



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 04:29 AM UTC

PDB ID : 1XBP / pdb_00001xbp
Title : Inhibition of peptide bond formation by pleuromutilins: The structure of the 50S ribosomal subunit from *Deinococcus radiodurans* in complex with Tiamulin
Authors : Schluenzen, F.; Pyetan, E.; Fucini, P.; Yonath, A.; Harms, J.M.
Deposited on : 2004-08-31
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)
Xtriage (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

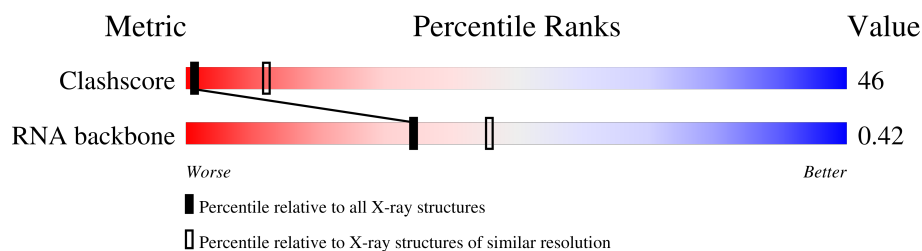
1 Overall quality at a glance

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)

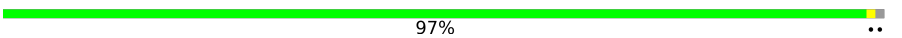
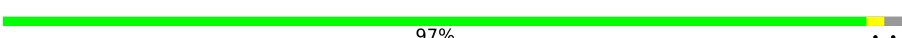
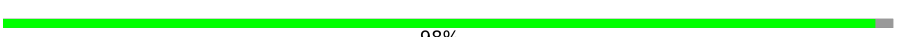
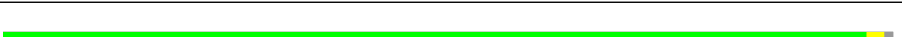
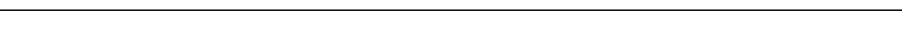
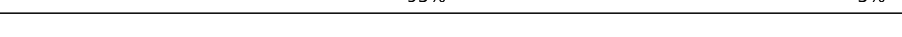
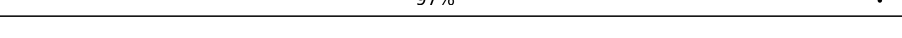
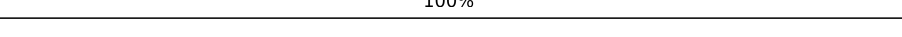
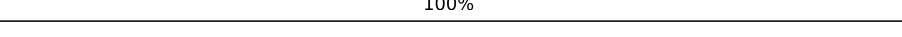
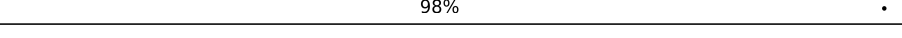
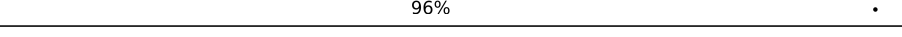
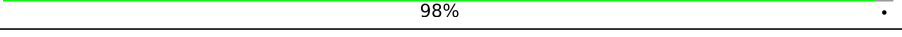
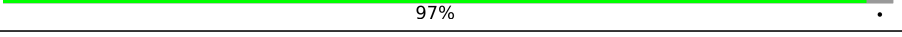
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	11% 62% 19% . .
2	9	124	13% 69% 14% 5%
3	A	274	98% ..
4	B	211	96% ..
5	C	204	97% .
6	D	180	99% .
7	E	185	95% . .
8	F	146	36% 64%
9	G	144	99% .

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Mol	Chain	Length	Quality of chain
10	H	174	
11	I	134	
12	J	156	
13	K	141	
14	L	116	
15	M	113	
16	N	166	
17	O	118	
18	P	100	
19	Q	134	
20	R	94	
21	S	115	
22	T	237	
23	U	91	
24	W	67	
25	X	55	
26	Y	73	
27	Z	59	
28	1	55	
29	2	47	
30	3	65	
31	4	37	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 65328 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
			2516	1124	464	811	117			

- 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	0	0	177
			177	177			

- Molecule 8 is a protein called 50S 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 50S 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 50S 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 50S 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 50S 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 50S 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 50S ribosomal protein L18.

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

- Molecule 16 is a protein called 50S 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 50S ribosomal protein L20.

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

- Molecule 18 is a protein called 50S 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 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
19	Q	127	Total	C	0	0	127
			127	127			

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

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

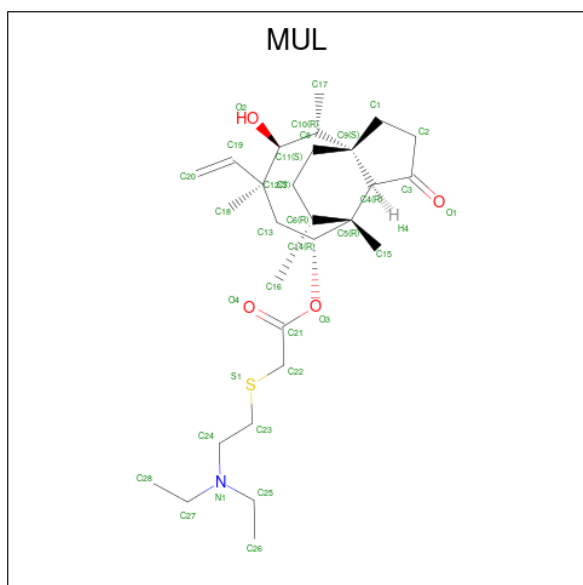
- Molecule 30 is a protein called 50S ribosomal protein L35.

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

- Molecule 32 is TIAMULIN (CCD ID: MUL) (formula: $C_{28}H_{47}NO_4S$).



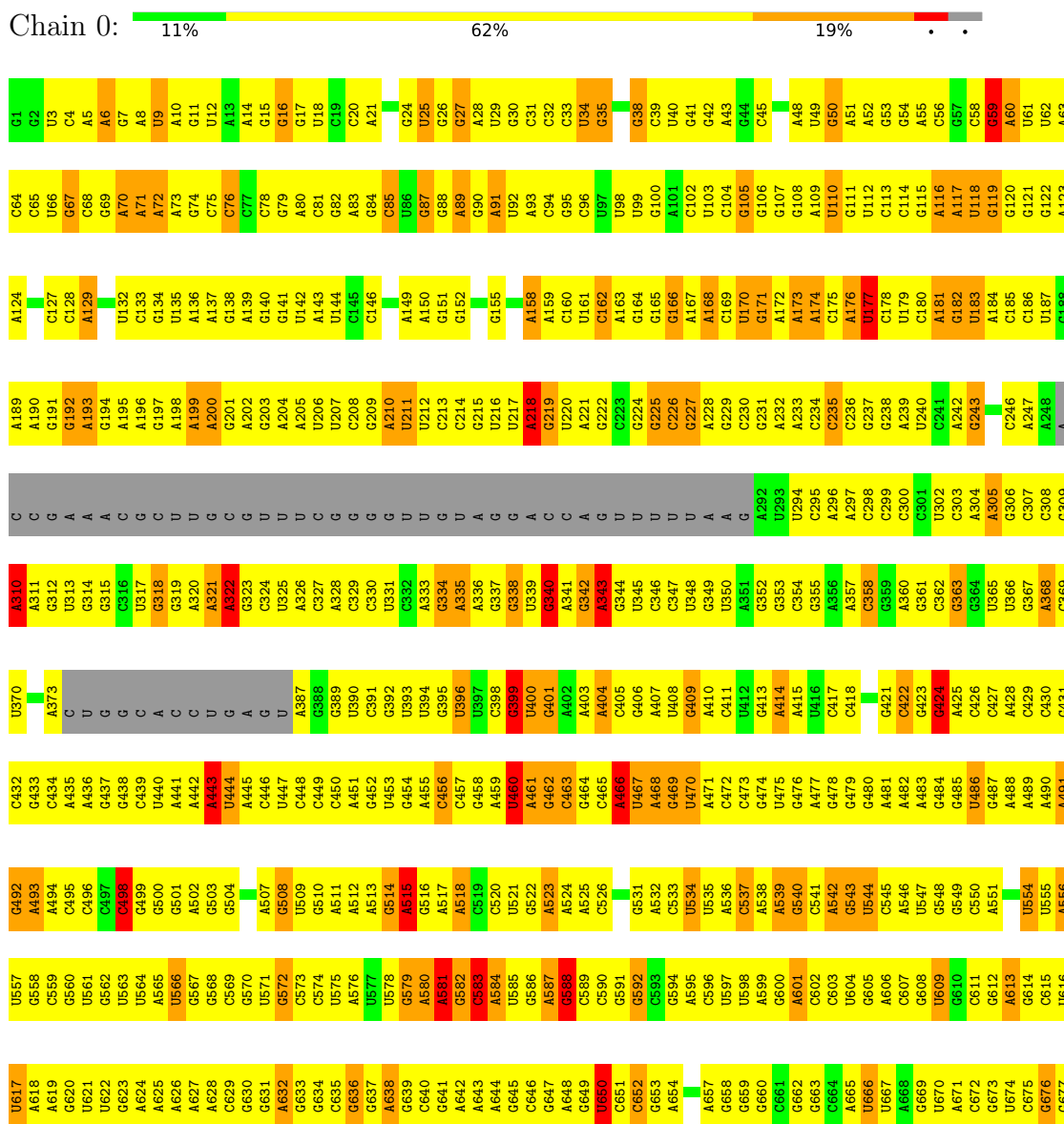
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	0	1	Total C N O S 34 28 1 4 1	0	0

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.

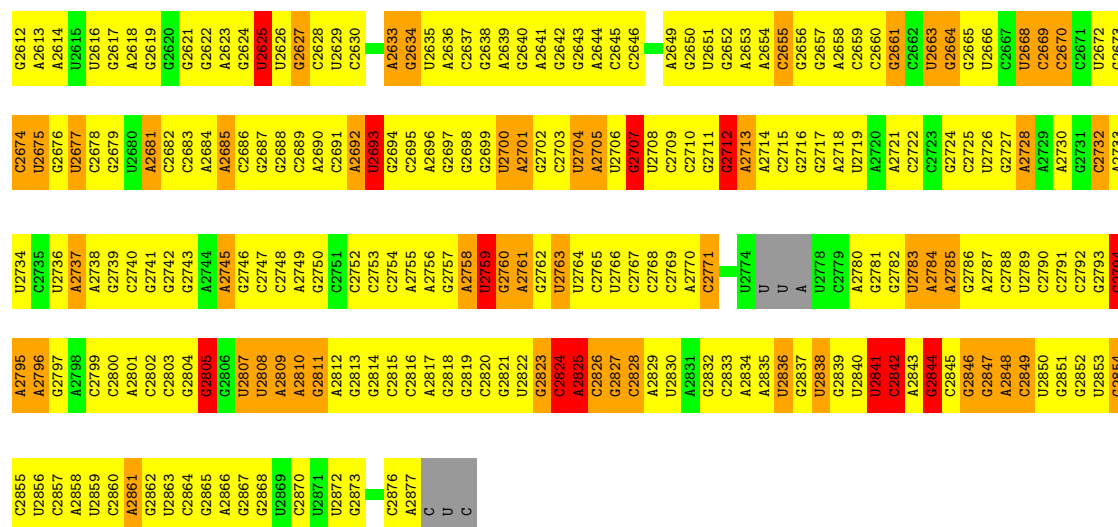
Note EDS was not executed.

• Molecule 1: 23S RIBOSOMAL RNA



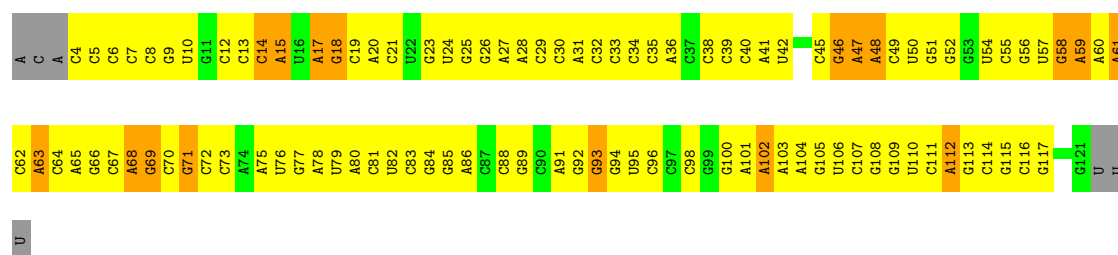
A1610	G1545	U1481	C1234	U1172	G1110	U1044	G983	A922	G861	A801	A740	G678
A1611	C1546	U1482	C1235	G1173	C1111	G1045	A984	A923	A862	A802	G741	C679
A1612	U1547	G1483	G1236	G1174	C1112	U1046	C985	C924	C863	C803	G742	U680
G1613	U1548	G1484	G1237	A1175	C1113	G1047	A986	U925	C864	C804	A743	A681
C1614	C1549	U1485	A1239	U1176	C1114	U1048	A987	C926	A865	G805	C744	G682
C1615	G1552	G1486	U1300	U1177	C1115	C1049	G988	G927	U866	A806	G745	A683
G1616	C1553	A1362	G1240	G1181	C1116	G1052	G989	G928	U867	A807	G746	C684
G1617	G1554	C1363	G1241	U1182	G1117	G1053	A990	A929	U868	C808	A747	U685
G1618	U1555	G1364	A1242	U1183	G1118	G1054	A991	A930	C869	C809	A748	C686
A1619	C1556	U1487	G1243	G1184	C1119	U1055	C992	G931	C870	U810	C749	G687
C1620	U1557	A1366	U1244	C1185	C1120	A1056	A993	G932	U871	G811	C750	A688
G1621	C1558	G1367	G1245	G1186	C1121	U1057	A994	G933	G872	G812	A751	A689
C1622	G1559	C1368	G1246	U1187	G1125	G1058	C995	G934	U873	A813	G752	A690
C1623	A1560	G1369	U1249	A1188	C1126	U1059	C996	C935	A874	G814	U753	C691
A1624	G1561	U1370	A1250	U1189	A1127	A1060	C997	A936	C875	A815	G754	C692
A1625	U1562	C1371	C1251	G1128	C1127	C1060	C998	C937	A876	U816	C755	A693
A1626	G1563	A1372	C1252	G1129	C1128	G1061	A999	G940	C877	A817	G756	G694
C1627	U1564	G1373	U1253	U1190	C1129	C1062	U1000	U941	C878	G818	U757	G695
G1628	C1565	C1374	G1254	G1191	U1130	A1065	A1001	U942	A879	C819	G758	U696
C1629	U1566	A1375	A1255	G1192	G1131	U1066	C1002	U943	C880	U820	C759	G697
A1630	G1567	G1376	C1256	U1193	C1132	G1067	C1003	U944	U881	A821	G760	A698
C1631	U1568	A1377	U1257	U1194	G1133	U1068	C1004	C982	A882	U822	G761	C699
A1632	A1569	G1378	G1258	G1195	C1134	C1069	U1005	G945	A883	U823	A762	C700
C1633	G1572	U1379	A1259	U1197	C1135	G1070	C1006	U946	A886	U824	A763	U701
A1634	U1573	C1380	U1260	U1198	G1136	U1071	A1007	C947	C887	C825	A764	A702
G1635	G1574	G1381	G1261	U1199	A1137	U1072	G1008	C948	C888	U826	C765	A703
C1636	U1575	C1382	U1262	G1200	A1138	G1073	G1009	C949	C889	C827	A766	G704
G1637	A1576	G1383	C1263	U1201	C1139	G1074	U1010	G950	C890	C828	C767	C705
G1638	C1577	U1448	C1264	U1202	G1140	C1075	U1011	G951	U890	C829	A768	A706
U1639	U1578	G1449	G1265	A1203	U1141	U1076	A1012	A952	A891	C830	U770	U707
C1640	G1579	C1450	G1266	U1204	G1142	U1077	G1013	G953	G	G831	C771	G708
G1641	U1580	A1386	U1267	G1205	A1143	A1078	G1014	U954	C	A832	C772	A709
C1642	C1581	G1387	U1268	G1206	U1144	G1079	U1015	G955	G	A833	C773	C710
A1643	U1582	C1388	C1269	U1207	C1145	A1080	C1016	A956	G	U834	A774	C711
G1644	G1583	G1389	C1270	A1208	G1146	A1081	C1017	G957	G	U835	C775	A712
U1645	A1584	U1391	C1271	G1209	G1147	C1082	U1018	G958	C	G836	G776	G713
C1646	U1585	C1392	G1272	U1210	G1148	C1083	U1019	C959	C	U837	A777	G714
U1647	G1586	G1393	G1273	G1211	G1149	A1084	A1020	U960	U	A838	G778	U715
C1648	U1587	G1394	C1274	U1212	C1150	G1085	A1021	G961	A	U839	C779	U716
A1649	C1588	A1395	A1275	U1213	U1151	C1086	A1022	C962	C	U840	U780	G717
U1650	U1589	G1396	U1276	C1214	C1152	G1087	U1023	G963	C	G841	G781	A718
G1651	C1590	C1397	G1277	A1215	A1153	A1088	G1024	A964	A	A842	U782	A719
C1652	U1591	G1398	A1278	G1216	G1154	C1089	A1025	G965	C	G843	G783	A720
G1653	U1592	C1399	G1279	U1217	C1155	C1090	U1026	A966	C	G844	U784	C721
A1654	C1593	A1400	U1280	U1218	U1156	C1091	C1027	G967	U	U845	C722	C723
C1655	U1594	G1401	A1281	C1219	G1157	C1094	G1028	C968	U	A846	U786	G726
U1656	C1595	U1402	A1282	U1220	A1158	A1095	C1029	U969	A	C847	A787	U727
A1657	U1596	C1403	C1283	C1221	U1159	A1096	U1030	A970	C	A848	G788	G728
C1658	G1597	U1404	G1284	G1222	C1160	A1097	C1031	A971	C	G849	A790	A729
G1659	U1598	A1405	A1285	G1223	U1161	A1098	A1032	C972	A911	C850	G791	C730
C1660	C1599	C1346	U1286	A1224	C1162	G1098	G1033	U973	A912	C851	U792	G733
G1661	U1600	G1407	A1287	G1225	U1163	C1099	U1034	U974	A913	U852	G793	A734
C1662	A1601	A1408	A1288	A1226	C1164	G1102	G1036	C975	C914	C853	A794	G735
G1663	U1602	C1348	A1289	A1227	G1165	G1103	U1037	C976	C915	G854	A795	G736
A1664	C1603	U1409	A1290	G1228	A1166	G1104	U1038	G977	U916	G855	A796	G737
C1665	U1604	G1410	G1291	C1229	U1167	U1105	A1039	A979	A918	U857	A797	G738
G1666	C1605	C1411	A1292	C1230	G1168	A1106	A1040	C980	U919	G858	G798	C739
A1667	U1606	U1412	A1293	U1231	C1169	A1107	G1041	C982	A921	U859	U800	
G1668	C1607	U1413	A1294	U1232	U1170							
C1669	U1608	G1414	G1294	U1233	A1171							
U1669	G1609	C1415	U1295	A1233								





• Molecule 2: 5S RIBOSOMAL RNA

Chain 9: 13% 69% 14% 5%



• Molecule 3: 50S ribosomal protein L2

Chain A: 98% ..



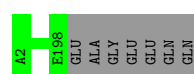
• Molecule 4: 50S ribosomal protein L3

Chain B: 96% ..

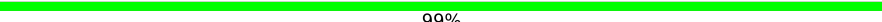


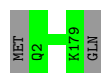
• Molecule 5: 50S ribosomal protein L4

Chain C: 97% .



• Molecule 6: 50S ribosomal protein L5

Chain D:  99% .



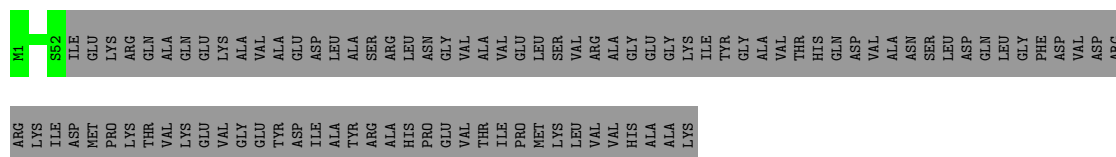
- Molecule 7: 50S ribosomal protein L6

Chain E:  95% ..

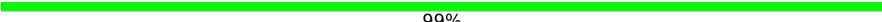


- Molecule 8: 50S ribosomal protein L9

Chain F:  36% 64%



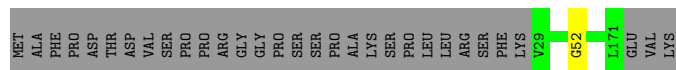
- Molecule 9: 50S ribosomal protein L11

Chain G:  99% .



- Molecule 10: 50S ribosomal protein L13

Chain H:  82% 18%



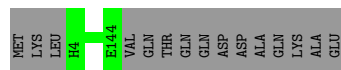
- Molecule 11: 50S ribosomal protein L14

Chain I:  97% ..



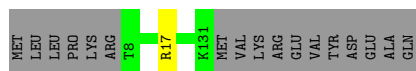
- Molecule 12: 50S ribosomal protein L15

Chain J:  90% 10%

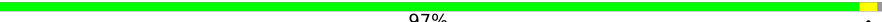


- Molecule 13: ribosomal protein L16

Chain K:  87% 12%

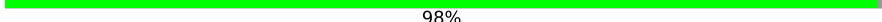


- Molecule 14: 50S ribosomal protein L17

Chain L:  97%



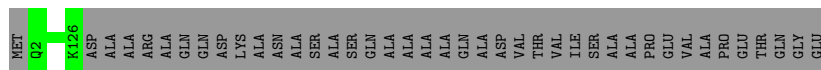
- Molecule 15: 50S ribosomal protein L18

Chain M:  98%

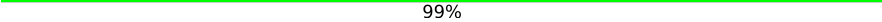


- Molecule 16: 50S ribosomal protein L19

Chain N:  75% 25%



- Molecule 17: 50S ribosomal protein L20

Chain O:  99%

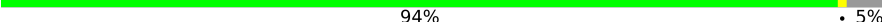


- Molecule 18: 50S ribosomal protein L21

Chain P:  100%

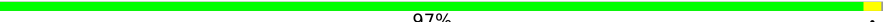
There are no outlier residues recorded for this chain.

- Molecule 19: 50S ribosomal protein L22

Chain Q:  94% 5%

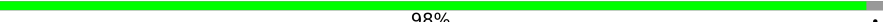


- Molecule 20: 50S ribosomal protein L23

Chain R:  97% ..



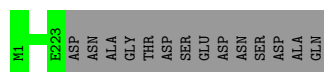
- Molecule 21: 50S ribosomal protein L24

Chain S:  98% .

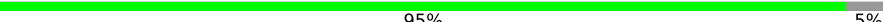


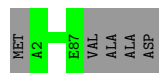
- Molecule 22: 50S ribosomal protein L25

Chain T:  94% 6%



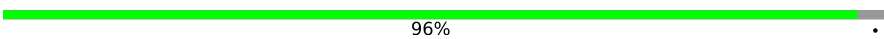
- Molecule 23: 50S ribosomal protein L27

Chain U:  95% 5%



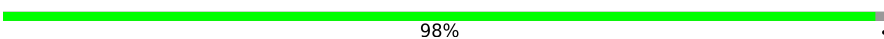


- Molecule 28: 50S ribosomal protein L33

Chain 1:  96% .

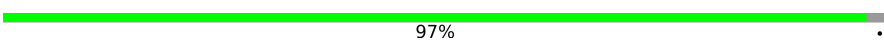


- Molecule 29: 50S ribosomal protein L34

Chain 2:  98% .

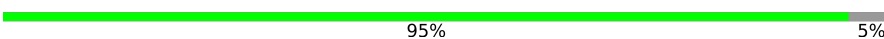


- Molecule 30: 50S ribosomal protein L35

Chain 3:  97% .



- Molecule 31: 50S 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	168.70 Å 405.00 Å 693.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.50	Depositor
% Data completeness (in resolution range)	88.3 (15.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.290 , 0.360	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	65328	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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: MUL

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	0.54	0/66467	0.90	145/103673 (0.1%)
2	9	0.37	0/2813	0.72	0/4384
All	All	0.54	0/69280	0.89	145/108057 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	260

There are no bond length outliers.

The worst 5 of 145 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2482	A	N9-C1'-C2'	8.91	125.37	112.00
1	0	192	G	C2'-C3'-O3'	8.37	122.06	109.50
1	0	1775	A	C4'-C3'-O3'	-8.06	100.91	113.00
1	0	1938	U	C2'-C3'-O3'	7.89	121.34	109.50
1	0	1710	U	N1-C1'-C2'	7.52	123.28	112.00

There are no chirality outliers.

5 of 260 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	16	G	Sidechain
1	0	27	G	Sidechain
1	0	6	A	Sidechain

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Mol	Chain	Res	Type	Group
1	0	67	G	Sidechain
1	0	9	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	29916	4242	0
2	9	2516	0	1286	147	0
3	A	270	0	0	2	0
4	B	205	0	0	3	0
5	C	197	0	0	0	0
6	D	178	0	0	0	0
7	E	177	0	0	1	0
8	F	52	0	0	0	0
9	G	143	0	0	0	0
10	H	143	0	0	1	0
11	I	132	0	0	2	0
12	J	141	0	0	0	0
13	K	124	0	0	1	0
14	L	114	0	0	3	0
15	M	111	0	0	0	0
16	N	125	0	0	0	0
17	O	117	0	0	0	0
18	P	100	0	0	0	0
19	Q	127	0	0	1	0
20	R	93	0	0	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	0	34	0	47	4	0
All	All	65328	0	31249	4380	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 46.

The worst 5 of 4380 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)
1:0:584:A:H4'	1:0:2038:C:N4	1.53	1.23
1:0:1621:C:H4'	1:0:1626:A:N6	1.57	1.19
1:0:918:A:H2'	1:0:919:U:H5''	1.24	1.18
1:0:1339:U:H5''	1:0:1994:U:H1'	1.21	1.18
1:0:1938:U:O2'	1:0:1939:U:H5'	1.42	1.18

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%)	514 (18%)	5 (0%)
2	9	117/124 (94%)	17 (14%)	1 (0%)
All	All	2874/3004 (95%)	531 (18%)	6 (0%)

5 of 531 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	34	U

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

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	2810	A
1	0	2824	C
2	9	58	G
1	0	2404	A
1	0	2377	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 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	MUL	0	2881	-	36,36,36	1.33	5 (13%)	55,55,55	1.62	7 (12%)

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	MUL	0	2881	-	-	4/18/79/79	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	2881	MUL	C5-C14	4.41	1.59	1.56
32	0	2881	MUL	C12-C11	3.24	1.58	1.55
32	0	2881	MUL	O3-C14	2.50	1.50	1.46
32	0	2881	MUL	C17-C10	2.08	1.57	1.53
32	0	2881	MUL	C10-C11	2.04	1.58	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	2881	MUL	O3-C21-C22	5.48	119.56	110.52
32	0	2881	MUL	C18-C12-C11	5.26	111.76	108.16
32	0	2881	MUL	C16-C6-C7	-2.99	105.97	110.33
32	0	2881	MUL	C9-C10-C11	2.92	115.19	112.46
32	0	2881	MUL	C17-C10-C11	-2.73	110.00	112.20

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	0	2881	MUL	C28-C27-N1-C24
32	0	2881	MUL	C28-C27-N1-C25
32	0	2881	MUL	C26-C25-N1-C27
32	0	2881	MUL	C26-C25-N1-C24

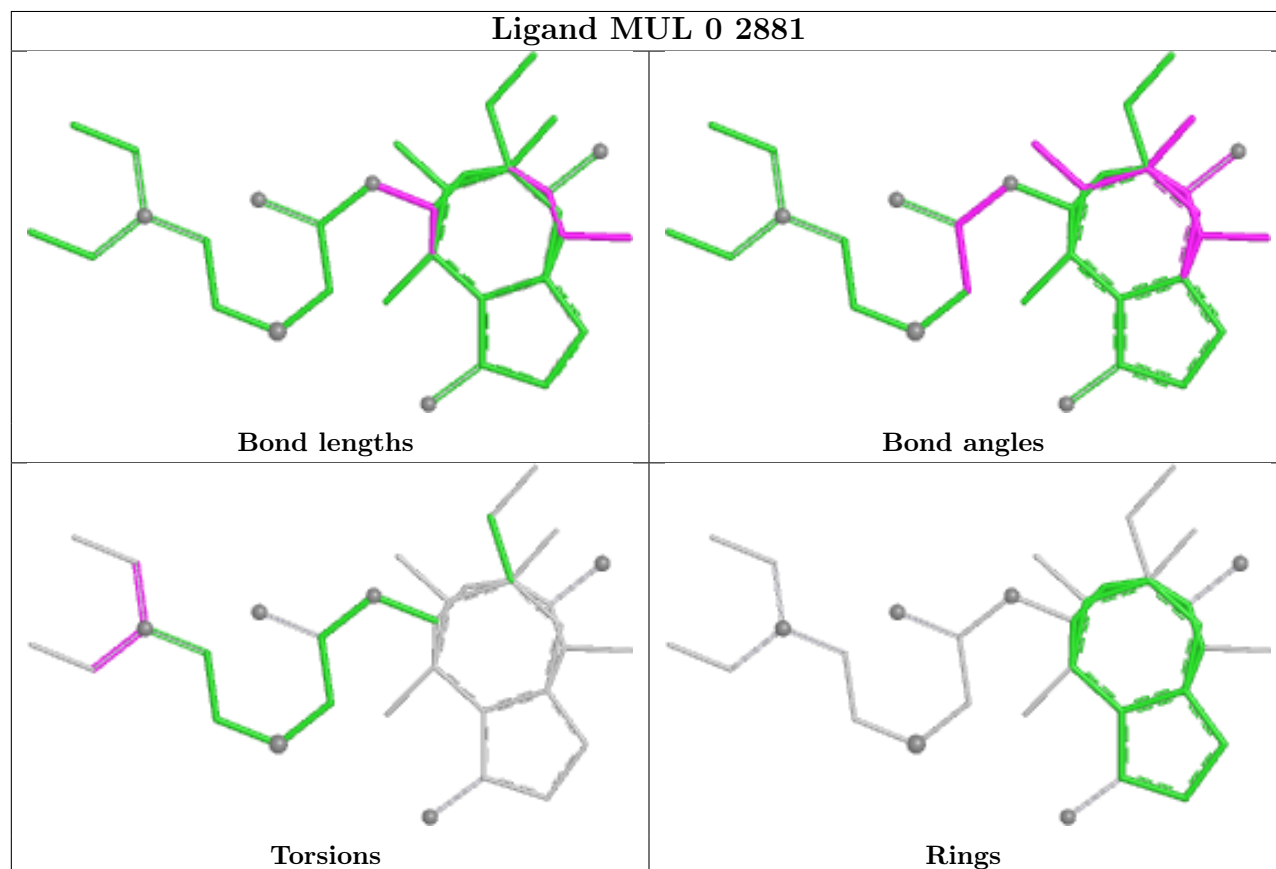
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	0	2881	MUL	4	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 [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.