



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:12 PM GMT

PDB ID : 1NKW  
Title : Crystal Structure Of The Large Ribosomal Subunit From Deinococcus Radiodurans  
Authors : Harms, J.M.; Schlutzen, F.; Zarivach, R.; Bashan, A.; Gat, S.; Agmon, I.; Bartels, H.; Franceschi, F.; Yonath, A.  
Deposited on : 2003-01-05  
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

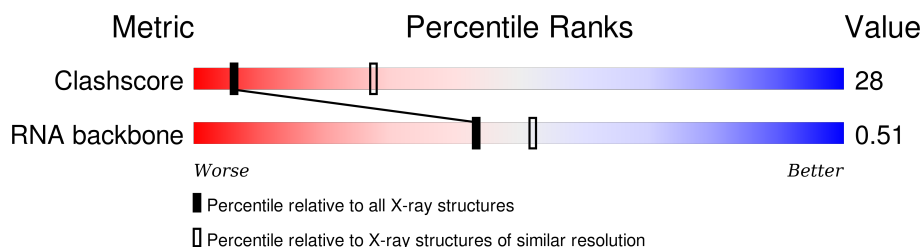
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

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))
Clashscore	102246	1222 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)



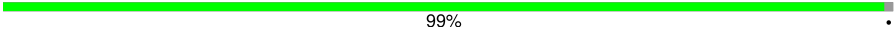


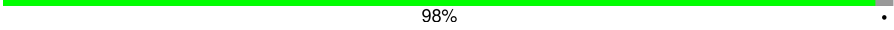
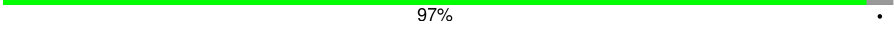

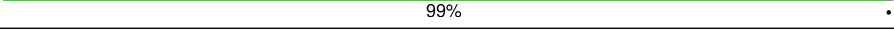
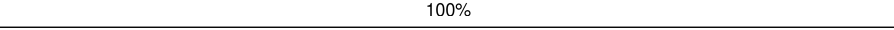
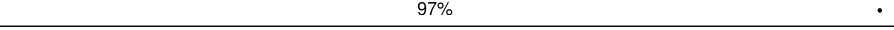
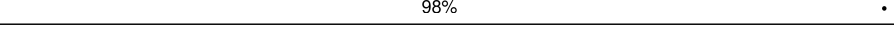
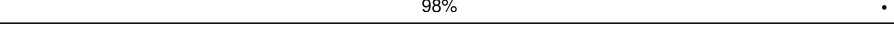
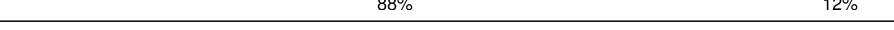
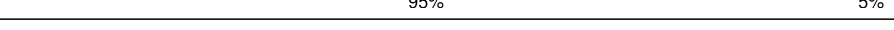
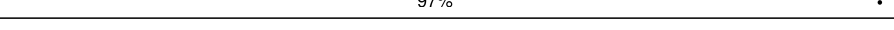
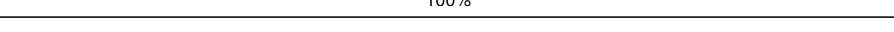
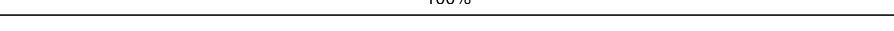
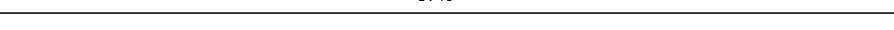


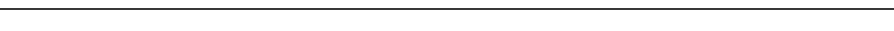

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	2880	
2	9	124	
3	A	275	
4	B	211	
5	C	205	
6	D	180	
7	E	212	
8	F	146	

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Mol	Chain	Length	Quality of chain
9	G	144	 99% .
10	H	174	 82% 18%
11	I	134	 99% .
12	J	156	 90% 10%
13	K	142	 87% . 13%
14	L	116	 98% .
15	M	114	 97% .
16	N	166	 74% . 25%
17	O	118	 99% .
18	P	100	 100%
19	Q	134	 97% .
20	R	95	 98% .
21	S	115	 98% .
22	T	253	 88% 12%
23	U	91	 95% 5%
24	W	67	 97% .
25	X	55	 100%
26	Y	73	 100%
27	Z	60	 97% .
28	1	82	 65% 35%
29	2	47	 98% .
30	3	64	 98% .
31	4	36	 97% .

## 2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 65300 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2766	Total	C	N	O	P	0	0	0
			59359	26479	10949	19166	2765			

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	118	Total	C	N	O	P	0	0	0
			2519	1124	464	813	118			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	A	270	Total	C	0	0	270
			270	270			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	B	205	Total	C	0	0	205
			205	205			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
5	C	197	Total	C	0	0	197
			197	197			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
6	D	178	Total	C	0	0	178
			178	178			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	E	177	Total C 177 177	0	0	177

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	F	52	Total C 52 52	0	0	52

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	G	143	Total C 143 143	0	0	143

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	H	143	Total C 143 143	0	0	143

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	I	132	Total C 132 132	0	0	132

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	J	141	Total C 141 141	0	0	141

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	K	124	Total C 124 124	0	0	124

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	L	114	Total C 114 114	0	0	114

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	M	111	Total C 111 111	8	0	111

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
16	N	125	Total C 125 125	0	0	125

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
17	O	117	Total C 117 117	16	0	117

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
18	P	100	Total C 100 100	0	0	100

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
19	Q	130	Total C 130 130	0	0	130

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
20	R	93	Total C 93 93	0	0	93

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	S	113	Total C 113 113	0	0	113

- Molecule 22 is a protein called general stress protein CTC.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	T	223	Total C 223 223	43	0	223

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
23	U	86	Total C 86 86	0	0	86

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
24	W	65	Total C 65 65	0	0	65

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
25	X	55	Total C 55 55	4	0	55

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	Y	73	Total C 73 73	0	0	73

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	Z	58	Total C 58 58	0	0	58

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	1	53	Total C 53 53	0	0	53

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	2	46	Total C 46 46	0	0	46

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	3	63	Total C 63 63	0	0	63

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
31	4	35	Total C 35 35	0	0	35

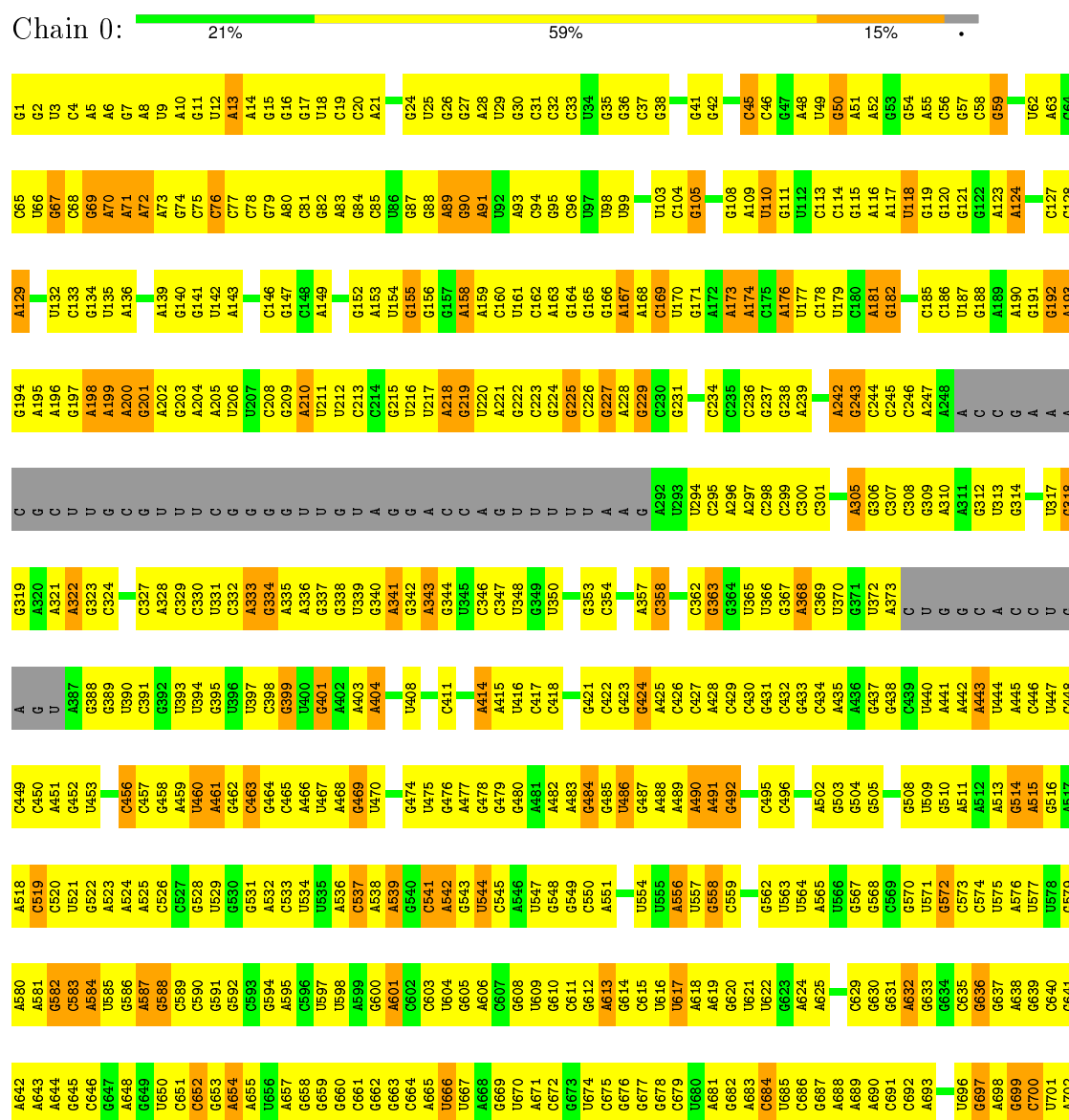


### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

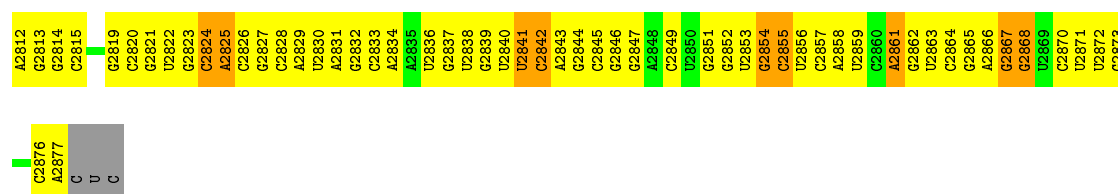
Note EDS was not executed.

#### • Molecule 1: 23S ribosomal RNA

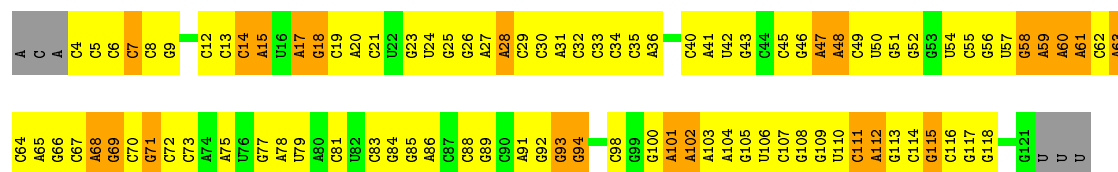
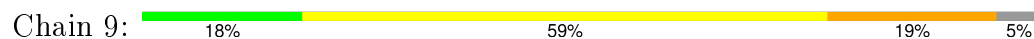


U1697	C1633	A1437	G1374	G1310	A1179	A1106	U1034	C968	C	A911	A834	C771	A703
C1698	A1634	G1438	C1375	C1311	A1180	A1107	G1035	U969	U	A912	U835	G772	G704
A1699	G1635	G1439	G1376	G1312	A1181		G1036	A970	U	A913	G836	G773	C705
G1703	G1636	G1440	G1377	U1313	U1182	G1110	U1037	A971	A	C914	U837	A774	A706
G1704	C1637	A1441	A1378	A1314	C1183	C1111	U1038	C972	C	U916	A838	U775	U707
U1705	G1638	C1442	A1379	A1315	G1184	U1112	A1039	U973		U917	U839	G776	
U1706	U1639	G1443	C1380	G1316	C1185	C1113	A1040	U974		A918	U840	A777	A712
A1707	C1640	C1444	G1381	G1317	C1190	A1114	G1041	C975		U919	G841	G778	G713
G1708	A1642	A1445	G1382	A1318	C1191	C1115	U1044	C976		A920	A842		U716
A1643	G1643	U1446	C1383	C1319	A1192	U1116	G1045	U977		C923	G843	G781	G717
G1644	A1644	U1447	G1384	A1320	A1193	G1117	U1046	U978		U924	G844	U782	A718
G1645		A1448	C1385	U1321	G1194	G1121	U1047	A979		U925	U845	G783	A719
		G1449	A1386	G1322	U1195	A1122	G1048	G980		A926	A846	U784	A720
		G1450	G1387	G1323	U1196		U1049	C981		A927	C847	U785	C721
		C1451	C1388	G1324	G1197	G1123	G1053	C982		A928	U848	U786	C722
		U1452	C1389	U1325	C1198	U1124	C1054	G983		U929	U849	U787	
		A1453	G1390	C1326	U1199	G1125	A1055	A984		U930	U850	G788	G726
		U1454	A1391	G1327	U1199	A1126	C1056	A985		U931	G851	G789	U727
		C1455	U1392	C1328	G1200		U1056	A986		U932	C852	A790	
		C1456	G1393	U1329	G1201	U1130	U1057	G987		C926	U857	G791	G728
		A1457			C1202	G1131	G1058			C927	G858	U792	
		A1458	G1398	G1332	A1203	C1132	U1059			G928	U859	G793	G732
		U1459	C1399	G1333	G1204	G1133	G1062	A991		A929	U860	G794	G733
		C1460	A1400	A1334	G1205	C1134	C1063			U930	A795	G734	G734
		C1461	G1401	G1335	G1206	U1135	C1064	A994		G931	U796	G735	G735
		A1462	G1402	G1337	G1207	G1136	A1065	A995		U932	A797	G736	G736
		A1463	U1403	C1338	A1208	A1137	G1066	C996		G933	U798	G737	G737
		G1464	G1404	U1339	G1209	A1138	U1067	A999		C934	U799	G738	G738
		C1465	A1405	G1340	U1210	A1139	A1068	A999		U935	U800	G739	G739
		U1466	G1406	G1341	U1211	U1141	G1069	A1001		C937	A801	A740	A740
		A1467	G1407	U1342	U1212	G1142	U1072	C1002		U943	A802	G741	G741
		A1468	A1408	C1343	U1217		A1081	C1003		G938	C803	G742	G742
		U1469	U1409	G1344	C1218	C1145	G1082	C1003		C939	C804	A743	A743
		G1470	U1410	G1345	G1219	C1152	C1083	A1004		G940	G872	G744	G744
		C1471	C1411	C1346	C1220	G1146	U1075	U1005		U941	U873	A806	C745
		U1472	C1412	C1347	G1221	G1147	U1076	C1006		U942	A874	A807	G746
		A1473	U1413	G1348	C1222	G1148	U1077	A1007		U943	G875	A747	A747
		U1474	G1414	G1349	G1223	G1149		G1008		A944	A876	A748	A748
		U1475	C1415	G1350	A1224	C1150	A1081	C1009		G945		G811	C749
		G1476	U1416	G1351	A1225	C1151	G1082	U1010		U946	A879	G812	C750
		C1477	C1417	G1352	G1291	C1152	C1083	A1011		C947	A813	A813	G751
		U1478	G1418	A1353	A1226	A1153	C1090	A1021		U954	G814	G752	G752
		G1479	C1419	A1354	A1227	A1154	U1092	G955		A956	A815	U753	U753
		U1480	U1419	A1355	C1228	G1155	C1086	A887		C948	U816	G754	G754
		U1481	G1356	G1356	C1229	U1156	A1087	C888			U817	C755	C755
		C1482	G1357		G1295		C1088	C889		A952	A817	G756	G756
		U1483	C1359		G1296	A1162	A1089	U953		U953	C819	U757	U757
		G1484	U1424		A1297	C1163	C1090	A1021		G955	G820	G758	G758
		U1485	G1425		G1298	C1164	U1092	A1022		A956	A821	C759	C759
		A1486	U1426		A1299	G1165	U1092	U1023		G957	G	U760	U760
		C1487	G1427		A1300	A1166	A1095	G1024		G958	U824	G761	G761
		U1488	G1428		C1364	A1167	A1096	A1025		C959	C825	A762	A762
		A1489	U1429		C1302	G1168	U1096	U1026		U960	U826	A763	A763
		U1490	G1430		U1303	A1171	A1099	C1027		G961	C827	A764	A764
		C1491	U1431		U1304	U1172	G1100	G1028		G962	C828	G765	G765
		A1492	G1432		C1305	A1173	U1101	C1029		G963	C829	A766	A766
		A1493	U1433		U1306	G1173	G1102	U1030		A964	C830	G767	G767
		G1494	U1434		U1307	A1174	G1103	C1031		G965	C831	U768	U768
		U1495	G1435		C1308	A1175	G1104	A1032		A966	A832	C769	C769
		G1496	G1436		G1309		U1105	G1033		G967	G	A833	U770

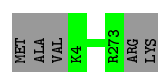




• Molecule 2: 5S ribosomal RNA



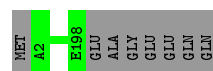
• Molecule 3: 50S ribosomal protein L2



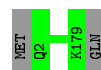
• Molecule 4: 50S ribosomal protein L3



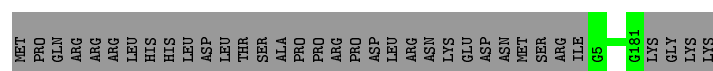
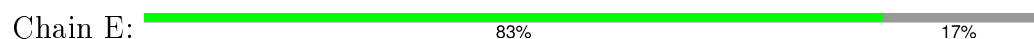
• Molecule 5: 50S ribosomal protein L4



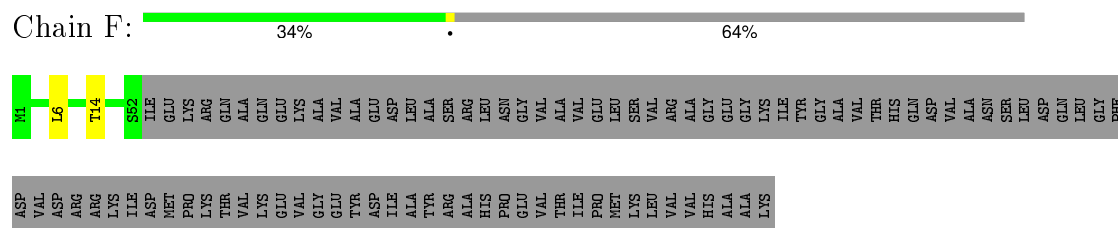
• Molecule 6: 50S ribosomal protein L5



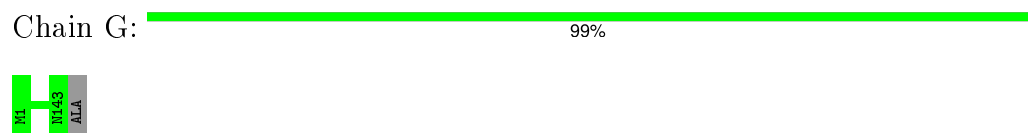
• Molecule 7: 50S ribosomal protein L6



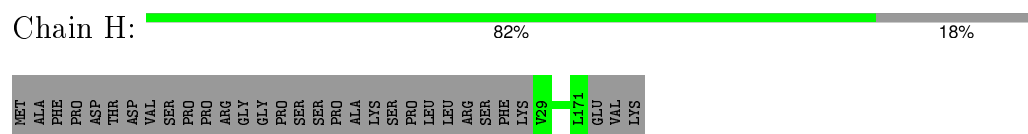
- Molecule 8: 50S ribosomal protein L9



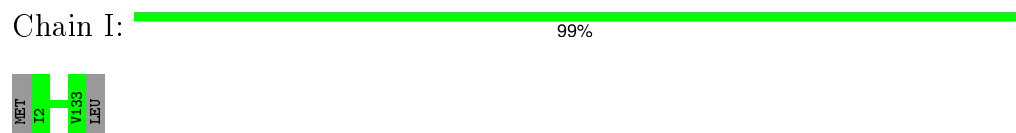
- Molecule 9: 50S ribosomal protein L11



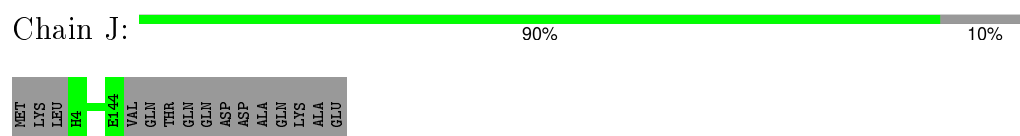
- Molecule 10: 50S ribosomal protein L13



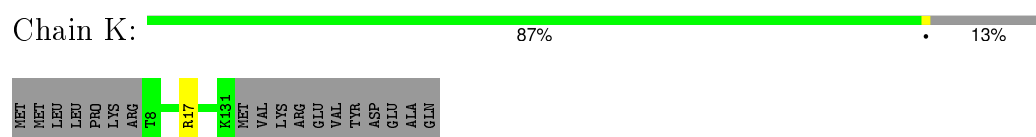
- Molecule 11: 50S ribosomal protein L14



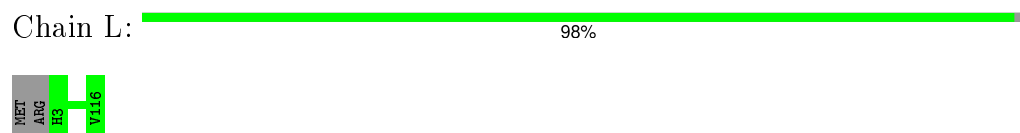
- Molecule 12: 50S ribosomal protein L15



- Molecule 13: 50S ribosomal protein L16

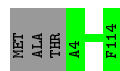


- Molecule 14: 50S ribosomal protein L17



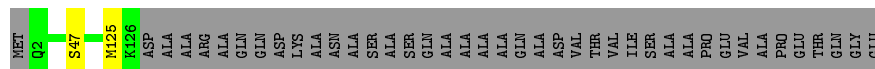
- Molecule 15: 50S ribosomal protein L18

Chain M:  97%



- Molecule 16: 50S ribosomal protein L19

Chain N:  74%



- Molecule 17: 50S ribosomal protein L20

Chain O:  99%



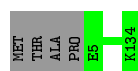
- Molecule 18: 50S ribosomal protein L21

Chain P:  100%

There are no outlier residues recorded for this chain.

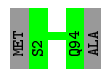
- Molecule 19: 50S ribosomal protein L22

Chain Q:  97%



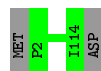
- Molecule 20: 50S ribosomal protein L23

Chain R:  98%




- Molecule 21: 50S ribosomal protein L24

Chain S:  98%



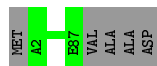
- Molecule 22: general stress protein CTC

Chain T:  88%



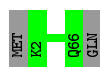
- Molecule 23: 50S ribosomal protein L27

Chain U: 95% 5%



- Molecule 24: 50S ribosomal protein L29

Chain W: 97% .



- Molecule 25: 50S ribosomal protein L30

Chain X: 100%

There are no outlier residues recorded for this chain.

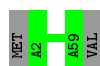
- Molecule 26: 50S ribosomal protein L31

Chain Y: 100%

There are no outlier residues recorded for this chain.

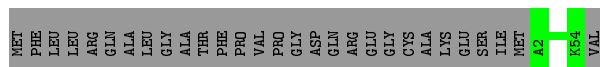
- Molecule 27: 50S ribosomal protein L32

Chain Z: 97% .



- Molecule 28: 50S ribosomal protein L33

Chain 1: 65% 35%



- Molecule 29: 50S ribosomal protein L34

Chain 2: 98% .



- Molecule 30: 50S ribosomal protein L35

Chain 3:  98% .



- Molecule 31: 50S ribosomal protein L36

Chain 4:  97% .





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.00Å 410.00Å 697.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.240 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	65300	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.25	0/66467	0.70	6/103673 (0.0%)
2	9	0.59	0/2816	0.81	1/4388 (0.0%)
All	All	0.27	0/69283	0.70	7/108061 (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
1	0	0	5

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	9	94	G	N9-C1'-C2'	-6.58	104.76	112.00
1	0	2428	U	N1-C1'-C2'	6.19	122.04	114.00
1	0	1279	G	N9-C1'-C2'	5.63	121.32	114.00
1	0	843	G	C2'-C3'-O3'	5.44	122.40	113.70
1	0	2660	C	N1-C1'-C2'	5.26	120.84	114.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1264	C	Sidechain
1	0	1342	U	Sidechain
1	0	2251	U	Sidechain
1	0	2668	U	Sidechain
1	0	788	G	Sidechain

## 5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59359	0	29917	2555	1
2	9	2519	0	1285	147	0
3	A	270	0	0	0	0
4	B	205	0	0	0	0
5	C	197	0	0	0	0
6	D	178	0	0	0	0
7	E	177	0	0	0	0
8	F	52	0	0	1	0
9	G	143	0	0	0	0
10	H	143	0	0	0	0
11	I	132	0	0	0	0
12	J	141	0	0	0	0
13	K	124	0	0	1	0
14	L	114	0	0	0	0
15	M	111	0	0	0	0
16	N	125	0	0	1	1
17	O	117	0	0	0	0
18	P	100	0	0	0	0
19	Q	130	0	0	0	0
20	R	93	0	0	0	0
21	S	113	0	0	0	0
22	T	223	0	0	0	0
23	U	86	0	0	0	0
24	W	65	0	0	0	0
25	X	55	0	0	0	0
26	Y	73	0	0	0	0
27	Z	58	0	0	0	0
28	1	53	0	0	0	0
29	2	46	0	0	0	0
30	3	63	0	0	0	0
31	4	35	0	0	0	0
All	All	65300	0	31202	2696	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

The worst 5 of 2696 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1679:U:H2'	1:0:1680:U:H5''	1.22	1.12
1:0:362:C:H2'	1:0:363:G:H4'	1.34	1.10
1:0:918:A:H2'	1:0:919:U:H5''	1.29	1.10
1:0:2548:G:H2'	1:0:2549:G:H5''	1.10	1.09
1:0:2058:U:H1'	1:0:2576:G:H21	1.08	1.08

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1552:C:OP1	16:N:47:SER:CA[8_455]	1.97	0.23

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2757/2880 (95%)	523 (18%)	48 (1%)
2	9	117/124 (94%)	23 (19%)	1 (0%)
All	All	2874/3004 (95%)	546 (18%)	49 (1%)

5 of 546 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	13	A
1	0	35	G
1	0	45	C
1	0	48	A
1	0	49	U

5 of 49 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1495	G
1	0	1820	G
1	0	2660	C
1	0	1651	U
1	0	1938	U

#### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

#### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

#### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

#### 5.7 Other polymers [i](#)

There are no such residues in this entry.

#### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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