



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 26, 2026 – 11:02 PM UTC

PDB ID : 1NWX / pdb_00001nwx
Title : COMPLEX OF THE LARGE RIBOSOMAL SUBUNIT FROM DEINOCOC-
CUS RADIODURANS WITH ABT-773
Authors : Schlutzen, F.; Harms, J.; Franceschi, F.; Hansen, H.A.S.; Bartels, H.; Zari-
vach, R.; Yonath, A.
Deposited on : 2003-02-07
Resolution : 3.50 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

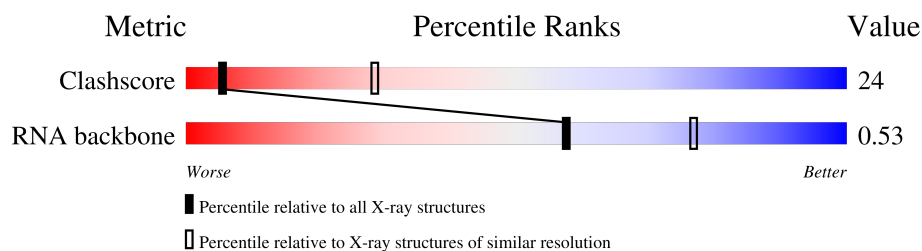
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	190562	1140 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

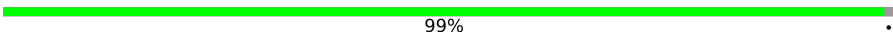
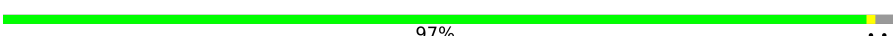
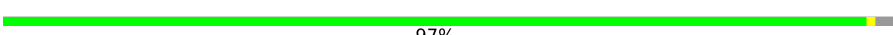
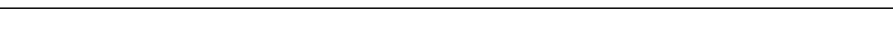
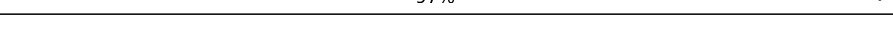
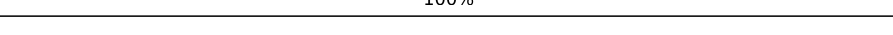
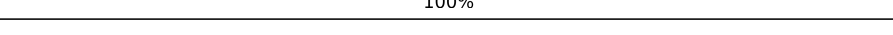
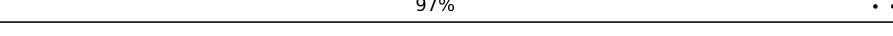
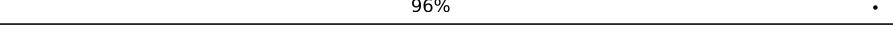
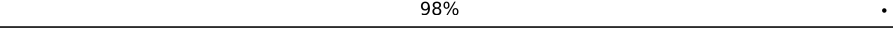
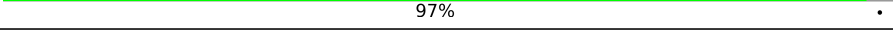
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	2880	26% 56% 13% .
2	9	124	19% 60% 16% . 5%
3	A	274	99% .
4	B	211	96% ..
5	C	204	97% .
6	D	180	98% ..
7	E	185	95% . .
8	F	146	34% . 64%
9	G	144	99% .

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Mol	Chain	Length	Quality of chain
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%

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 65355 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 114	C 114	0	0	114

- Molecule 15 is a protein called ribosomal protein L18.

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

- Molecule 16 is a protein called ribosomal protein L19.

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

- Molecule 17 is a protein called ribosomal protein L20.

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

- Molecule 18 is a protein called ribosomal protein L21.

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

- Molecule 19 is a protein called ribosomal protein L22.

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

- Molecule 20 is a protein called ribosomal protein L23.

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

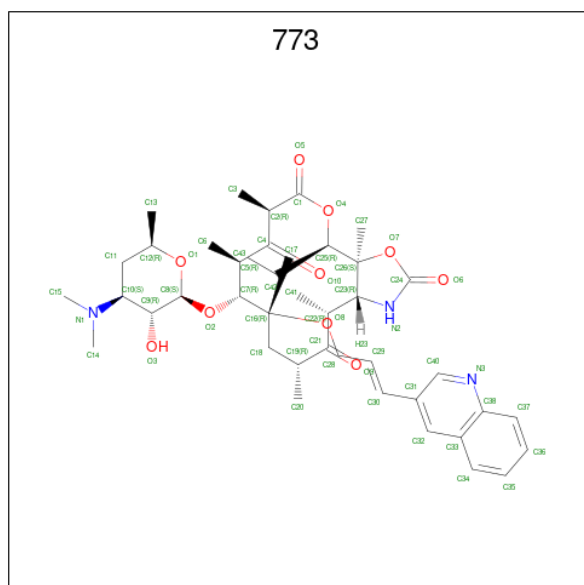
- Molecule 30 is a protein called ribosomal protein L35.

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 CETHROMYCIN (CCD ID: 773) (formula: $C_{42}H_{59}N_3O_{10}$).



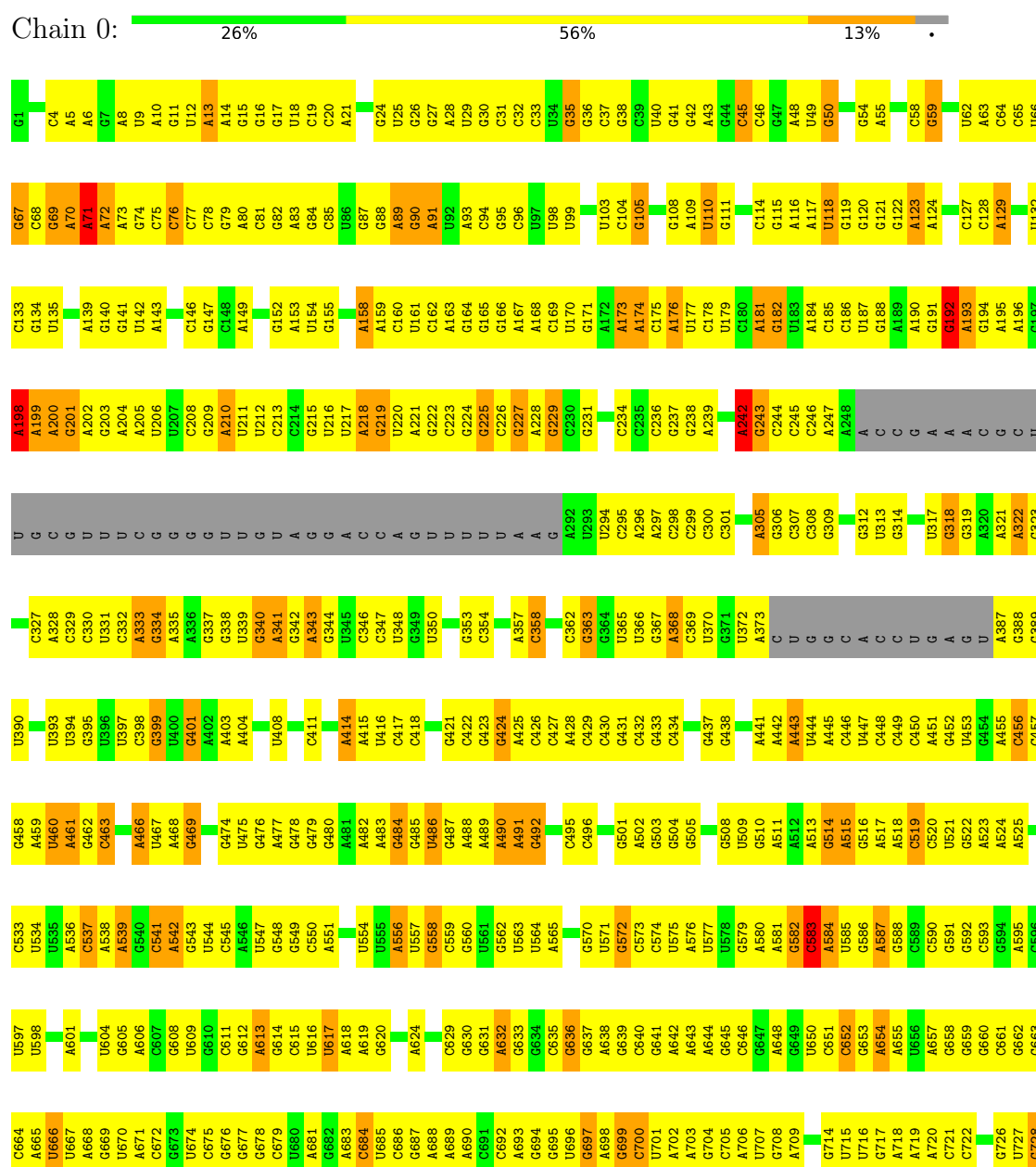
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	0	1	Total C N O 55 42 3 10	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

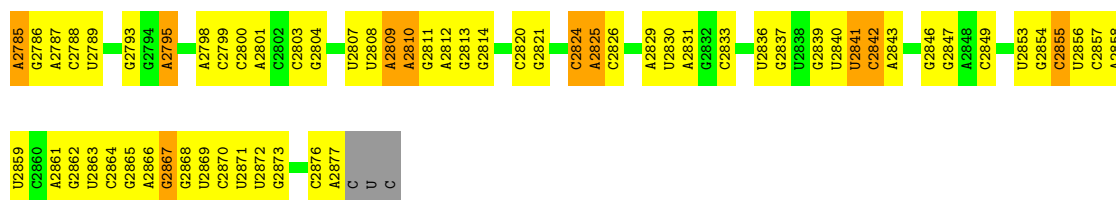
Note EDS was not executed.

• Molecule 1: 23S RIBOSOMAL RNA



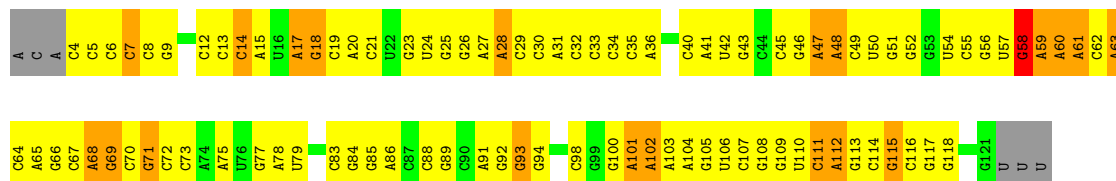
C1691	C1692	A1693	A1694	A1695	A1696	A1697	A1698	A1699	C1703	C1704	U1705	A1706	A1707	C1708	U1709	U1710	C1711	G1712	G1713	A1714	A1715	G1716	A1717	A1718	G1719	G1720	A1721	G1722	G1723	C1724	C1725	C1726	C1727	A1728	C1729	G1730	C1731	C1736	C1737	U1738	G1739	G1740	G1741	G1742	C1743	G1747	U1748	A1749	A1750	A1751	U1752	A1753	G1754	G1755	C1756	U1757	C1758	C1759	C1760	C1761	A1762	A1763	A1764	C1765	A1766	C1767	U1768	C1769	U1770	C1771	A1772	G1773	A1774	U1775	G1776	A1777	G1778	G1781	U1782	G1783	U1784	U1785	U1786	A1787	A1788	U1789	A1790	U1791	U1792	G1793
G1488	C1489	U1490	C1491	A1492	C1493	U1494	A1495	G1496	U1500	C1501	G1502	G1503	G1504	U1505	A1509	A1512	U1513	C1514	U1515	A1516	C1517	C1518	A1585	A1586	A1587	A1588	A1589	C1590	U1591	U1592	C1593	A1594	A1595	A1596	A1597	C1598	G1599	U1600	U1601	A1602	A1603	A1604	A1605	U1608	G1609	A1610	U1611	U1612	A1613	C1614	C1615	C1552	G1553	G1554	A1555	A1618	A1619	C1620																																
U1426	G1427	A1428	C1429	U1430	C1431	G1432	A1433	G1436	A1437	G1438	G1439	G1440	A1441	C1442	G1443	A1444	U1445	U1446	A1448	C1449	G1450	U1451	U1452	C1455	C1456	A1457	A1458	U1459	G1460	C1461	A1463	A1464	G1465	C1466	U1467	A1468	U1469	G1470	G1471	C1472	U1473	U1474	U1475	G1476	G1477	U1478	G1479	A1480	U1481	U1482	G1483	G1484	U1485	A1486	C1487																																			
U1357	C1358	G1359	C1360	C1361	C1362	U1363	C1364	U1365	G1368	G1367	A1368	G1369	A1370	C1371	A1372	G1373	G1374	C1375	C1376	G1377	A1378	A1379	C1380	G1381	C1382	C1383	G1384	C1385	A1386	G1387	C1388	C1389	C1390	A1391	U1392	G1393	A1397	G1398	C1399	A1400	G1401	U1402	A1403	A1404	A1405	A1406	G1407	U1408	U1409	U1410	C1411	C1412	A1416	C1417	A1418	G1419	C1422	A1423	U1424	G1425																														
G1296	A1297	G1298	A1299	C1300	U1301	C1302	U1303	U1304	C1305	U1306	U1307	C1308	G1309	C1310	G1311	G1312	U1313	A1314	A1315	G1316	A1317	A1318	C1319	U1320	U1321	A1322	G1323	G1324	U1325	U1326	C1327	C1328	U1329	G1332	G1333	A1334	G1335	G1336	G1337	U1338	C1339	A1340	U1341	C1342	C1343	G1344	C1345	C1346	C1347	A1348	A1349	A1350	G1351	G1352	A1353	A1354	G1355	G1356																																
C1230	C1231	A1233	C1234	C1235	A1238	G1241	A1242	G1243	U1244	G1245	U1246	U1247	C1248	A1249	A1250	G1251	C1252	C1253	A1254	A1255	C1256	U1257	G1258	A1259	A1260	G1261	U1262	C1263	C1264	G1265	G1266	U1267	U1268	A1269	C1270	C1271	G1272	G1273	U1274	A1275	A1276	A1277	A1278	A1279	U1280	A1281	G1282	A1283	U1284	A1285	U1286	A1287	A1288	A1289	A1290	G1291	A1292	A1293	A1294	U1295																														
G1082	C1083	C1086	C1087	C1088	C1089	C1090	C1091	U1092	A1095	A1096	A1099	U1100	U1101	C1102	C1103	G1110	U1111	U1112	C1113	A1114	C1115	U1116	G1117	C1121	A1122	G1123	U1124	G1125	A1126	U1130	G1131	C1132	G1133	C1134	C1135	A1136	A1137	A1138	A1139	A1140	U1141	G1142	C1145	G1146	G1147	G1148	G1149	C1150	U1151	C1152	A1153	A1154																																						
C1002	C1003	U1004	C1006	A1007	G1008	C1009	U1010	U1011	A1012	C1016	C1017	C1018	U1019	A1020	A1021	A1022	U1023	G1024	A1025	U1026	C1027	G1028	C1029	U1030	C1031	A1032	G1033	U1034	C1035	G1036	U1037	U1038	A1039	A1040	G1041	U1044	C1054	A1055	U1056	A1057	G1058	C1064	A1065	G1066	G1067	A1068	G1069	C1073	C1074	C1075	U1076	A1081																																						
G933	A936	C937	G938	C939	G940	U941	U942	U943	A944	G945	A951	A952	G953	U954	G955	A956	G957	G958	U960	G961	A964	G965	C968	U969	A970	A971	C972	U973	C974	C975	C976	G977	U978	A979	G980	C981	C982	G983	A984	G985	U986	A987	A988	A989	A990	A991	A994	A995	C996	C997	C998	A999	G1000	A1001																																				
C864	U865	U866	U867	U868	C869	C870	U871	U872	U873	A874	G875	A876	A886	G887	G888	C889	U890	A891	G892	A893	A894	A895	A896	A897	C898	U899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	C914	C915	U916	U917	U918	U919	A922	A923	C926	G927	G928	A929	A930	U931	G932																																			
A794	A795	A796	A797	G798	G799	U800	A801	A802	C803	C804	G805	A806	A807	C808	G809	G810	G811	G812	A813	G814	A815	U816	G817	A818	A819	A820	A821	U824	C825	U826	C829	C830	G831	A832	U837	A838	U839	U840	G841	A842	G843	G844	A847	U848	U852	C853	G854	G855	A856	U857	G858	A790	U859	U860	G861																																			
G732	G733	G734	G735	G736	G737	G738	G739	A740	C741	G742	A743	C744	G745	G746	C750	G751	G752	U753	C754	C755	C756	U757	G758	U759	U760	G761	A762	A763	A764	C765	A766	C767	U768	C769	U770	C771	A772	G773	A774	U775	G776	A777	G778	G781	U782	G783	U784	U785	U786	A787	G788	G789	A790	U791	U792	G793																																		





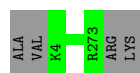
• Molecule 2: 5S RIBOSOMAL RNA

Chain 9: 19% 60% 16% 5%



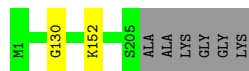
• Molecule 3: ribosomal protein L2

Chain A: 99%



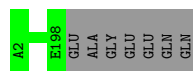
• Molecule 4: ribosomal protein L3

Chain B: 96%



• Molecule 5: ribosomal protein L4

Chain C: 97%



• Molecule 6: ribosomal protein L5

Chain D: 98%



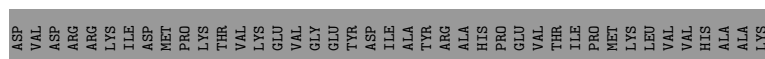
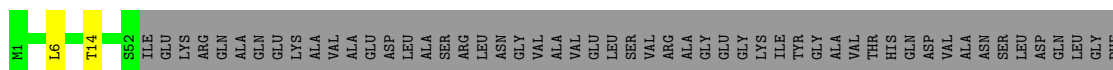
• Molecule 7: ribosomal protein L6

Chain E: 95%



- Molecule 8: ribosomal protein L9

Chain F: 34% 64%



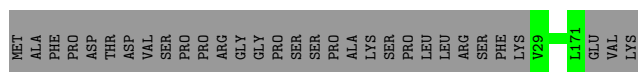
- Molecule 9: ribosomal protein L11

Chain G: 99%



- Molecule 10: ribosomal protein L13

Chain H: 82% 18%



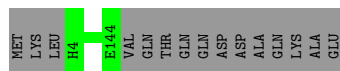
- Molecule 11: ribosomal protein L14

Chain I: 99%



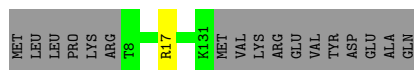
- Molecule 12: ribosomal protein L15

Chain J: 90% 10%

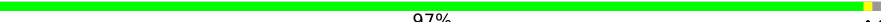


- Molecule 13: ribosomal protein L16

Chain K: 87% 12%

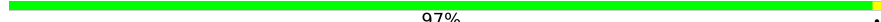


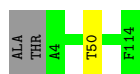
- Molecule 14: ribosomal protein L17

Chain L:  97% ..



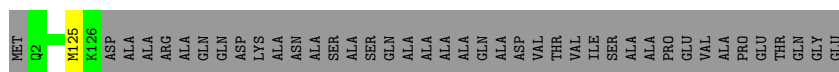
- Molecule 15: ribosomal protein L18

Chain M:  97% ..

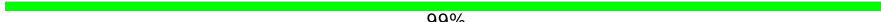


- Molecule 16: ribosomal protein L19

Chain N:  75% . 25%

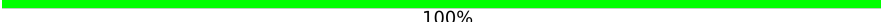


- Molecule 17: ribosomal protein L20

Chain O:  99% .

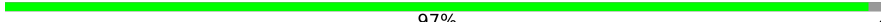


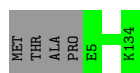
- Molecule 18: ribosomal protein L21

Chain P:  100%

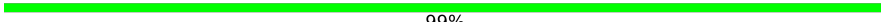
There are no outlier residues recorded for this chain.

- Molecule 19: ribosomal protein L22

Chain Q:  97% .

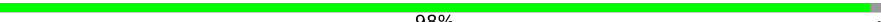


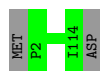
- Molecule 20: ribosomal protein L23

Chain R:  99% .



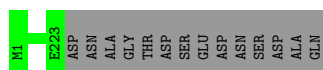
- Molecule 21: ribosomal protein L24

Chain S:  98% .



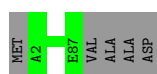
- Molecule 22: general stress protein Ctc

Chain T: 94% 6%



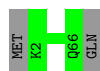
- Molecule 23: ribosomal protein L27

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.

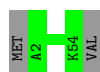
- Molecule 27: ribosomal protein L32

Chain Z: 97% ..

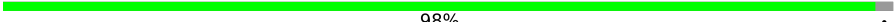


- Molecule 28: ribosomal protein L33

Chain 1: 96% .

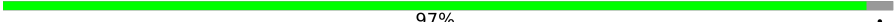


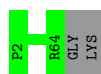
- Molecule 29: ribosomal protein L34

Chain 2:  98% .



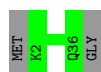
- Molecule 30: ribosomal protein L35

Chain 3:  97% .



- Molecule 31: ribosomal protein L36

Chain 4:  95% 5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	171.00 Å 409.50 Å 695.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.285 , 0.313	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	65355	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 773

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	0.26	0/66467	0.59	15/103673 (0.0%)
2	9	0.45	0/2816	0.80	1/4388 (0.0%)
All	All	0.27	0/69283	0.60	16/108061 (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.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2018	G	C2'-C3'-O3'	7.19	120.28	109.50
1	0	242	A	C2'-C3'-O3'	6.85	119.77	109.50
1	0	192	G	C2'-C3'-O3'	6.31	118.97	109.50
1	0	71	A	C2'-C3'-O3'	5.77	118.16	109.50
1	0	1279	G	C4'-C3'-O3'	-5.77	104.34	113.00

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 ⓘ

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	2133	0
2	9	2519	0	1285	147	0
3	A	270	0	0	0	0
4	B	205	0	0	2	0
5	C	197	0	0	0	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	55	0	59	9	0
All	All	65355	0	31261	2278	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 2278 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)
1:0:2041:A:N6	32:0:2881:773:H143	1.54	1.19
1:0:2548:G:H2'	1:0:2549:G:H5''	1.21	1.17
1:0:1679:U:H2'	1:0:1680:U:H5''	1.27	1.16
1:0:2041:A:H61	32:0:2881:773:C14	1.58	1.16
1:0:1966:C:H4'	1:0:2585:C:H4'	1.22	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%)	482 (17%)	41 (1%)
2	9	117/124 (94%)	23 (19%)	1 (0%)
All	All	2874/3004 (95%)	505 (17%)	42 (1%)

5 of 505 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 42 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1975	G

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Mol	Chain	Res	Type
1	0	2261	G
1	0	2015	G
1	0	2161	C
1	0	2404	A

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	773	0	2881	-	58,59,59	1.82	11 (18%)	74,88,88	1.46	12 (16%)

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	773	0	2881	-	-	2/67/98/98	0/4/5/5

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	2881	773	C35-C34	-5.90	1.24	1.36
32	0	2881	773	C37-C38	-5.34	1.33	1.41
32	0	2881	773	C5-C4	-5.29	1.44	1.52
32	0	2881	773	C2-C4	4.06	1.58	1.52
32	0	2881	773	C22-C21	-3.04	1.47	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	2881	773	O7-C24-N2	-5.29	105.73	109.80
32	0	2881	773	O6-C24-N2	4.11	134.05	129.19
32	0	2881	773	O9-C21-C22	3.03	124.85	120.64
32	0	2881	773	C23-N2-C24	2.99	116.29	112.39
32	0	2881	773	C42-C25-C26	2.81	119.11	115.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

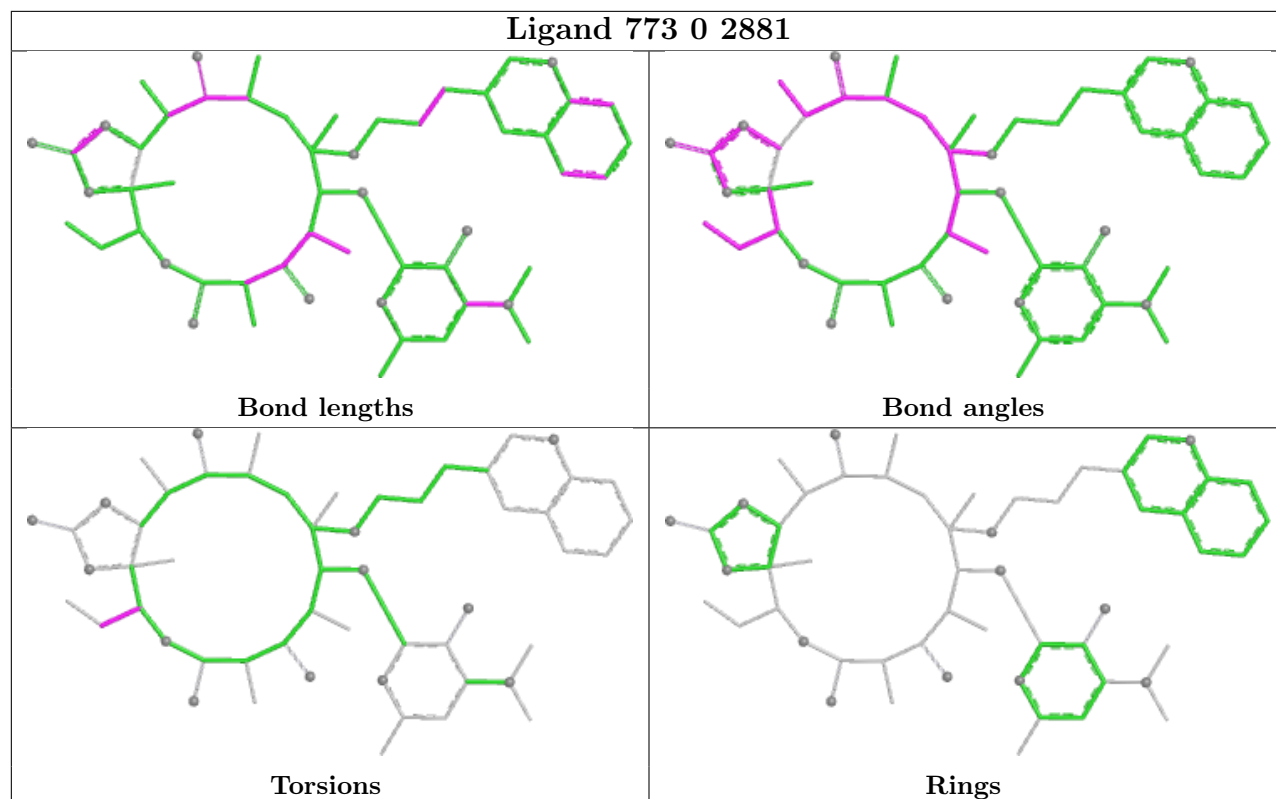
Mol	Chain	Res	Type	Atoms
32	0	2881	773	O4-C25-C42-C43
32	0	2881	773	C26-C25-C42-C43

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	0	2881	773	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.