



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:15 PM GMT

PDB ID : 1NWY
Title : COMPLEX OF THE LARGE RIBOSOMAL SUBUNIT FROM DEINOCOC-
CUS RADIODURANS WITH AZITHROMYCIN
Authors : Schlutzen, F.; Harms, J.; Franceschi, F.; Hansen, H.A.S.; Bartels, H.; Zari-
vach, R.; Yonath, A.
Deposited on : 2003-02-07
Resolution : 3.30 Å(reported)

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

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

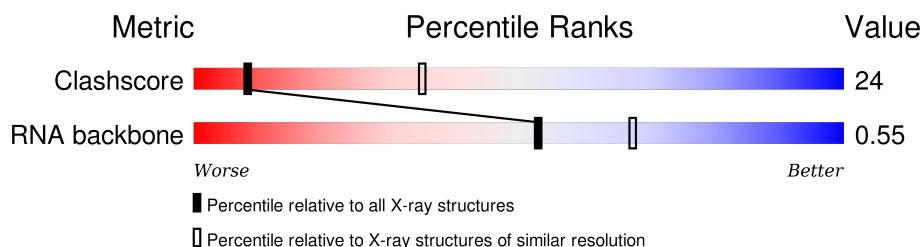
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

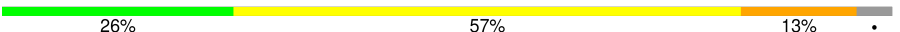
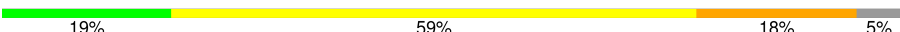
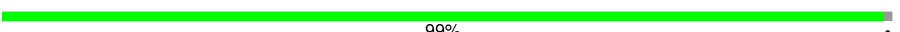
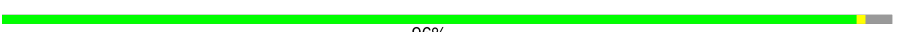



Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1058 (3.38-3.22)
RNA backbone	2183	1005 (3.82-2.78)

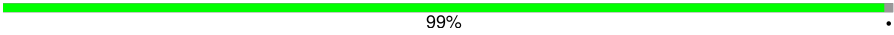

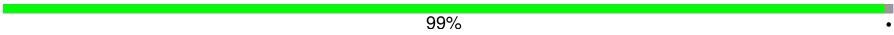


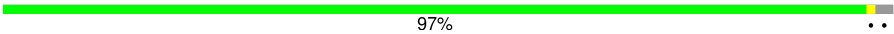
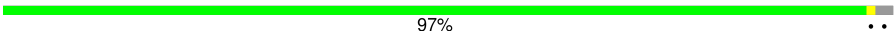

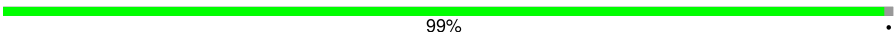

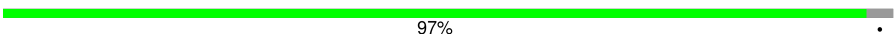
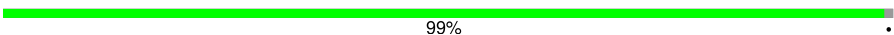
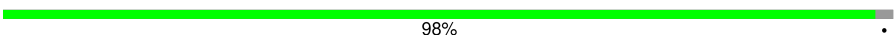


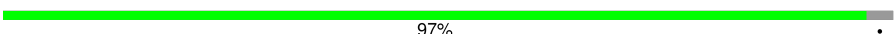
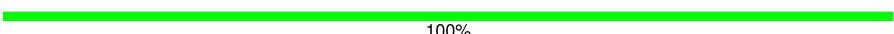
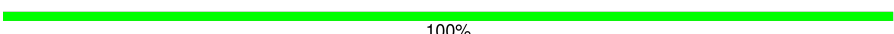
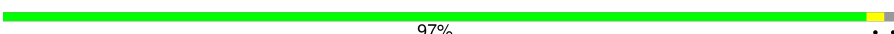
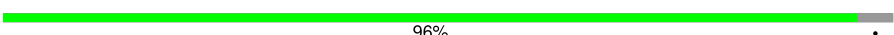
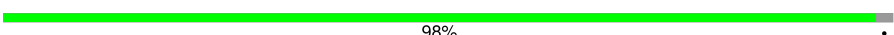
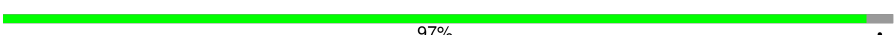
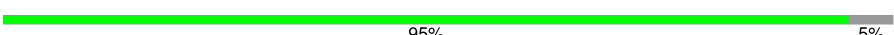
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey 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	274	
4	B	211	
5	C	204	
6	D	180	
7	E	185	
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	141	 87% . 12%
14	L	116	 97% ..
15	M	113	 97% ..
16	N	166	 75% . 25%
17	O	118	 99% .
18	P	100	 100%
19	Q	134	 97% .
20	R	94	 99% .
21	S	115	 98% .
22	T	237	 94% 6%
23	U	91	 95% 5%
24	W	67	 97% .
25	X	55	 100%
26	Y	73	 100%
27	Z	59	 97% ..
28	1	55	 96% .
29	2	47	 98% .
30	3	65	 97% .
31	4	37	 95% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	ZIT	0	2881	-	-	X	-
32	ZIT	0	2882	-	-	X	-

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 65404 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 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 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 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 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 ribosomal protein L6.

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

- Molecule 8 is a protein called ribosomal protein L9.

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

- Molecule 9 is a protein called ribosomal protein L11.

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

- Molecule 10 is a protein called ribosomal protein L13.

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

- Molecule 11 is a protein called ribosomal protein L14.

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

- Molecule 12 is a protein called ribosomal protein L15.

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

- Molecule 13 is a protein called ribosomal protein L16.

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

- Molecule 14 is a protein called ribosomal protein L17.

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

- Molecule 15 is a protein called ribosomal protein L18.

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

- Molecule 16 is a protein called ribosomal protein L19.

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

- Molecule 17 is a protein called ribosomal protein L20.

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

- Molecule 18 is a protein called ribosomal protein L21.

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

- Molecule 19 is a protein called ribosomal protein L22.

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

- Molecule 20 is a protein called ribosomal protein L23.

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

- Molecule 21 is a protein called 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 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 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 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 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 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 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 ribosomal protein L34.

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

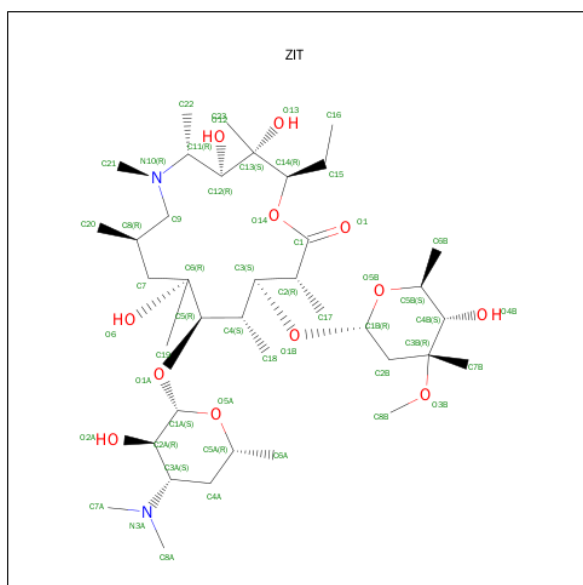
- Molecule 30 is a protein called ribosomal protein L35.

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

- Molecule 31 is a protein called ribosomal protein L36.

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

- Molecule 32 is AZITHROMYCIN (three-letter code: ZIT) (formula: $C_{38}H_{72}N_2O_{12}$).



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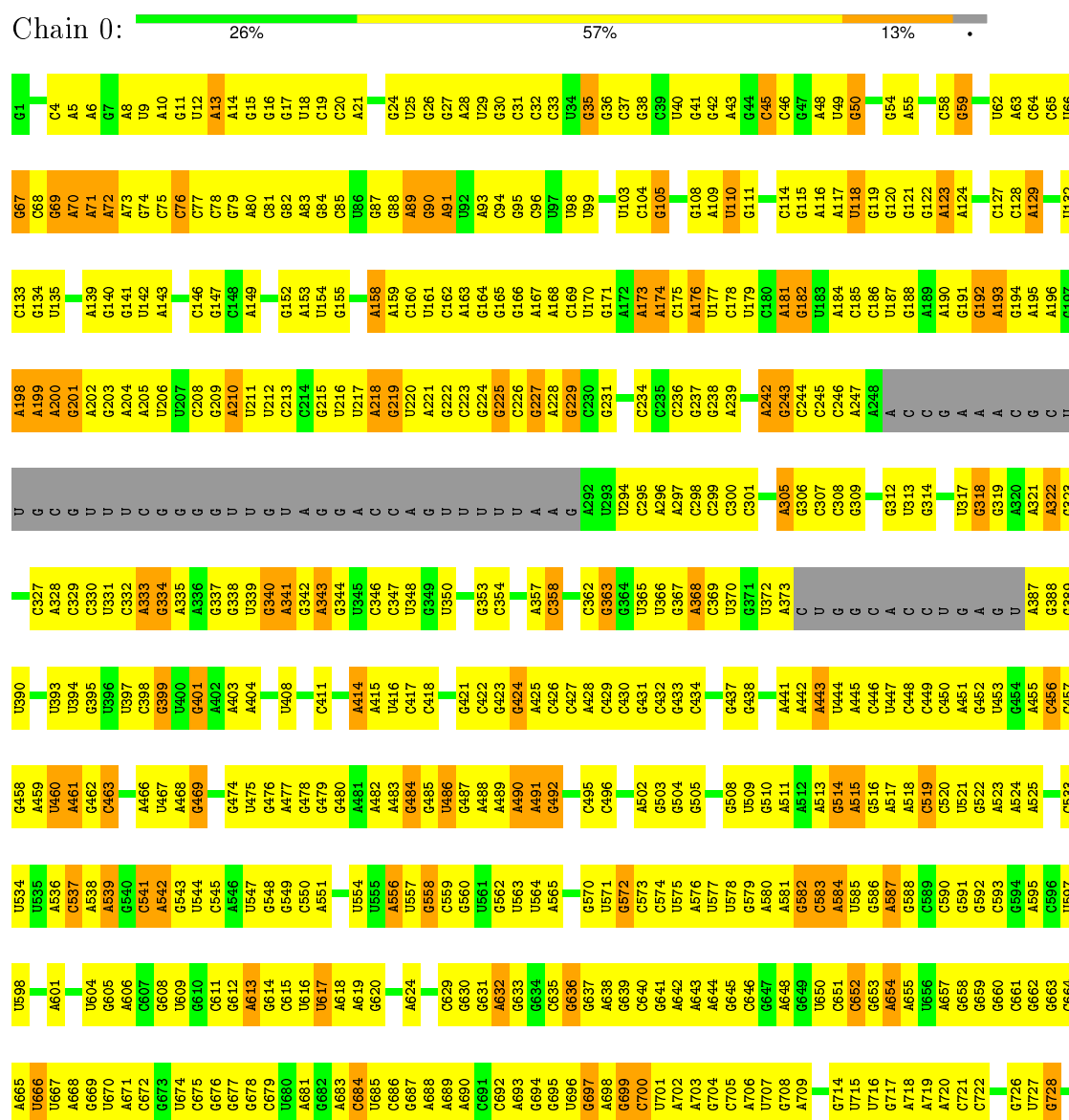
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
32	0	1	52	38	2	12	0	0

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.

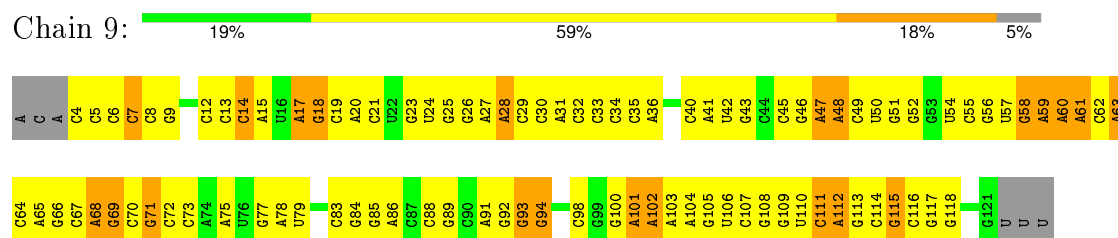
• Molecule 1: 23S RIBOSOMAL RRNA



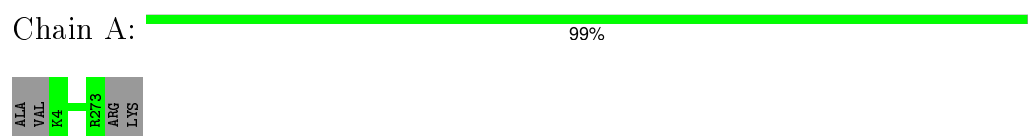
G1760	G1691	G1622	G1559	G1489	G1427	G1358	G1297	G1233	G1156	G1082	G1002	G933	C864	A794	G732
G1761	G1692	C1623	A1560	U1490	G1428	G1359	G1298	A1233	A1162	C1083	C1003	A936	C865	A795	G733
G1762	A1561	A1624	G1561	C1491	A1429	G1363	A1299	C1234	C1163	C1086	U1005	C937	A866	A796	G734
G1763	A1694	A1625	G1562	A1492	G1430	C1363	A1300	C1235	C1164	C1087	U1006	C938	U866	A797	G735
G1764	G1695	A1626	G1566	A1493	U1431	C1364	C1301	C1236	G1165	A1088	A1007	C939	U868	C799	G736
G1765	G1696	C1627	A1567	G1495	G1432	U1365	U1302	A1238	A1166	C1089	G1008	C940	C869	U800	G737
U1766	A1697	A1433	G1496	G1496	A1433	G1368	U1303	G1241	A1167	C1090	G1039	U941	C870	U801	G738
G1698	A1568	A1434	G1497	G1497	A1434	G1368	U1304	G1242	G1168	C1091	U1010	U942	C871	A802	A740
A1699	A1569	A1435	G1498	G1498	A1435	G1368	U1305	G1243	G1169	C1092	A1012	U943	C872	A803	G741
G1703	G1570	G1436	G1499	U1500	G1436	G1371	U1306	U1244	A1171	A1095	C1016	U944	C873	C804	G742
U1704	G1571	G1437	C1501	G1438	G1437	A1372	U1307	G1245	U1170	A1096	U1011	U945	A874	G805	A743
G1705	C1572	G1439	G1502	G1439	G1439	G1373	U1308	G1246	G1171	C1097	C1017	U946	A875	A806	C744
U1706	G1573	G1440	G1503	G1440	G1440	G1374	G1309	G1247	U1172	C1098	U1012	U947	A876	A807	C745
A1706	A1574	A1441	G1504	G1441	A1441	G1375	C1310	U1248	U1173	C1099	C1018	U948	A877	C808	G746
A1707	C1575	G1442	U1505	G1442	G1442	G1376	C1311	G1249	A1179	A1099	U1019	U949	A878	C809	
G1708	G1576	G1443	U1506	G1443	G1443	G1377	C1312	G1250	A1180	G1100	U1020	U950	A879	C810	
G1709	G1577	G1444	A1509	G1444	G1444	A1378	U1313	G1251	A1181	G1101	A1021	U951	A880	U810	C749
U1710	U1578	G1445	U1510	G1445	G1445	A1379	U1314	G1252	U1182	G1102	A1022	U952	A881	G811	C750
G1711	G1579	U1446	U1511	U1446	U1446	C1380	A1315	C1253	U1183	C1103	U1023	U953	A882	G812	G751
G1712	C1580	U1447	U1512	U1447	U1447	G1381	G1316	C1254	G1184	G1110	G1024	U954	A883	A813	G752
G1713	U1513	U1448	U1513	U1448	U1448	G1382	G1317	G1255	G1185	G1111	U1025	U955	A884	G814	U753
U1714	U1514	G1451	U1514	G1451	G1451	G1383	C1318	A1256	U1191	U1112	U1026	U956	A885	A815	G754
A1715	A1515	U1452	U1515	U1452	U1452	G1384	C1319	G1257	U1192	U1113	G1027	U957	A886	U816	C755
G1716	G1584	U1453	U1516	G1453	U1453	G1385	A1320	U1258	A1193	U1114	G1028	U958	A887	A817	G756
A1717	G1585	U1454	U1517	G1454	U1454	G1386	A1321	G1259	G1194	G1115	U1029	U959	A888	U818	U757
A1718	A1586	U1455	U1518	G1455	U1455	G1387	G1322	A1260	U1195	U1116	U1030	U960	A889	U819	G758
G1719	A1587	G1456	G1520	G1456	G1456	G1388	G1323	G1261	U1196	G1117	U1031	U961	A890	A820	C759
U1720	A1588	C1457	C1524	C1457	C1457	C1389	U1325	U1262	G1197	A1122	G1032	U962	A891	U821	G761
G1721	G1589	A1458	U1525	A1458	A1458	G1390	U1326	G1263	U1198	G1121	A1033	U963	A892	U822	A762
G1722	C1590	U1459	U1526	U1459	U1459	G1391	U1327	C1264	C1198	U1123	U1034	U964	A893	C825	A763
U1723	U1591	U1460	G1527	U1460	U1460	G1392	C1328	G1265	U1199	G1124	G1035	U965	A894	U826	A764
G1724	U1592	G1461	C1528	G1461	G1461	G1393	U1329	G1266	U1200	U1125	G1036	U966	A895	U827	C765
C1725	C1593	A1462	U1529	A1462	A1462	G1394	G1332	G1267	G1201	G1126	U1037	U967	A896	U828	A766
A1726	U1594	C1463	U1530	C1463	C1463	G1395	G1333	U1268	U1202	A1127	U1038	U968	A897	C830	G767
G1727	A1595	A1464	C1531	A1464	A1464	G1396	G1334	G1269	A1203	G1128	U1039	U969	A898	C831	U768
A1728	A1596	G1465	U1532	G1465	G1465	A1400	A1334	G1270	G1204	U1130	A1040	U970	A899	A832	C769
C1729	G1597	C1466	G1533	C1466	C1466	G1401	A1335	G1271	G1205	G1131	G1041	U971	A900	U833	G770
G1730	C1598	U1467	U1535	U1467	U1467	G1402	G1336	G1272	G1206	C1132	U1044	U972	A901	U834	C771
C1731	G1599	A1468	G1536	A1468	A1468	U1403	G1337	G1273	G1207	C1133	C1054	U973	A902	U835	C772
C1736	U1601	U1469	U1537	U1469	U1469	C1404	G1338	G1277	U1212	C1134	C1055	U974	A903	U836	G773
G1737	U1602	G1470	U1538	G1470	G1470	A1405	U1339	A1278	U1213	G1135	A1056	U975	A904	U837	A774
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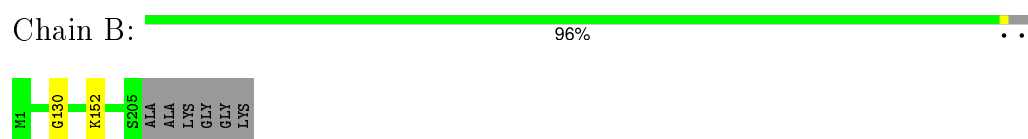
- Molecule 2: 5S RIBOSOMAL RRNA



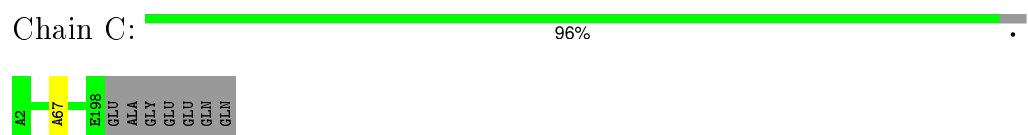
- Molecule 3: ribosomal protein L2



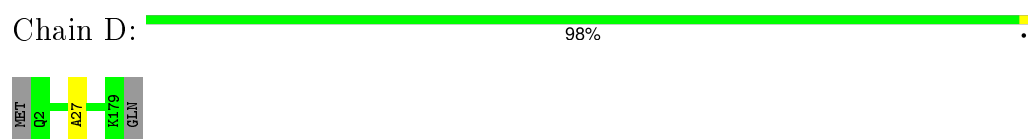
- Molecule 4: ribosomal protein L3



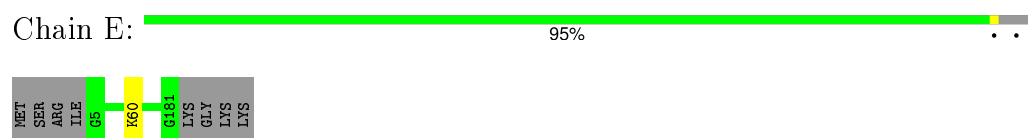
- Molecule 5: ribosomal protein L4



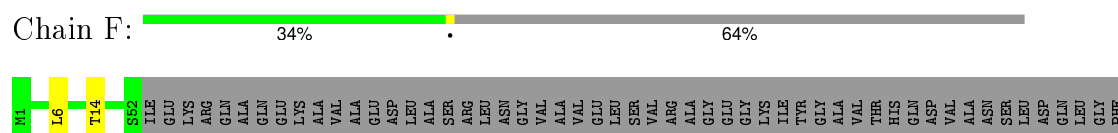
- Molecule 6: ribosomal protein L5



- Molecule 7: ribosomal protein L6



- Molecule 8: ribosomal protein L9




ASP VAL ASP ARG ARG LYS ILE ASP MET PRO LYS THR VAL LYS GLU VAL GLY TYR ASP ILE ALA TYR ARG ALA HIS PRO GLU VAL THR ILE PRO MET LYS LEU VAL VAL HIS ALA ALA LYS

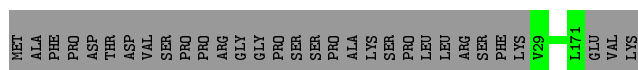
- Molecule 9: ribosomal protein L11

Chain G:  99%

 MET ILE ALA

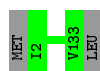
- Molecule 10: ribosomal protein L13

Chain H:  82% 18%

 MET ALA PHE PRO ASP THR ASP VAL SER PRO ARG GLY PRO SER PRO ALA LYS SER PRO LEU ARG SER PHE LYS V29 L171 GLU VAL LYS

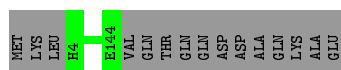
- Molecule 11: ribosomal protein L14

Chain I:  99%


 MET ILE V133 LEU

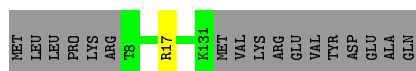
- Molecule 12: ribosomal protein L15

Chain J:  90% 10%

 MET LYS LEU H4 F144 VAL GLN THR GLN ASP ASP ALA GLN LYS ALA GLU

- Molecule 13: ribosomal protein L16

Chain K:  87% 12%

 MET LEU LEU PRO LYS ARG T8 R17 K131 MET VAL LYS ARG GLU VAL TYR ASP GLU ALA GLN

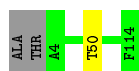
- Molecule 14: ribosomal protein L17

Chain L:  97%

 MET ARG R3 S15 V116

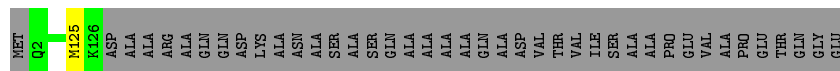
- Molecule 15: ribosomal protein L18

Chain M:  97%

 ALA THR A4 T50 F114

- Molecule 16: ribosomal protein L19

Chain N:  75% 25%



- Molecule 17: ribosomal protein L20

Chain O:  99%



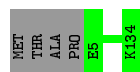
- Molecule 18: ribosomal protein L21

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 19: ribosomal protein L22

Chain Q:  97%



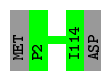
- Molecule 20: ribosomal protein L23

Chain R:  99%



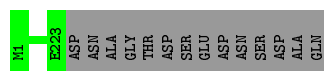
- Molecule 21: ribosomal protein L24

Chain S:  98%



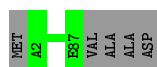
- Molecule 22: general stress protein Ctc

Chain T:  94% 6%



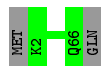
- Molecule 23: ribosomal protein L27

Chain U:  95% 5%



- Molecule 24: ribosomal protein L29

Chain W: 97%



- Molecule 25: ribosomal protein L30

Chain X: 100%

There are no outlier residues recorded for this chain.

- Molecule 26: ribosomal protein L31

Chain Y: 100%

There are no outlier residues recorded for this chain.

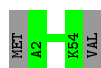
- Molecule 27: ribosomal protein L32

Chain Z: 97%



- Molecule 28: ribosomal protein L33

Chain 1: 96%



- Molecule 29: ribosomal protein L34

Chain 2: 98%



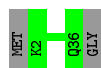
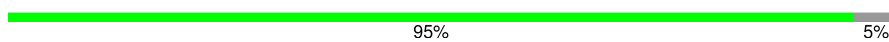
- Molecule 30: ribosomal protein L35

Chain 3: 97%



- Molecule 31: ribosomal protein L36

Chain 4:



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, α , β , γ	170.80 Å 409.50 Å 695.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.279 , 0.304	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	65404	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZIT

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	0.23	0/66467	0.67	0/103673
2	9	0.59	0/2816	0.81	1/4388 (0.0%)
All	All	0.26	0/69283	0.67	1/108061 (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	1

There are no bond length outliers.

All (1) 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

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1342	U	Sidechain

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59359	0	29917	2160	0
2	9	2519	0	1285	147	0
3	A	270	0	0	0	0
4	B	205	0	0	3	0
5	C	197	0	0	1	0
6	D	178	0	0	1	0
7	E	177	0	0	1	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	1	0
15	M	111	0	0	1	0
16	N	125	0	0	1	0
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	1	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
32	0	104	0	144	47	0
All	All	65404	0	31346	2342	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

The worst 5 of 2342 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)
32:0:2882:ZIT:H6A1	32:0:2882:ZIT:C6B	1.61	1.30
32:0:2881:ZIT:C6B	32:0:2881:ZIT:H6A1	1.61	1.29
1:0:1679:U:H2'	1:0:1680:U:H5''	1.27	1.16
1:0:2058:U:H1'	1:0:2576:G:H21	1.10	1.14
1:0:2548:G:H2'	1:0:2549:G:H5''	1.26	1.14

There are no symmetry-related clashes.

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%)	485 (17%)	43 (1%)
2	9	117/124 (94%)	23 (19%)	1 (0%)
All	All	2874/3004 (95%)	508 (17%)	44 (1%)

5 of 508 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 44 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1410	U
1	0	1685	A

Continued on next page...

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Mol	Chain	Res	Type
1	0	2633	A
1	0	1495	G
1	0	1651	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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	ZIT	0	2881	-	54,54,54	0.82	1 (1%)	76,83,83	1.30	6 (7%)
32	ZIT	0	2882	-	54,54,54	0.82	1 (1%)	76,83,83	1.30	6 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	ZIT	0	2881	-	-	0/72/107/107	0/3/3/3
32	ZIT	0	2882	-	-	0/72/107/107	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	2881	ZIT	C3A-N3A	-2.26	1.42	1.48
32	0	2882	ZIT	C3A-N3A	-2.17	1.42	1.48

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	2882	ZIT	C1A-O1A-C5	-6.96	103.82	116.30
32	0	2881	ZIT	C1A-O1A-C5	-6.89	103.94	116.30
32	0	2881	ZIT	C4A-C3A-C2A	-3.17	105.42	110.03
32	0	2882	ZIT	C4A-C3A-C2A	-3.13	105.47	110.03
32	0	2882	ZIT	C2A-C3A-N3A	2.01	116.25	110.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	0	2881	ZIT	21	0
32	0	2882	ZIT	26	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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