.06	1.52
24:N:76:SER:HB3	36:A:2641:G:C5'	1.44	1.48
24:N:78:TYR:CD2	36:A:2642:G:H5'	1.35	1.36

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%)	108 (48%)	66 (29%)	52 (23%)	0	2
2	D	273/275 (99%)	179 (66%)	57 (21%)	37 (14%)	0	11
3	E	203/205 (99%)	133 (66%)	41 (20%)	29 (14%)	0	10
4	F	206/208 (99%)	126 (61%)	55 (27%)	25 (12%)	1	14
5	G	179/181 (99%)	121 (68%)	43 (24%)	15 (8%)	1	26
6	H	165/167 (99%)	121 (73%)	26 (16%)	18 (11%)	1	17
8	K	138/140 (99%)	91 (66%)	35 (25%)	12 (9%)	1	25
9	O	120/122 (98%)	90 (75%)	22 (18%)	8 (7%)	2	35
10	P	144/146 (99%)	88 (61%)	35 (24%)	21 (15%)	0	9
11	Q	139/141 (99%)	99 (71%)	26 (19%)	14 (10%)	1	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	R	115/117 (98%)	78 (68%)	26 (23%)	11 (10%)	1	22
13	S	97/99 (98%)	52 (54%)	24 (25%)	21 (22%)	0	3
14	T	136/138 (99%)	89 (65%)	28 (21%)	19 (14%)	0	10
15	U	115/117 (98%)	84 (73%)	20 (17%)	11 (10%)	1	22
16	V	99/101 (98%)	63 (64%)	22 (22%)	14 (14%)	0	10
17	W	111/113 (98%)	90 (81%)	10 (9%)	11 (10%)	1	20
18	X	91/93 (98%)	69 (76%)	17 (19%)	5 (6%)	3	41
19	Y	105/107 (98%)	50 (48%)	34 (32%)	21 (20%)	0	4
20	Z	183/185 (99%)	120 (66%)	45 (25%)	18 (10%)	1	21
21	0	82/84 (98%)	55 (67%)	20 (24%)	7 (8%)	1	26
22	1	91/93 (98%)	55 (60%)	17 (19%)	19 (21%)	0	3
23	4	33/35 (94%)	17 (52%)	11 (33%)	5 (15%)	0	8
24	N	136/138 (99%)	94 (69%)	26 (19%)	16 (12%)	1	15
25	2	69/71 (97%)	51 (74%)	14 (20%)	4 (6%)	3	39
26	3	58/60 (97%)	45 (78%)	10 (17%)	3 (5%)	3	42
27	5	57/59 (97%)	37 (65%)	13 (23%)	7 (12%)	1	14
28	6	48/50 (96%)	26 (54%)	11 (23%)	11 (23%)	0	2
29	7	47/49 (96%)	34 (72%)	9 (19%)	4 (8%)	1	26
30	8	62/64 (97%)	37 (60%)	17 (27%)	8 (13%)	0	13
31	9	35/37 (95%)	19 (54%)	12 (34%)	4 (11%)	1	16
32	e	70/103 (68%)	40 (57%)	23 (33%)	7 (10%)	1	20
All	All	3633/3726 (98%)	2361 (65%)	815 (22%)	457 (13%)	0	14

5 of 457 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	17	PRO
1	C	43	GLU
1	C	52	PRO
1	C	54	ARG
1	C	59	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	C	180/180 (100%)	130 (72%)	50 (28%)	0	6
2	D	217/217 (100%)	173 (80%)	44 (20%)	2	14
3	E	165/165 (100%)	134 (81%)	31 (19%)	2	17
4	F	165/165 (100%)	126 (76%)	39 (24%)	1	9
5	G	155/155 (100%)	121 (78%)	34 (22%)	1	11
6	H	136/136 (100%)	115 (85%)	21 (15%)	4	29
8	K	105/105 (100%)	88 (84%)	17 (16%)	3	26
9	O	100/100 (100%)	84 (84%)	16 (16%)	3	27
10	P	112/112 (100%)	91 (81%)	21 (19%)	2	17
11	Q	111/111 (100%)	85 (77%)	26 (23%)	1	9
12	R	100/100 (100%)	81 (81%)	19 (19%)	2	17
13	S	77/77 (100%)	60 (78%)	17 (22%)	1	11
14	T	120/120 (100%)	99 (82%)	21 (18%)	3	21
15	U	93/93 (100%)	76 (82%)	17 (18%)	2	18
16	V	82/82 (100%)	60 (73%)	22 (27%)	1	7
17	W	92/92 (100%)	74 (80%)	18 (20%)	2	15
18	X	75/75 (100%)	60 (80%)	15 (20%)	2	15
19	Y	88/88 (100%)	72 (82%)	16 (18%)	2	19
20	Z	162/162 (100%)	128 (79%)	34 (21%)	1	12
21	0	66/66 (100%)	56 (85%)	10 (15%)	4	30
22	1	78/78 (100%)	53 (68%)	25 (32%)	0	4
23	4	31/31 (100%)	25 (81%)	6 (19%)	2	16
24	N	117/117 (100%)	100 (86%)	17 (14%)	5	32
25	2	66/66 (100%)	58 (88%)	8 (12%)	7	42
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%)	37 (76%)	12 (24%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	7	42/42 (100%)	36 (86%)	6 (14%)	5	33
30	8	54/54 (100%)	40 (74%)	14 (26%)	1	7
31	9	34/34 (100%)	29 (85%)	5 (15%)	4	31
32	e	54/54 (100%)	46 (85%)	8 (15%)	4	31
All	All	3029/3029 (100%)	2424 (80%)	605 (20%)	2	15

5 of 605 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	Q	1	MET
14	T	27	THR
27	5	58	LEU
11	Q	42	ILE
12	R	28	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
12	R	23	ASN
14	T	43	GLN
25	2	9	GLN
13	S	34	HIS
13	S	38	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
35	B	118/119 (99%)	19 (16%)	1 (0%)
36	A	2878/2879 (99%)	692 (24%)	22 (0%)
All	All	2996/2998 (99%)	711 (23%)	23 (0%)

5 of 711 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
35	B	2	C
35	B	13	A
35	B	15	A
35	B	16	G
35	B	25	A

5 of 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	A	1420	U
36	A	1558	A
36	A	2780	G
36	A	1542	G
36	A	1815	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, 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%)	-0.02	12 (5%) 25 21	73, 140, 196, 228	0
2	D	275/275 (100%)	0.87	57 (20%) 1 2	18, 59, 122, 191	0
3	E	205/205 (100%)	1.08	54 (26%) 1 2	20, 74, 138, 209	0
4	F	208/208 (100%)	0.46	24 (11%) 5 7	26, 76, 155, 199	0
5	G	181/181 (100%)	0.55	26 (14%) 3 4	40, 94, 165, 199	0
6	H	167/167 (100%)	0.09	15 (8%) 10 11	11, 67, 139, 168	0
7	J	0/170	-	-	-	-
8	K	140/140 (100%)	0.13	12 (8%) 11 11	30, 110, 178, 234	0
9	O	122/122 (100%)	-0.15	2 (1%) 68 52	20, 58, 106, 159	0
10	P	146/146 (100%)	0.66	30 (20%) 1 2	28, 78, 141, 189	0
11	Q	141/141 (100%)	0.07	3 (2%) 60 44	22, 68, 140, 174	0
12	R	117/117 (100%)	0.40	10 (8%) 11 11	18, 69, 143, 195	0
13	S	99/99 (100%)	1.51	36 (36%) 1 2	18, 106, 167, 216	0
14	T	138/138 (100%)	0.13	7 (5%) 27 22	19, 75, 153, 238	0
15	U	117/117 (100%)	1.25	40 (34%) 1 2	24, 61, 118, 158	0
16	V	101/101 (100%)	0.43	14 (13%) 4 5	20, 72, 127, 200	0
17	W	113/113 (100%)	0.74	18 (15%) 3 4	5, 65, 136, 178	0
18	X	93/93 (100%)	0.59	11 (11%) 5 7	34, 63, 128, 170	0
19	Y	107/107 (100%)	1.05	22 (20%) 1 2	35, 76, 151, 176	0
20	Z	185/185 (100%)	-0.06	5 (2%) 52 38	36, 82, 147, 226	0
21	0	84/84 (100%)	1.69	32 (38%) 1 1	19, 85, 145, 160	0
22	1	93/93 (100%)	1.80	31 (33%) 1 2	38, 92, 166, 194	0
23	4	35/35 (100%)	-0.05	3 (8%) 11 11	82, 115, 164, 187	0
24	N	138/138 (100%)	0.61	22 (15%) 3 4	58, 84, 107, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	2	71/71 (100%)	0.26	3 (4%) 35 26	42, 70, 130, 187	0
26	3	60/60 (100%)	0.58	12 (20%) 2 3	53, 68, 130, 149	0
27	5	59/59 (100%)	0.76	13 (22%) 1 2	16, 83, 166, 185	0
28	6	50/50 (100%)	-0.25	0 100 100	61, 118, 161, 188	0
29	7	49/49 (100%)	1.10	11 (22%) 1 2	33, 61, 140, 186	0
30	8	64/64 (100%)	1.70	27 (42%) 1 1	28, 75, 142, 191	0
31	9	37/37 (100%)	3.48	19 (51%) 0 1	102, 132, 185, 210	0
32	e	72/103 (69%)	-0.59	0 100 100	46, 118, 183, 199	0
33	f	0/31	-	-	-	-
33	g	0/31	-	-	-	-
34	h	0/30	-	-	-	-
35	B	119/119 (100%)	-0.04	9 (7%) 14 13	35, 118, 182, 220	0
36	A	2879/2879 (100%)	0.39	306 (10%) 7 8	5, 79, 177, 310	0
All	All	6693/6986 (95%)	0.49	886 (13%) 4 5	5, 82, 169, 310	0

The worst 5 of 886 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	A	2585	U	15.5
31	9	11	CYS	12.8
31	9	27	CYS	12.7
22	1	40	ARG	11.9
36	A	2506	U	11.7

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.