



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:03 am GMT

PDB ID : 1NJP
Title : The crystal structure of the 50S Large ribosomal subunit from *Deinococcus radiodurans* complexed with a tRNA acceptor stem mimic (ASM)
Authors : Bashan, A.; Agmon, I.; Zarivatch, R.; Schlutzen, F.; Harms, J.M.; Berisio, R.; Bartels, H.; Hansen, H.A.; Yonath, A.
Deposited on : 2003-01-02
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

<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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

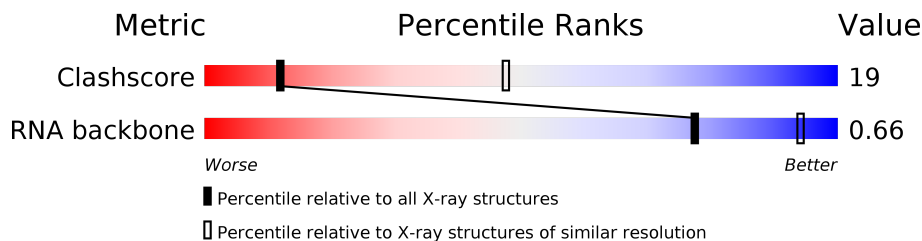
1 Overall quality at a glance

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	112137	1322 (3.60-3.40)
RNA backbone	2435	1024 (4.10-2.86)

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	5	35	
3	K	141	
4	T	237	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 60249 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 tRNA acceptor stem mimic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	5	25	Total	C	N	O	P	0	0	0
			543	249	97	173	24			

- Molecule 3 is a protein called 50S ribosomal protein L16.

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

- Molecule 4 is a protein called GENERAL STRESS PROTEIN CTC.

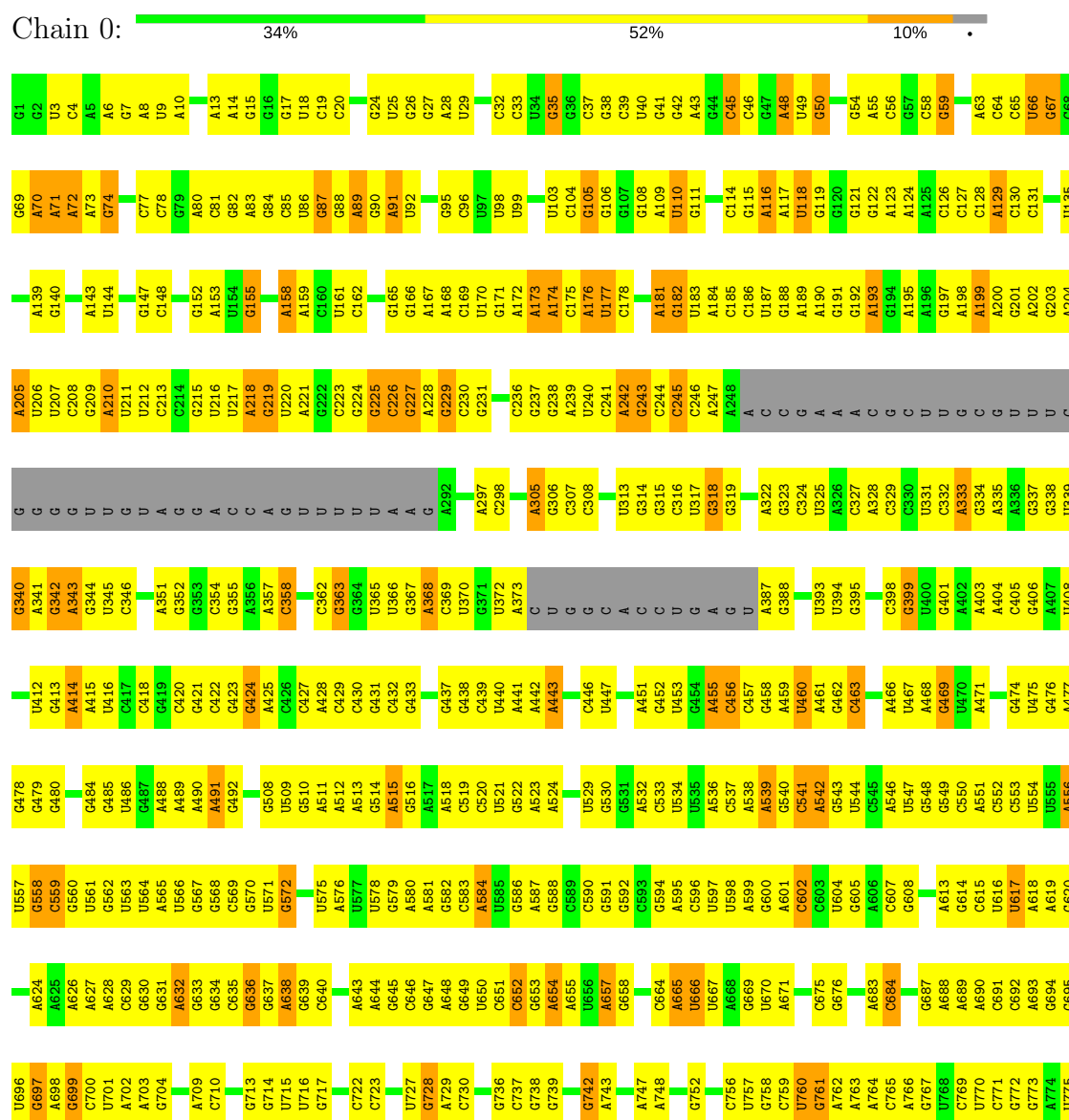
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	T	223	Total	C	0	0	223
			223	223			

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 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



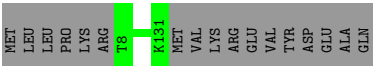
U1909	U1819	G1659	A1587	G1508	A1441	U1357	A1288	C1214	U1141	U1044	U978	A	A838	G776
A1910	A1820	G1742	U1591	A1509	G1442	C1358	A1289	U1217	A1142	G1045	U979	C	U839	A777
A1911	C1821	C1743	U1592	A1510	G1443	G1359	A1290	U1218	G1143	U1046	A979	C	U840	A778
G1912	C1822	G1662	U1593	A1511	C1444	U1365	G1291	C1218	C1144	G1047	G980	A911	C	G841
G1913	C1823	C1745	U1594	A1512	A1445	U1365	A1292	C1219	C1145	C981	U981		A842	U779
U1825	C1825	G1746	U1594	A1513	U1446	A1366	A1293	G1220	G1146	C1052	A984		G843	G781
U1826	U1826	C1665	A1595	C1514	U1447	A1367	G1298	C1221	G1147	G1053	U917		G844	G782
A1915	U1827	G1666	A1596	U1515	A1448	G1368	U1301	G1222	G1148	C1054	G985		U845	U783
G1916	C1829	U1748	A1597	U1516	A1449	G1368	U1302	G1223	G1149	A1055	A986		U846	G784
C1830	G1968	U1749	A1597	C1517	G1450	G1373	U1301	A1224	G1150	U1056	G987		U847	U785
A1918	C1831	U1750	U1599	C1518	C1451	U1373	U1302	G1225	U1151	A1057	G988		U848	U786
G1919	G1831	G1754	U1600	G1519	U1452	G1377	U1307	A1226	U1152	G1058	A921		U849	U787
A1920	U1835	A1670	U1601	G1520	U1453	G1377	U1308	A1227	A1153	G1059	A922		U850	A788
A1921	C1836	G1755	U1602	G1521	C1454	C1380	U1309	A1228	A1154	A1060	A923		C851	G789
U1922	C1837	U1672	A1603	C1522	C1455	G1381	G1309	A1229	U1155	G1061	U924		G852	U790
U1923	G1838	G1760	U1604	U1523	A1456	G1382	C1310	A1230	G1156	A1062	A925		G853	A791
A1924	C1839	G1761	A1605	G1524	A1457	C1383	C1311	U1231	U1157	G1063	A926		U854	G792
C1925	A1839	C1762	A1606	G1525	U1458	U1384	U1312	A1232	A1162	A1064	C995		U855	U793
U1926	A1840	G1763	C1606	C1526	U1459	A1386	U1313	C1233	C1163	G1065	C996		G856	G794
U1927	G1841	U1674	A1607	C1527	U1460	G1387	A1314	C1234	C1164	G1066	A997		U857	A795
G1928	U1928	A1681	U1608	U1530	A1463	C1388	U1315	C1235	G1165	U1067	A998		U858	U796
U1929	C1850	G1765	C1609	C1531	A1464	G1389	G1316	A1242	A1166	G1073	G1000		G859	A797
A1930	A1851	U1766	A1610	A1532	G1465	C1390	G1317	G1243	U1167	G1074	A1001		U860	G798
G1931	U1855	G1767	U1611	G1533	C1466	U1391	A1318	U1244	G1168	C1075	C1002		C861	A799
U1932	G1856	A1685	G1612	U1534	U1467	U1392	C1319	G1245	C1169	U1076	C1003		A862	U800
A1933	U1857	C1686	U1613	G1540	A1468	G1393	A1320	U1246	U1172	A1081	U1004		U863	G799
U1934	C1857	U1687	C1614	C1541	U1469	U1397	G1323	G1249	U1173	U1082	A927		U864	U801
U1935	G1858	G1687	G1615	G1542	G1470	A1397	U1324	A1250	G1174	A1083	U1005		U865	A802
A1936	A1859	U1688	U1616	U1543	U1471	G1398	U1325	G1251	G1175	A1084	C939		C866	C803
U1946	A1860	C1692	G1617	G1544	C1472	C1399	U1326	C1252	U1176	G1085	A1007		C867	C804
C1947	G1861	A1777	U1618	A1544	U1473	U1402	U1327	G1253	C1177	C1086	G1008		U868	G805
U1948	C1862	U1778	A1619	G1545	U1474	G1403	C1328	G1254	C1178	U1087	C1009		G869	A806
A1949	U1865	G1779	U1620	U1546	U1475	U1404	U1329	U1257	A1179	C1088	A943		U870	A807
C1950	G1866	U1780	C1621	C1552	U1476	U1405	U1330	G1258	A1180	G1088	A944		U871	C808
A1951	U1866	G1704	G1622	C1553	U1477	G1407	U1331	A1259	U1181	C1089	G945		G872	C809
U1952	G1867	C1708	C1623	G1557	G1479	U1410	G1332	G1260	U1182	C1090	U1015		A873	U810
A1953	U1868	U1785	A1624	C1558	U1480	C1411	G1333	U1261	C1183	C1091	C1017		G874	G811
U1954	C1869	C1786	U1709	A1561	U1481	U1410	U1334	G1262	G1184	U1092	C1018		C875	G812
G1955	U1880	U1787	A1625	G1562	U1482	C1411	A1335	G1263	C1185	U1093	G951		A876	A813
U1956	A1881	G1788	U1710	U1563	U1483	G1412	A1336	C1264	G1186	U1094	A952		C880	G814
C1957	G1882	U1789	C1627	G1563	U1484	G1413	U1337	G1265	A1187	G1098	A953		G887	A815
U1958	A1883	G1790	G1628	G1566	A1486	C1414	G1338	G1266	A1188	A1099	U954		G888	U816
A1959	U1884	C1792	U1713	A1567	G1487	C1415	G1339	A1267	C1189	G1100	U1023		C889	A817
U1961	C1885	U1793	A1632	U1568	G1488	C1416	U1340	U1268	C1190	U1024	A956		U890	G818
C1962	U1886	A1714	U1632	A1569	U1489	U1418	C1340	G1269	G1191	A1114	A1025		A891	C819
A1963	G1887	G1715	C1633	U1570	U1490	G1419	G1341	U1270	A1192	U1026	G957		U892	U820
U1964	C1888	U1716	A1634	G1571	C1491	U1424	U1342	C1271	G1193	C1120	C959		G	A821
G1965	U1889	A1799	G1635	C1572	A1492	G1425	U1343	G1272	U1194	G1121	U960		G	G822
C1966	G1890	U1800	U1643	G1573	U1493	U1426	C1344	U1273	U1195	A1122	G961		G	U823
U1967	U1893	C1801	G1644	A1574	G1494	G1427	G1345	G1274	G1196	U1036	U1037		G	A824
A1968	C1894	U1722	C1648	C1575	U1495	U1428	U1346	A1275	U1197	C1031	A964		G	C825
U1969	U1894	C1727	U1651	G1576	G1496	G1429	A1429	G1276	C1198	G1128	A1032		C	U826
A1970	A1895	A1728	U1652	U1577	G1497	U1430	C1347	U1277	U1199	A1129	G965		C	C827
C1971	G1896	G1729	U1653	U1578	G1498	G1431	U1348	G1278	U1200	U1130	G967		U	G828
G1972	U1897	U1810	C1654	C1580	U1499	U1432	A1349	A1279	G1203	G1034	U1034		A	C829
U1973	A1899	C1730	G1655	C1581	U1500	G1432	G1350	U1280	A1203	C1132	G1036		C	C830
C1974	U1900	G1731	C1656	U1582	C1501	A1433	G1351	A1281	G1204	G1133	U1037		C	G831
A1975	U1901	U1732	A1654	A1582	G1502	U1434	G1352	U1282	U1038	A1137	A970		A	A832
G1976	C1902	U1733	C1655	U1583	G1503	G1435	A1353	G1284	A1039	C972	A971		G	A833
U1977	U1906	G1814	U1656	G1584	G1504	G1436	A1354	A1285	A1040	U973	C		C	A834
C1978	C1907	C1736	A1657	U1585	U1505	A1437	A1355	U1286	G1211	A1139	G1041		U	U837
U1979	U1908	G1737	U1658	A1586	U1506	U1437	C1356	A1287	G1212	A1140	C975		U	A838



Chain K:

88%

12%

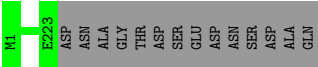


- Molecule 4: GENERAL STRESS PROTEIN CTC

Chain T:

94%

6%



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	169.90Å 409.90Å 695.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.244 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	60249	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.14	0/66467	0.63	0/103673
2	5	0.15	0/563	0.63	0/873
All	All	0.14	0/67030	0.63	0/104546

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	873	U	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59359	0	29917	1724	0
2	5	543	0	290	11	0
3	K	124	0	0	0	0
4	T	223	0	0	0	0
All	All	60249	0	30207	1731	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 19.

The worst 5 of 1731 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)
1:0:940:G:H3'	1:0:941:U:H5''	1.22	1.14
1:0:1141:U:H3	1:0:2008:C:H5''	1.20	1.04
1:0:1073:G:H2'	1:0:1074:G:H4'	1.40	1.01
1:0:2548:G:H2'	1:0:2549:G:H5''	1.44	1.00
1:0:2769:C:H2'	1:0:2867:G:H22	1.21	0.99

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%)	413 (14%)	0
2	5	22/35 (62%)	2 (9%)	0
All	All	2779/2915 (95%)	415 (14%)	0

5 of 415 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	15	G
1	0	35	G
1	0	45	C
1	0	48	A
1	0	49	U

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue 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	$\# Z > 2$
2	PPU	5	35	2	31,40,41	2.69	5 (16%)	34,57,60	1.18	4 (11%)

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
2	PPU	5	35	2	-	0/21/43/44	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	35	PPU	OC-CM	-4.94	1.28	1.42
2	5	35	PPU	CE2-CZ	2.63	1.44	1.38
2	5	35	PPU	CD2-CG	2.64	1.44	1.38
2	5	35	PPU	CE1-CZ	3.56	1.46	1.38
2	5	35	PPU	C-N3'	12.16	1.61	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	35	PPU	C-CA-N	2.19	117.94	109.10
2	5	35	PPU	C9-N6-C6	2.30	126.49	119.51
2	5	35	PPU	CM-OC-CZ	2.85	123.75	117.50
2	5	35	PPU	C2-N1-C6	3.29	119.89	111.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.