



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 08:58 am BST

PDB ID : 1SM1
Title : COMPLEX OF THE LARGE RIBOSOMAL SUBUNIT FROM DEINOCOC-
CUS RADIODURANS WITH QUINUPRISTIN AND DALFOPRISTIN
Authors : Harms, J.M.; Schlutzen, F.; Fucini, P.; Bartels, H.; Yonath, A.
Deposited on : 2004-03-08
Resolution : 3.42 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

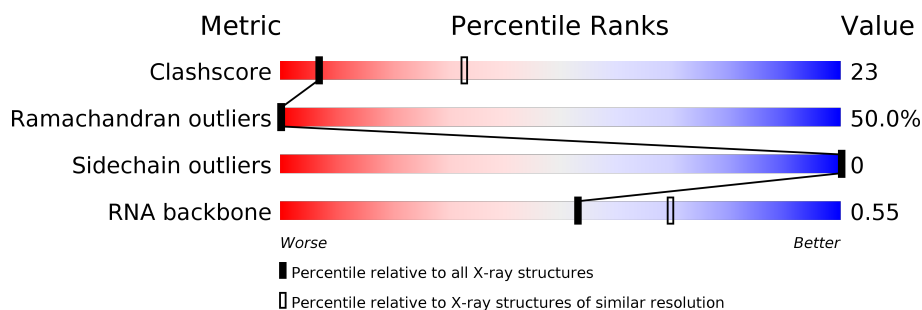
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.42 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	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RNA backbone	3102	1012 (3.88-2.96)

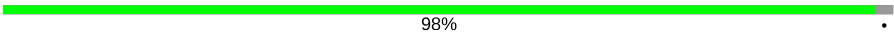

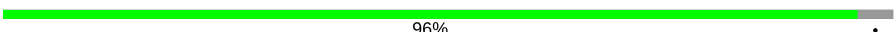











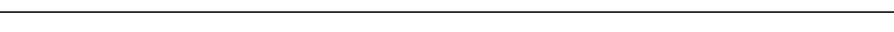
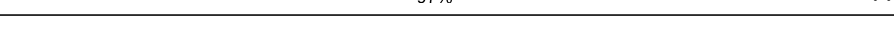
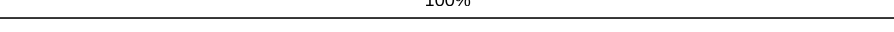
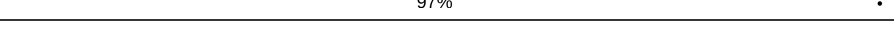
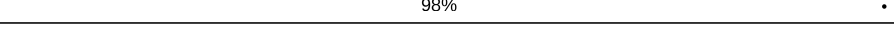
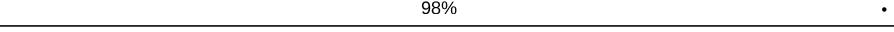

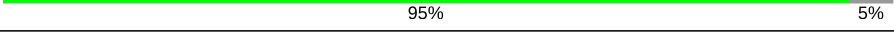
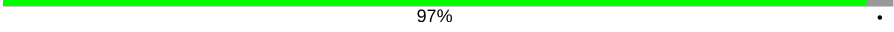
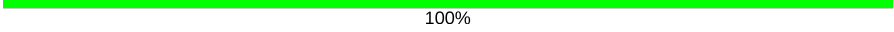
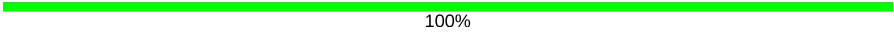
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	29% 53% 13% . .
2	1	82	65% 35%
3	2	47	98% .
4	3	66	95% 5%
5	4	37	95% 5%
6	5	8	63% 13% 25%
7	9	124	36% 54% 5% 5%

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Mol	Chain	Length	Quality of chain
8	A	275	 98%
9	B	211	 97%
10	C	205	 96%
11	D	180	 99%
12	E	212	 83%17%
13	F	146	 36%64%
14	G	144	 99%
15	H	174	 82%18%
16	I	134	 99%
17	J	156	 90%10%
18	K	142	 87%13%
19	L	116	 97%
20	M	114	 97%
21	N	166	 75%25%
22	O	118	 97%
23	P	100	 100%
24	Q	134	 97%
25	R	95	 98%
26	S	115	 98%
27	T	253	 88%12%
28	U	91	 95%5%
29	W	67	 97%
30	X	55	 100%
31	Y	73	 100%
32	Z	60	 95%

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
33	DOL	0	2882	X	-	-	-
6	DBB	5	3	-	-	X	-

2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 65418 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 protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	1	53	Total	C	0	0	53
			53	53			

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	2	46	Total	C	0	0	46
			46	46			

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	3	63	Total	C	0	0	63
			63	63			

- Molecule 5 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
5	4	35	Total	C	0	0	35
			35	35			

- Molecule 6 is a protein called QUINUPRISTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	5	8	Total	C	N	O	S	0	0	0
			73	53	9	10	1			

- Molecule 7 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	9	118	Total	C	N	O	P	0	0	0
			2516	1124	464	811	117			

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L6.

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

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L9.

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

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L11.

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

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L18.

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

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L19.

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

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

- Molecule 27 is a protein called GENERAL STRESS PROTEIN CTC.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L27.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L30.

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

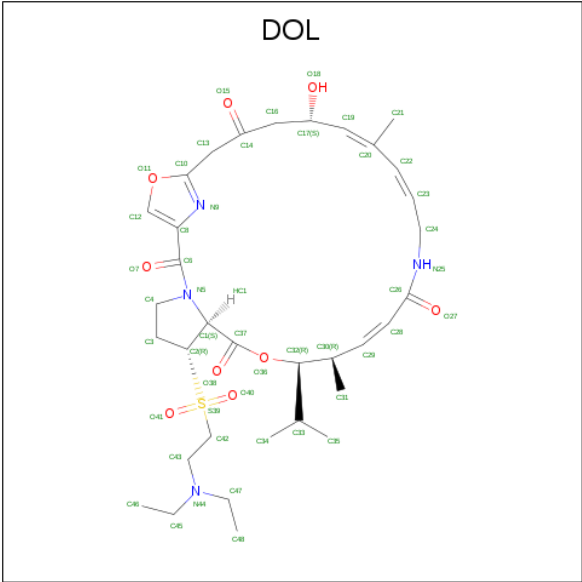
- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L31.

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L32.

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

- Molecule 33 is 5-(2-DIETHYLAMINO-ETHANESULFONYL)-21-HYDROXY-10-ISOPROPYL-11,19-DIMETHYL-9,26-DIOXA-3,15,28-TRIAZA-TRICYCLO[23.2.1.00,255]OCTACOSA-1(27),12,17,19,25(28)-PENTAENE-2,8,14,23-TETRAONE (three-letter code: DOL) (formula: C₃₄H₅₀N₄O₉S).



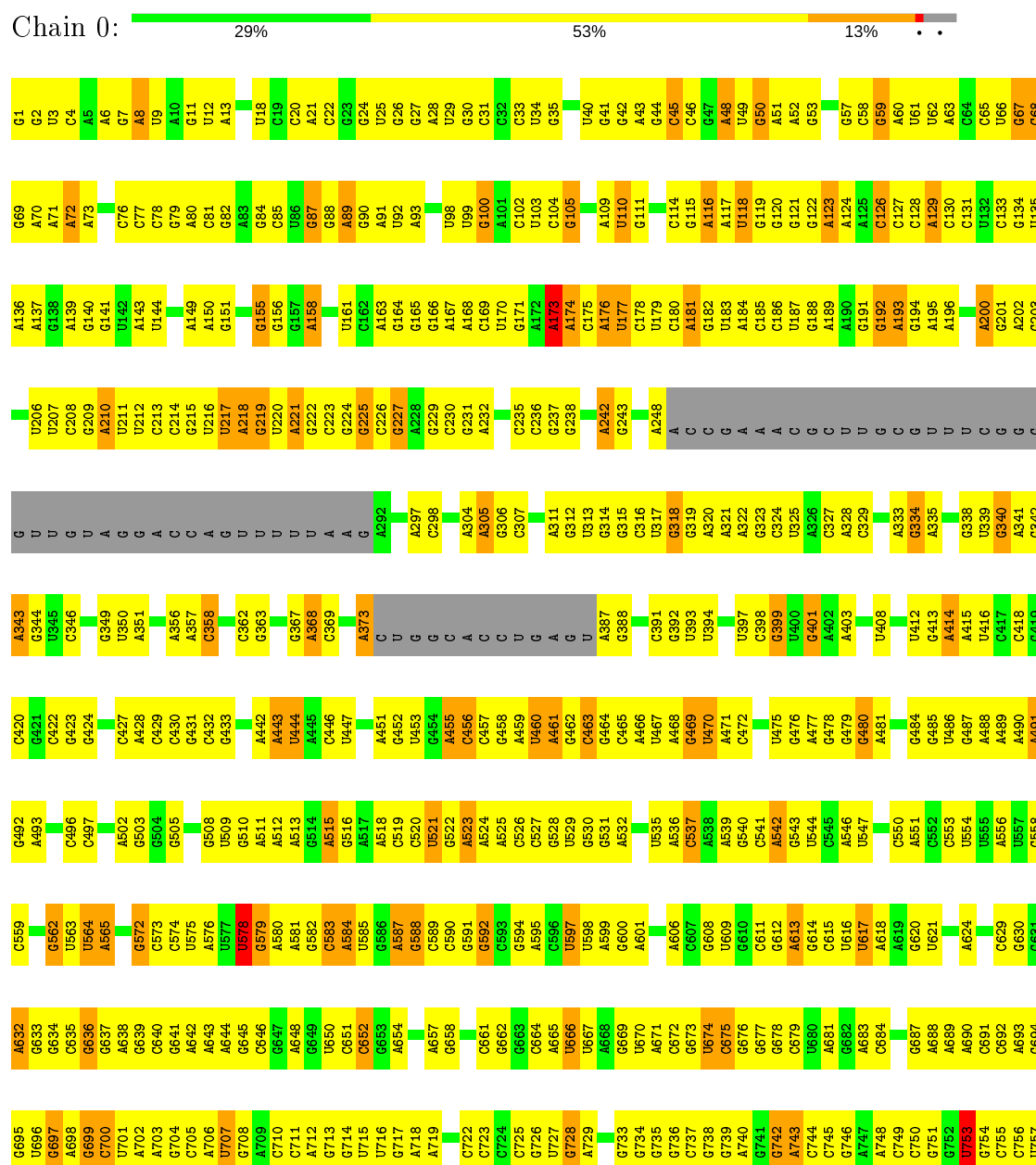
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	0	1	Total	C	N	O	S	0	0
			48	34	4	9	1		

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 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

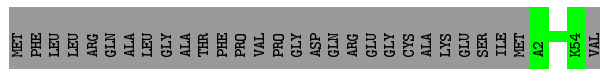


U1770	C1698	U1637	G1398	G1331	A1267	U1199	A1126	C1013	G957	G	A821	G758
A1771	A1699	G1638	C1399	G1332	U1268	G1200	A1131	A1022	G958	G	G822	C759
C1772	C1702	U1639	A1400	G1333	G1269	G1201	G1132	U1023	C959	G	U823	U760
C1773	G1702	C1640	A1560	A1334	C1270	U1202	G1133	G1024	U960	G	G824	G761
A1774	A1706	C1641	U1402	G1338	G1271	G1203	G1133	A1025	C962	C	G825	A762
A1775	A1707	G1642	U1403	U1339	G1272	G1204	G1136	U1026	C963	C	U826	A763
U1776	C1708	A1643	A1406	C1340	G1273	G1205	G1137	U1027	A964	U	C827	A764
C1779	U1709	U1645	A1407	G1341	C1274	G1206	A1138	C1027	G965	A	C828	C765
	G1710	G1646	U1408	U1342	U1275	G1207	A1139	U1028	G966	C	C829	
C1781	C1711	U1647	U1409	C1343	U1276	G1208	A1140	U1029	A967	C	C830	
A1782	G1712	U1648	U1410	C1344	U1277	G1209	U1141	U1030	G968	C	G831	
G1783	G1713	U1649	U1411	G1345	A1278	U1212	U1142	C1031	C969	A	A832	
C1784	A1714	A1650	G1414	C1346	U1280	U1213	A1143	A1032	U969	G	G772	
A1785	A1715	U1651	C1417	C1347	A1281	U1214	U1144	G1033	A970	C	A774	
G1786	G1716	U1652	C1418	U1348	A1282	A1215	U1145	U1034	A971	U	U775	
C1787	A1717	C1487	C1418	A1349	A1283		G1146	G1035	C972	U	G776	
U1788	A1718	U1488	U1418	A1352	G1284	G1218	G1147	G1036	U973	A	A777	
G1789	G1719	C1655	U1426	G1352	A1285	C1219	G1148	U1038	U974	C	G778	
C1790	G1720	U1656	G1427	A1353	U1286		G1149	A1039	C975	C	U779	
C1791	G1721	A1657	G1428	A1354	U1287	G1222	C1150	A1040	C976	A911	U840	
C1792	A1657	G1584	A1429	A1355	A1288	G1223	C1151	G1041	G977		G841	
A1793	G1722	A1585	G1430	G1356	A1289	A1224	C1152		U978		A842	
C1794	U1723	G1586	U1431	U1357	A1290	G1225	A1153	U1044	G980		G843	
C1795	G1724	A1587	G1432	C1358	G1291	A1226	A1154	G1045	U916		U844	
A1796	C1725	U1588	A1433	G1359	A1282	A1227	G1155	U1046	C981		U845	
C1797	C1726	G1662	U1433	U1360	A1283	G1228		U1047	C982		A846	
G1798	C1727	C1563	U1434	G1361	A1284	U1229	A1158		G983		C847	
A1799	G1730	G1664	G1435	C1363	A1285	C1230	U1159	C1052	A984		A848	
C1800	G1731	G1665	A1436	C1364	A1286	G1231	U1160	G1053	G985		U852	
A1801	C1731	G1666	A1437	G1365	A1300	U1232	U1161	C1054	G987		A790	
A1802	G1736	A1667	G1438	U1365	U1301	A1233	A1162	A1055	G988		G791	
G1803	G1737	G1668	A1441	A1366		A1234	C1163	U1056	G989		U792	
U1804	U1737	A1669	C1442	A1367	U1304	G1241	G1174	G1066	C996		G793	
G1805	G1744	A1670	G1443	G1368	A1510	C1235	C1164	A1067	C997		A856	
A1806	C1745	A1671	C1444	U1370	U1306		U1175	G1069	C998		A801	
C1807	A1746	U1672	U1445	G1371	U1307	A1242	A1177	G1073	A999		U866	
G1808	G1747	U1613	U1446	U1371	U1308	G1243	A1179	G1074	G1000		G867	
U1809		C1673	U1447	A1372	C1308	U1244	C1178	A1081	A1001		C803	
G1810	U1748	C1615	U1448	G1373	G1309		G1181	U1082	A1002		C804	
A1811	G1749	G1616	A1449	G1374	C1310		U1182	G1086	C1003		G805	
U1812	A1750	G1617	C1449	U1374	C1311	U1247	A1183	U1087	A1004		A806	
A1813	U1751	U1618	G1450		G1312	G1248	G1184		U941		C807	
	U1752	A1619	A1451	C1380	U1313	G1249	C1185		U942		U873	
G1816	A1753	C1620	A1453	G1381	A1314	A1250	G1186		U943		A874	
U1817	G1754	C1621	U1454	G1382	A1315	G1251	A1187		A1005		G875	
G1818	G1755	G1622	C1455	C1383	G1316	C1252	U1177		A1006		G876	
U1819	C1756	G1623	C1456	G1384	G1317	C1253	A1179		A1007		A877	
U1820	C1757	A1624	A1457	C1385	A1318	G1254	A1180		U944		G877	
A1821	G1758	A1625	A1458	C1386	C1319	A1255	G1181		A944		U878	
C1822	A1759	A1626	U1459	G1387	A1320	C1256	U1182		A1008		C809	
G1823	G1760	C1627	G1460	C1388	A1321	U1257	C1183		G1009		G811	
C1824	U1761	C1628	C1461	C1389	G1322	G1258	G1184		U1010		A812	
C1825	C1762	G1629	C1462	G1390	G1323	A1259	C1185		C947		G813	
U1826	G1763	A1630	A1463	A1391	G1324	A1260	G1186		C948		G814	
	A1764	C1631	G1464	U1392	U1325	G1261	A1187		G951		A883	
G1831	C1765	A1632	U1465	G1393	U1326	U1262	A1188		A952		C884	
G1832	U1766	C1633	C1466	G1394	C1327	G1263			G953		U816	
	G1767	U1695	U1467	A1395	C1328	C1264	G1196		U1015		C889	
	U1768	C1696	U1468	C1396	U1329	G1265	U1123		G954		G818	
		U1697	U1469	A1397	G1330	G1266	U1124		U1016		C890	
							G1125		C1017		A891	



- Molecule 2: 50S RIBOSOMAL PROTEIN L33

Chain 1:  65% 35%



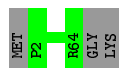
- Molecule 3: 50S RIBOSOMAL PROTEIN L34

Chain 2:  98%



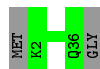
- Molecule 4: 50S RIBOSOMAL PROTEIN L35

Chain 3:  95% 5%



- Molecule 5: 50S RIBOSOMAL PROTEIN L36

Chain 4:  95% 5%



- Molecule 6: QUINUPRISTIN

Chain 5:  63% 13% 25%



- Molecule 7: 5S RIBOSOMAL RNA

Chain 9:  36% 54% 5% 5%



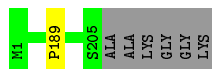
- Molecule 8: 50S RIBOSOMAL PROTEIN L2

Chain A:  98%



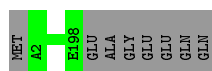
• Molecule 9: 50S RIBOSOMAL PROTEIN L3

Chain B: 97%



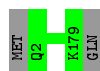
• Molecule 10: 50S RIBOSOMAL PROTEIN L4

Chain C: 96%



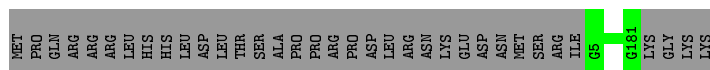
• Molecule 11: 50S RIBOSOMAL PROTEIN L5

Chain D: 99%



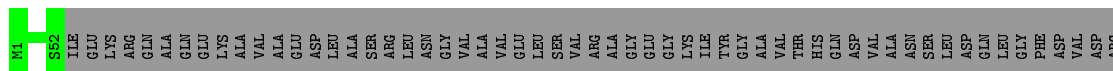
• Molecule 12: 50S RIBOSOMAL PROTEIN L6

Chain E: 83% 17%



• Molecule 13: 50S RIBOSOMAL PROTEIN L9

Chain F: 36% 64%



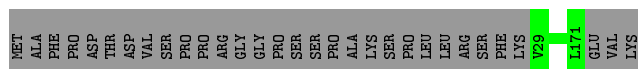
• Molecule 14: 50S RIBOSOMAL PROTEIN L11

Chain G: 99%



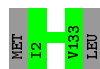
• Molecule 15: 50S RIBOSOMAL PROTEIN L13

Chain H: 82% 18%



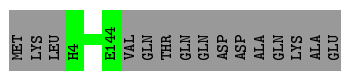
• Molecule 16: 50S RIBOSOMAL PROTEIN L14

Chain I: 99% .



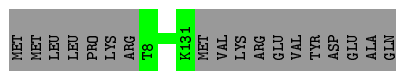
• Molecule 17: 50S RIBOSOMAL PROTEIN L15

Chain J: 90% 10%



• Molecule 18: 50S RIBOSOMAL PROTEIN L16

Chain K: 87% 13%



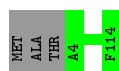
• Molecule 19: 50S RIBOSOMAL PROTEIN L17

Chain L: 97% ..



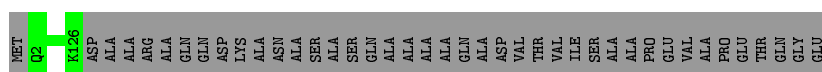
• Molecule 20: 50S RIBOSOMAL PROTEIN L18

Chain M: 97% .



• Molecule 21: 50S RIBOSOMAL PROTEIN L19

Chain N: 75% 25%



• Molecule 22: 50S RIBOSOMAL PROTEIN L20

Chain O: 97% ..



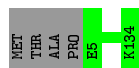
- Molecule 23: 50S RIBOSOMAL PROTEIN L21

Chain P: 100%

There are no outlier residues recorded for this chain.

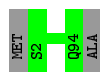
- Molecule 24: 50S RIBOSOMAL PROTEIN L22

Chain Q: 97%



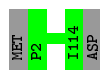
- Molecule 25: 50S RIBOSOMAL PROTEIN L23

Chain R: 98%



- Molecule 26: 50S RIBOSOMAL PROTEIN L24

Chain S: 98%



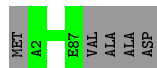
- Molecule 27: GENERAL STRESS PROTEIN CTC

Chain T: 88%



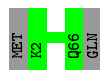
- Molecule 28: 50S RIBOSOMAL PROTEIN L27

Chain U: 95%



- Molecule 29: 50S RIBOSOMAL PROTEIN L29

Chain W: 97%



- Molecule 30: 50S RIBOSOMAL PROTEIN L30

Chain X:  100%

There are no outlier residues recorded for this chain.

- Molecule 31: 50S RIBOSOMAL PROTEIN L31

Chain Y:  100%

There are no outlier residues recorded for this chain.

- Molecule 32: 50S RIBOSOMAL PROTEIN L32

Chain Z:  95%



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	168.50 Å 406.00 Å 693.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.42	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.42)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.278 , 0.348	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	65418	wwPDB-VP
Average B, all atoms (Å ²)	80.0	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: DOL, DBB, 004, MHV, MHW, MHT, MHU

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	0.70	16/66467 (0.0%)	0.74	12/103673 (0.0%)
6	5	0.85	0/13	0.67	0/15
7	9	0.50	0/2813	0.65	0/4384
All	All	0.70	16/69293 (0.0%)	0.73	12/108072 (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	146
6	5	1	1
7	9	0	1
All	All	1	148

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	1962	C	N1-C2	-7.46	1.32	1.40
1	0	2255	G	C5-C6	-7.28	1.35	1.42
1	0	2789	U	N1-C2	6.94	1.44	1.38
1	0	868	U	N1-C2	6.93	1.44	1.38
1	0	806	A	C5-C6	6.88	1.47	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	994	A	N9-C1'-C2'	-6.36	105.00	112.00
1	0	800	U	OP2-P-O3'	6.27	119.00	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2056	C	N1-C1'-C2'	-6.04	105.36	112.00
1	0	1686	A	C5'-C4'-O4'	5.86	116.13	109.10
1	0	1938	U	C2'-C3'-O3'	5.75	122.90	113.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	5	8	MHT	C3

5 of 148 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	126	C	Sidechain
1	0	174	A	Sidechain
1	0	211	U	Sidechain
1	0	33	C	Sidechain
1	0	8	A	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	2138	0
2	1	53	0	0	0	0
3	2	46	0	0	0	0
4	3	63	0	0	0	0
5	4	35	0	0	0	0
6	5	73	0	64	6	0
7	9	2516	0	1286	66	0
8	A	270	0	0	1	0
9	B	205	0	0	1	0
10	C	197	0	0	0	0
11	D	178	0	0	0	0
12	E	177	0	0	0	0
13	F	52	0	0	0	0
14	G	143	0	0	0	0
15	H	143	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	I	132	0	0	0	0
17	J	141	0	0	0	0
18	K	124	0	0	0	0
19	L	114	0	0	1	0
20	M	111	0	0	0	0
21	N	125	0	0	0	0
22	O	117	0	0	2	0
23	P	100	0	0	0	0
24	Q	130	0	0	0	0
25	R	93	0	0	0	0
26	S	113	0	0	0	0
27	T	223	0	0	0	0
28	U	86	0	0	0	0
29	W	65	0	0	0	0
30	X	55	0	0	0	0
31	Y	73	0	0	0	0
32	Z	58	0	0	2	0
33	0	48	0	47	16	0
All	All	65418	0	31314	2213	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 23.

The worst 5 of 2213 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)
1:0:1463:A:H1'	1:0:1543:G:H22	1.05	1.14
1:0:128:C:H2'	1:0:129:A:H5''	1.19	1.10
1:0:1656:U:H2'	1:0:1657:A:H5''	1.34	1.10
1:0:940:G:H3'	1:0:941:U:H5''	1.23	1.09
1:0:2607:C:H3'	1:0:2608:A:H5'	1.10	1.08

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	5	2/8 (25%)	1 (50%)	0	1 (50%)	0 0

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	5	2	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	5	2/2 (100%)	2 (100%)	0	100 100

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2757/2880 (95%)	433 (15%)	19 (0%)
7	9	117/124 (94%)	12 (10%)	0
All	All	2874/3004 (95%)	445 (15%)	19 (0%)

5 of 445 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	45	C
1	0	48	A
1	0	49	U
1	0	50	G
1	0	59	G

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1354	A
1	0	1664	G
1	0	2093	G
1	0	1313	U
1	0	2261	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

5 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
6	DBB	5	3	6	4,5,6	0.58	0	1,5,7	0.06	0
6	MHW	5	1	6	9,9,10	0.76	0	10,11,13	1.56	1 (10%)
6	004	5	7	6	9,10,11	1.69	2 (22%)	9,12,14	1.27	1 (11%)
6	MHU	5	5	6	14,15,16	1.14	1 (7%)	18,19,21	1.11	1 (5%)
6	MHV	5	6	6	7,9,10	0.67	0	7,11,13	1.68	2 (28%)

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
6	DBB	5	3	6	-	1/3/4/6	-
6	MHW	5	1	6	-	2/2/2/4	0/1/1/1
6	004	5	7	6	-	2/4/6/8	0/1/1/1
6	MHU	5	5	6	-	2/9/12/14	0/1/1/1
6	MHV	5	6	6	-	0/1/12/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5	7	004	CB-CA	3.12	1.55	1.52
6	5	7	004	CG2-CB	-2.70	1.34	1.39
6	5	5	MHU	CZ1-NZ	-2.59	1.39	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	1	MHW	O-C-CA	-4.20	120.24	124.22
6	5	6	MHV	CE-CD2-CG	3.22	117.29	111.89
6	5	5	MHU	O-C-CA	-2.83	117.37	124.78
6	5	7	004	CG2-CB-CA	2.31	124.38	120.65
6	5	6	MHV	CB-CA-N	-2.02	108.33	112.50

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	5	3	DBB	O-C-CA-CB
6	5	1	MHW	O-C-CA-N
6	5	1	MHW	O-C-CA-CB
6	5	5	MHU	N-CA-CB-CG
6	5	5	MHU	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	5	3	DBB	5	0
6	5	1	MHW	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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
33	DOL	0	2882	-	43,50,50	4.58	11 (25%)	51,70,70	3.94	18 (35%)

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
33	DOL	0	2882	-	2/2/14/20	20/58/77/77	0/2/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	0	2882	DOL	O40-S39	18.61	1.77	1.44
33	0	2882	DOL	O41-S39	18.41	1.76	1.44
33	0	2882	DOL	C28-C29	-8.71	1.11	1.32
33	0	2882	DOL	C1-C37	4.83	1.62	1.52
33	0	2882	DOL	C8-C6	-4.51	1.42	1.50

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	0	2882	DOL	C4-N5-C1	-14.71	94.37	112.45
33	0	2882	DOL	O18-C17-C16	13.82	145.78	109.73
33	0	2882	DOL	C28-C26-N25	-9.38	97.30	114.97
33	0	2882	DOL	O40-S39-O41	-7.23	109.95	118.19
33	0	2882	DOL	O27-C26-C28	6.58	138.02	123.03

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	0	2882	DOL	C2
33	0	2882	DOL	C17

5 of 20 torsion outliers are listed below:

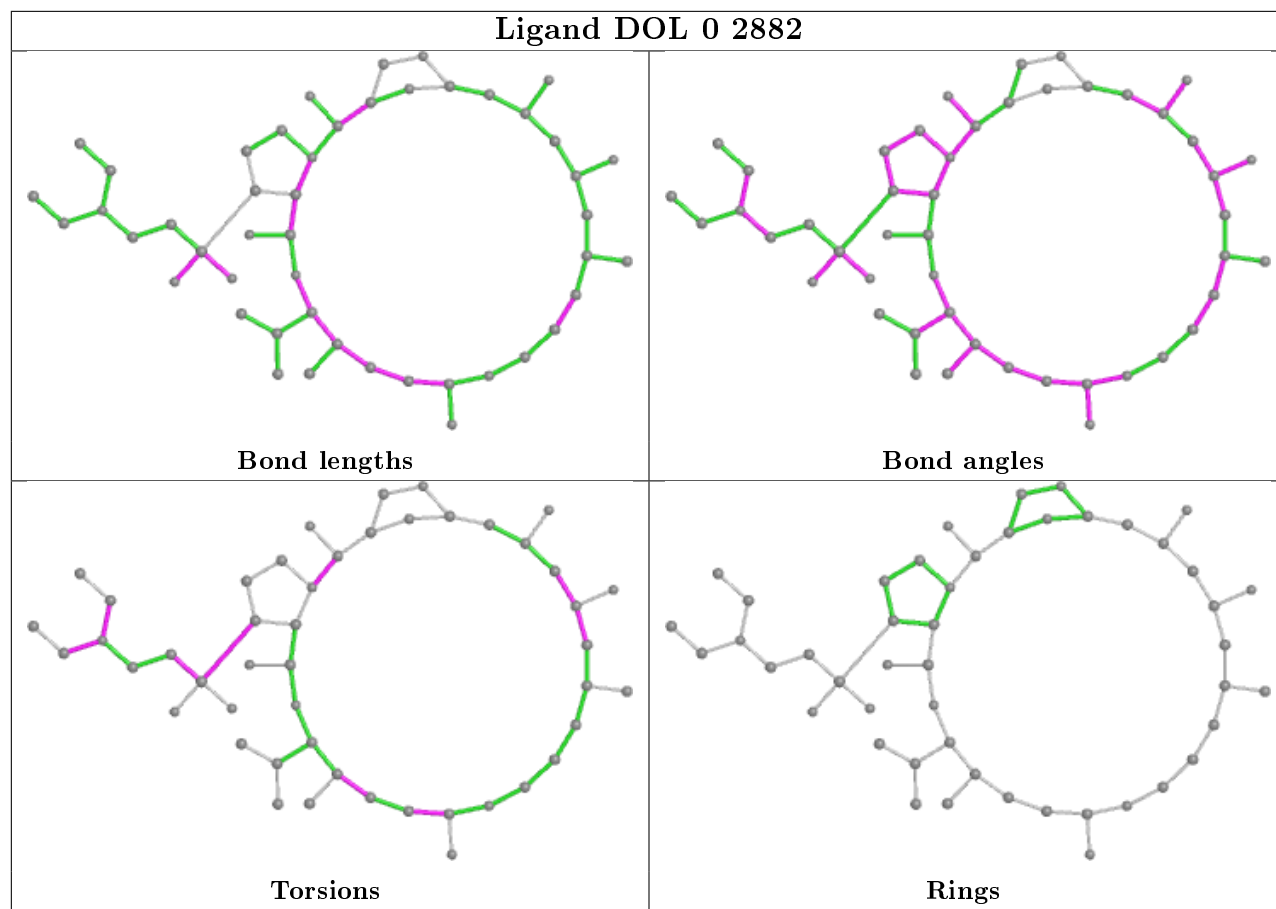
Mol	Chain	Res	Type	Atoms
33	0	2882	DOL	O7-C6-N5-C1
33	0	2882	DOL	C8-C6-N5-C1
33	0	2882	DOL	C1-C2-S39-O41
33	0	2882	DOL	C1-C2-S39-O40
33	0	2882	DOL	C1-C2-S39-C42

There are no ring outliers.

1 monomer is involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	0	2882	DOL	16	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.