



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:17 PM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

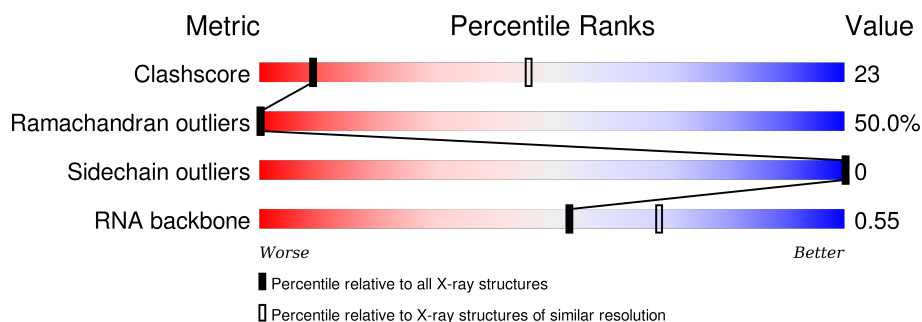
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.42 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	102246	1032 (3.50-3.34)
Ramachandran outliers	100387	1002 (3.50-3.34)
Sidechain outliers	100360	1003 (3.50-3.34)
RNA backbone	2183	1042 (4.02-2.80)


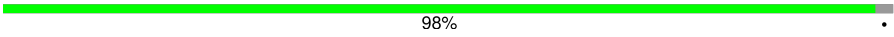
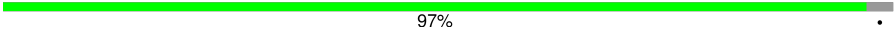
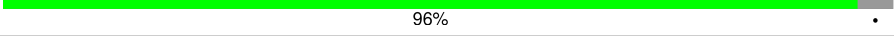
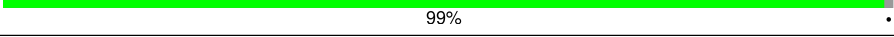


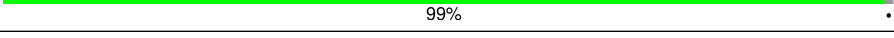
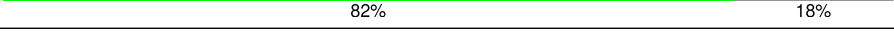
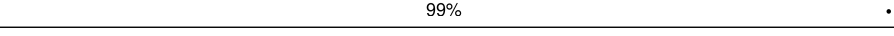
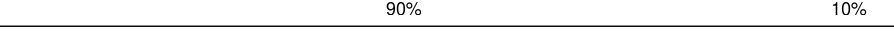
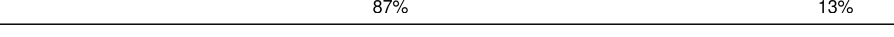
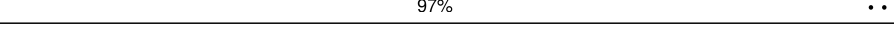
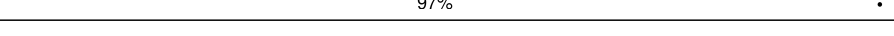

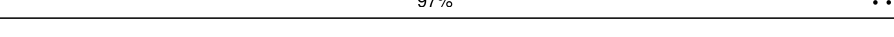
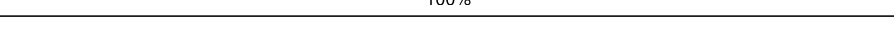
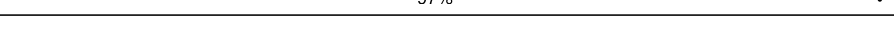
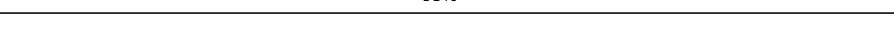






The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	2880	
2	1	82	
3	2	47	
4	3	66	
5	4	37	
6	5	8	


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Mol	Chain	Length	Quality of chain
7	9	124	 36%54%5%5%
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%

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Mol	Chain	Length	Quality of chain
32	Z	60	

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

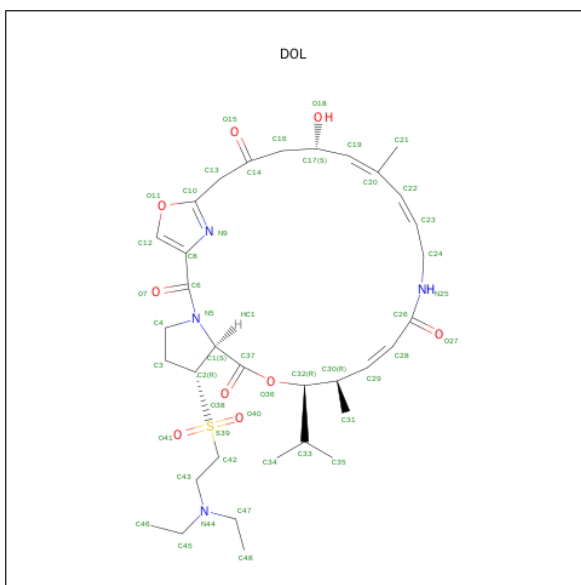
- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L31.

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).



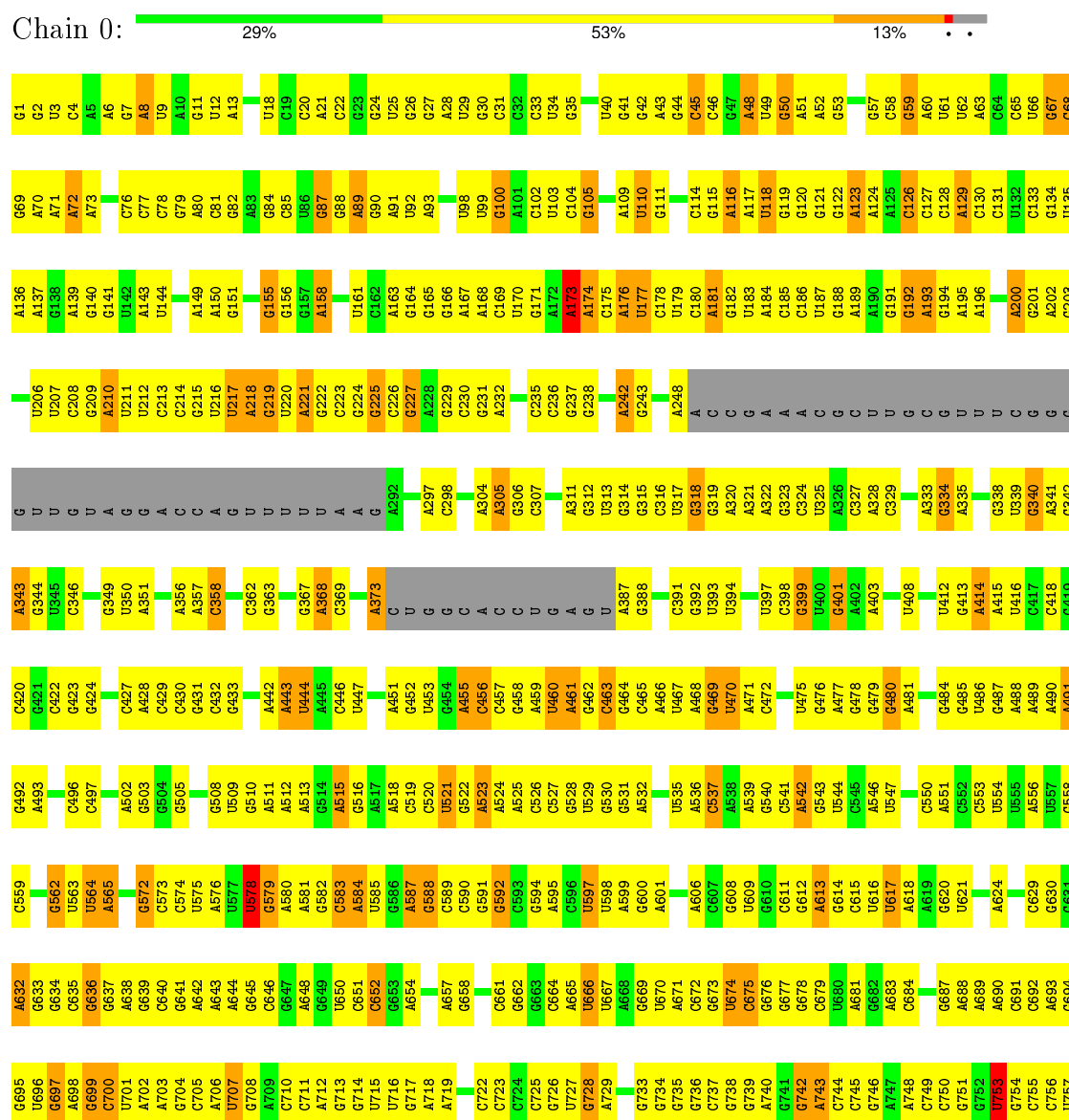
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	0	1	Total	C	N	O	S	0	0
			48	34	4	9	1		

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

Note EDS was not executed.

• Molecule 1: 23S RIBOSOMAL RNA



G1854	U1770	C1698	U1637	C1558	G1470	G1398	G1331	U1267	U1199	G1018	G957	G	A821	G758
G1855	A1771	A1699	G1638	C1559	G1471	C1399	G1332	U1268	G1200	G1022	G958	G	G822	C759
U1856	C1772	C1702	U1639	A1560	U1472	G1400	G1333	G1269	U1201	U1023	G959	G	U823	U760
A1774	C1773	C1702	C1640	U1473	U1473	G1401	A1334	C1270	U1202	G1024	U960	G	U824	G761
A1775	A1706	A1706	C1641	U1474	U1474	U1402	G1403	C1271	A1203	A1025	G961	G	C825	A762
A1860	A1707	A1707	G1642	U1562	U1475	U1403	G1338	G1272	G1204	G1026	G962	C	U826	A763
G1861	C1708	C1708	U1643	U1563	G1476	A1406	U1339	G1273	G1205	U1027	G963	C	C827	A764
G1862	U1709	U1709	G1644	U1564	G1477	A1407	C1340	C1274	G1206	C1027	G964	U	C828	C765
G1863	C1779	C1779	U1645	G1565	G1479	G1407	G1341	G1275	G1207	G1028	G965	A	C829	A766
G1864	U1710	U1710	U1646	U1566	U1480	A1408	U1342	U1276	G1208	C1029	A966	C	C830	
G1865	C1711	C1711	U1647	U1567	U1481	U1409	C1343	U1277	G1209	U1030	G967	C	G831	
G1866	G1782	G1712	C1648	G1571	U1482	U1410	C1344	G1278	U1212	C1031	G968	A	A832	C771
A1869	C1783	G1713	A1649	G1572	U1483	G1414	C1345	G1279	U1213	A1032	G969	G	A833	G772
U1870	A1784	A1714	U1650	C1572	G1484	G1414	C1346	U1280	U1214	G1033	U970	C	A834	A774
A1881	G1786	G1716	U1651	G1573	U1485	C1417	C1347	A1281	A1215	U1034	G971	U	U835	U775
G1882	U1787	G1717	U1652	A1574	U1486	C1418	C1348	A1282	G1216	G1036	G972	U	G836	G776
A1883	C1788	A1718	C1653	C1418	G1487	C1418	A1349	C1283	A1215	U1037	G973	A	U837	A777
A1884	G1789	G1719	U1654	G1577	U1488	C1418	A1349	C1284	G1218	U1038	G974	C	A838	G778
G1885	U1790	U1790	C1655	G1577	U1489	U1426	G1352	A1285	C1219	A1039	G975	C	U839	U779
A1886	C1791	G1720	U1656	A1583	U1490	G1427	A1353	U1286	G1222	A1040	G976	A911	U840	U780
G1887	G1792	G1721	U1657	G1584	U1491	G1428	A1354	A1287	G1223	G1041	G977		G841	G781
G1888	A1793	G1722	A1585	A1586	A1493	A1429	A1355	A1288	G1224	C1151	U978	C914	A842	U782
G1889	U1794	U1723	G1658	A1587	G1496	G1430	G1356	A1289	A1224	C1152	U979	C915	G843	G783
G1890	C1795	C1724	G1660	A1588	U1497	G1431	U1357	G1290	G1225	A1153	G980	U916	G844	U784
A1901	U1796	G1725	C1661	A1589	U1500	G1432	C1358	G1291	A1226	A1045	G981	U917	U845	U785
A1902	C1797	C1726	G1662	C1593	U1501	A1433	G1359	A1292	A1227	U1046	G982	A913	A846	U786
G1905	G1799	G1727	C1663	C1594	C1501	U1434	G1360	A1293	G1228	G1047	G983	U919	C847	A787
U1906	A1800	G1730	G1665	A1596	G1502	G1435	C1363	C1230	C1229	C1052	G984		A848	G788
C1907	C1801	C1731	U1666	A1597	G1503	G1436	C1364	A1299	A1231	G1053	G985	A922	U852	G789
U1909	A1802	A1802	A1667	G1598	U1504	A1437	U1365	A1300	U1232	C1054	G987	C926	G853	G791
G1803	G1803	C1736	G1668	G1599	U1505	G1438	A1366	U1301	C1235	A1055	G988		G854	U792
U1910	U1804	G1737	U1669	A1604	G1508	A1441	A1367	U1304	G1241	A1057	G989	C928	G855	G793
A1911	C1805	C1744	G1670	A1605	A1509	C1442	G1368	C1305	U1242	A1058	A992	A930	A856	A795
G1912	A1807	C1745	A1672	A1606	A1510	G1443	U1370	U1306	G1243	A1059	G993	G931	G858	A796
G1913	C1808	A1746	C1673	G1613	A1511	C1444	G1371	U1307	U1243	G1066	A994	G932	U859	A797
U1914	G1809	G1747	U1676	C1614	U1512	U1445	A1372	C1308	U1244	G1067	A995	G933	U860	G798
A1915	U1810	U1748	U1677	C1615	U1513	U1446	G1373	G1309	U1247	G1068	C996	G934	C864	C799
C1916	U1811	G1749	C1678	C1616	U1514	U1447	G1374	C1310	U1248	A1068	C997	C935	A865	U800
C1917	A1813	A1751	U1679	U1617	A1515	C1448	U1379	C1311	U1249	G1069	C998	A936	U866	A801
G1918	G1816	U1752	U1680	A1619	G1520	G1450	C1380	G1312	G1248	G1073	A999	G937	G867	A802
A1919	U1817	A1753	A1681	C1620	U1524	A1453	G1381	U1313	A1250	G1074	G1000	G938	U868	C803
A1920	G1818	G1754	A1682	C1621	G1524	U1454	G1382	A1314	G1251	A1081	A1001	C939	U869	C804
U1921	C1819	G1755	G1683	G1622	G1527	U1455	C1383	A1315	C1252	G1082	C1002	G940	C870	G805
U1922	U1819	C1756	G1684	C1623	G1527	C1456	G1384	G1317	G1253	A1083	A1003	U941	U871	A806
U1923	C1820	C1757	A1685	A1624	C1528	A1457	C1385	A1318	G1254	U1005	U1005	U943	G872	C808
C1924	A1821	C1758	A1686	A1625	C1529	A1458	A1386	C1319	A1255	C1086	C1006	A944	G873	C809
C1925	C1822	U1759	C1687	A1626	U1530	U1459	G1387	A1320	C1256	C1087	A1007	G945	A874	
U1926	G1823	G1760	C1688	C1627	U1530	G1460	C1388	A1321	U1257		G1008	U946	G875	U810
U1927	C1824	G1761	U1689	C1628	G1541	C1461	C1389	G1322	U1258	C1090	C1009	U946	A876	G811
G1928	U1825	C1762	U1690	G1629	G1542	C1462	G1390	G1323	A1259	C1091	G947	C948	G877	G812
U1929	U1826	G1763	G1691	A1630	G1543	A1463	A1391	G1324	G1260	U1092	A1010		G877	A813
C1930	A1764	A1764	C1692	C1631	A1544	A1464	G1392	G1325	U1261	C1087	A1012		A874	G814
G1931	G1831	C1765	A1693	A1632	U1545	G1465	U1393	U1326	G1262	A1099	G951		A883	A815
A1936	G1832	U1766	C1694	C1633	U1546	U1466	G1394	C1327	G1263		G952		C884	U816
G1937	U1768	G1767	A1695	C1634	C1549	U1467	A1395	C1328	G1264	G1123	G953		C889	A817
U1938	G1838	U1769	U1697	G1636	C1552	U1469	A1397	G1330	U1266	U1124	U954		C890	G818
										U1124	G955		U860	C819
										G1125	C1017		A891	U820

• Molecule 2: 50S RIBOSOMAL PROTEIN L33

35%

MET	PHE	LEU	LEU	ARG	GLN	ALA	ALA	GLY	THR	PHE	PRO	VAL	PRO	GLY	ASP	GLN	ARG	GLU	GLY	CYS	ALA	LYS	GLU	SER	ILE	MET	A2	K5-4	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	------	-----

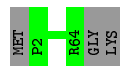
- Molecule 3: 50S RIBOSOMAL PROTEIN L34

Chain 2:  98%



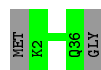
- Molecule 4: 50S RIBOSOMAL PROTEIN L35

Chain 3:  95%



- Molecule 5: 50S RIBOSOMAL PROTEIN L36

Chain 4:  95%

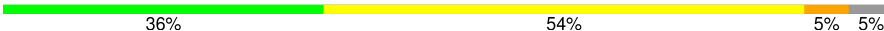


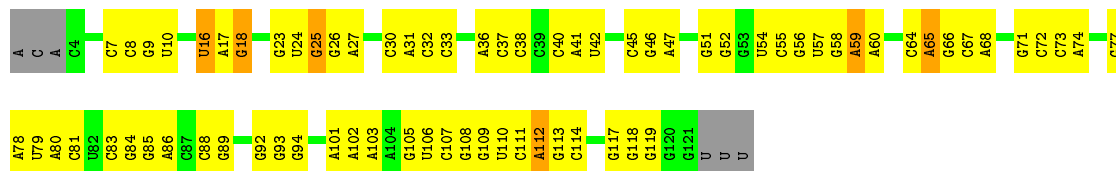
- Molecule 6: QUINUPRISTIN

Chain 5:  63% 13% 25%



- Molecule 7: 5S RIBOSOMAL RNA

Chain 9:  36% 54% 5% 5%



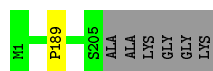
- Molecule 8: 50S RIBOSOMAL PROTEIN L2

Chain A:  98%



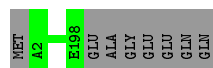
- Molecule 9: 50S RIBOSOMAL PROTEIN L3

Chain B:  97%



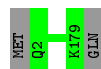
- Molecule 10: 50S RIBOSOMAL PROTEIN L4

Chain C:  96%

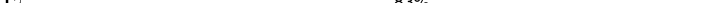


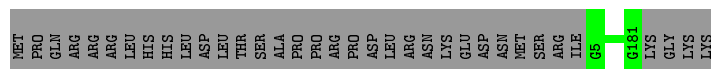
- Molecule 11: 50S RIBOSOMAL PROTEIN L5

Chain D: 99%



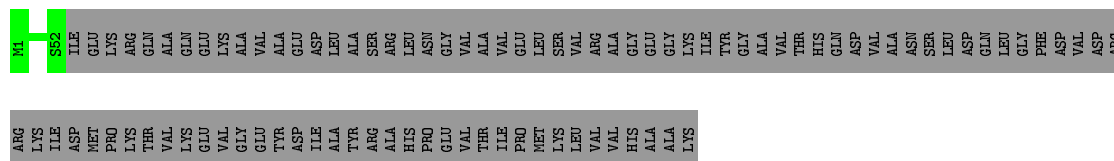
- Molecule 12: 50S RIBOSOMAL PROTEIN L6

Chain E:  83% 17%



- Molecule 13: 50S RIBOSOMAL PROTEIN L9

Chain F: 36% 64%

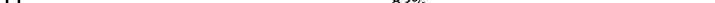


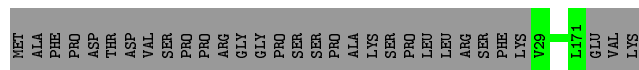
- Molecule 14: 50S RIBOSOMAL PROTEIN L11

Chain G:  99%



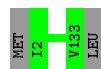
- Molecule 15: 50S RIBOSOMAL PROTEIN L13

Chain H:  82% 18%




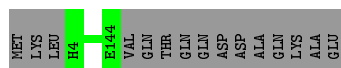
- Molecule 16: 50S RIBOSOMAL PROTEIN L14

Chain I: 99%




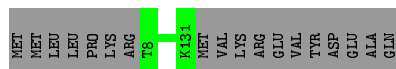
- Molecule 17: 50S RIBOSOMAL PROTEIN L15

Chain J:  90% 10%



- Molecule 18: 50S RIBOSOMAL PROTEIN L16

Chain K:  87% 13%



- Molecule 19: 50S RIBOSOMAL PROTEIN L17

Chain L:  97% ..



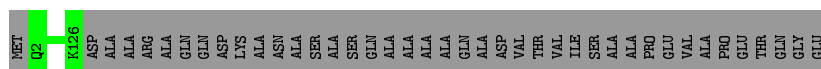
- Molecule 20: 50S RIBOSOMAL PROTEIN L18

Chain M:  97% .



- Molecule 21: 50S RIBOSOMAL PROTEIN L19

Chain N:  75% 25%



- Molecule 22: 50S RIBOSOMAL PROTEIN L20

Chain O:  97% ..



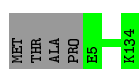
- Molecule 23: 50S RIBOSOMAL PROTEIN L21

Chain P:  100%

There are no outlier residues recorded for this chain.

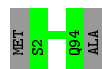
- Molecule 24: 50S RIBOSOMAL PROTEIN L22

Chain Q:  97% .



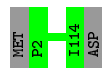
- Molecule 25: 50S RIBOSOMAL PROTEIN L23

Chain R:  98%





- Molecule 26: 50S RIBOSOMAL PROTEIN L24

Chain S:  98%



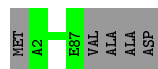
- Molecule 27: GENERAL STRESS PROTEIN CTC

Chain T:  88%  12%



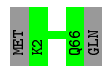
- Molecule 28: 50S RIBOSOMAL PROTEIN L27

Chain U:  95%  5%



- 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 will therefore be 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 1.0	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 ⓘ

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 [i](#)

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	MHW	5	1	6	9,9,10	0.78	0	8,11,13	0.74	0
6	DBB	5	3	6	4,5,6	0.51	0	3,5,7	1.40	1 (33%)
6	MHU	5	5	6	13,15,16	1.14	1 (7%)	15,19,21	1.11	1 (6%)
6	MHV	5	6	6	7,9,10	0.67	0	8,11,13	1.48	1 (12%)
6	004	5	7	6	9,10,11	1.75	2 (22%)	10,12,14	1.41	2 (20%)

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	MHW	5	1	6	-	1/2/2/4	0/1/1/1
6	DBB	5	3	6	-	0/2/4/6	0/0/0/0
6	MHU	5	5	6	-	0/8/12/14	0/1/1/1
6	MHV	5	6	6	-	0/1/12/14	0/1/1/1
6	004	5	7	6	-	0/4/6/8	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	CG2-CB	-2.62	1.34	1.39
6	5	5	MHU	CZ1-NZ	-2.45	1.39	1.45
6	5	7	004	CB-CA	3.51	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	5	MHU	O-C-CA	-3.05	117.37	125.44
6	5	3	DBB	O-C-CA	-2.42	119.18	125.49
6	5	7	004	CG2-CB-CA	2.13	124.38	120.70
6	5	7	004	C-CA-N	2.45	114.44	109.12
6	5	6	MHV	CE-CD2-CG	3.03	117.29	112.01

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	5	1	MHW	O-C-CA-N

There are no ring outliers.

2 monomers are involved in 5 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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
33	DOL	0	2882	-	43,50,50	4.25	13 (30%)	50,70,70	4.09	18 (36%)

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	0/58/77/77	0/1/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	0	2882	DOL	C28-C29	-7.72	1.11	1.32
33	0	2882	DOL	C8-C6	-3.86	1.42	1.50
33	0	2882	DOL	C1-C2	-3.01	1.50	1.55
33	0	2882	DOL	C6-N5	-2.04	1.31	1.35
33	0	2882	DOL	C22-C23	2.46	1.38	1.31

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	-16.51	94.37	112.39
33	0	2882	DOL	O40-S39-O41	-8.35	109.95	117.98
33	0	2882	DOL	C28-C26-N25	-7.63	97.30	114.87
33	0	2882	DOL	C23-C22-C20	-4.76	118.48	125.75
33	0	2882	DOL	C16-C17-C19	-3.73	103.99	111.38

All (2) chirality outliers are listed below:

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

There are no torsion outliers.

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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