



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:28 am GMT

PDB ID : 1NJO  
Title : The crystal structure of the 50S Large ribosomal subunit from *Deinococcus radiodurans* complexed with a short substrate analog ACCPuromycin (ACCP)  
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 : 3.70 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](mailto: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.

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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

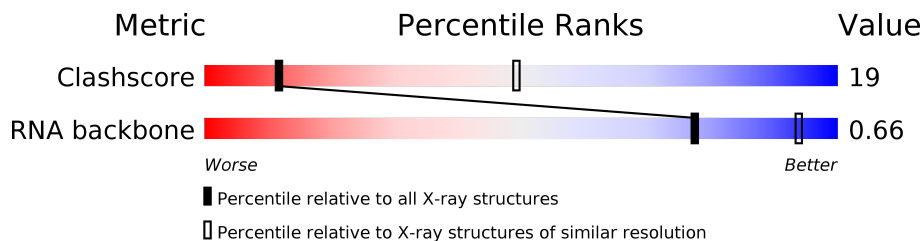
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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	1377 (3.90-3.50)
RNA backbone	2435	1010 (4.50-2.90)

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  $\geq 3$ , 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	4	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 59455 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 RNA ACC(Puromycin).

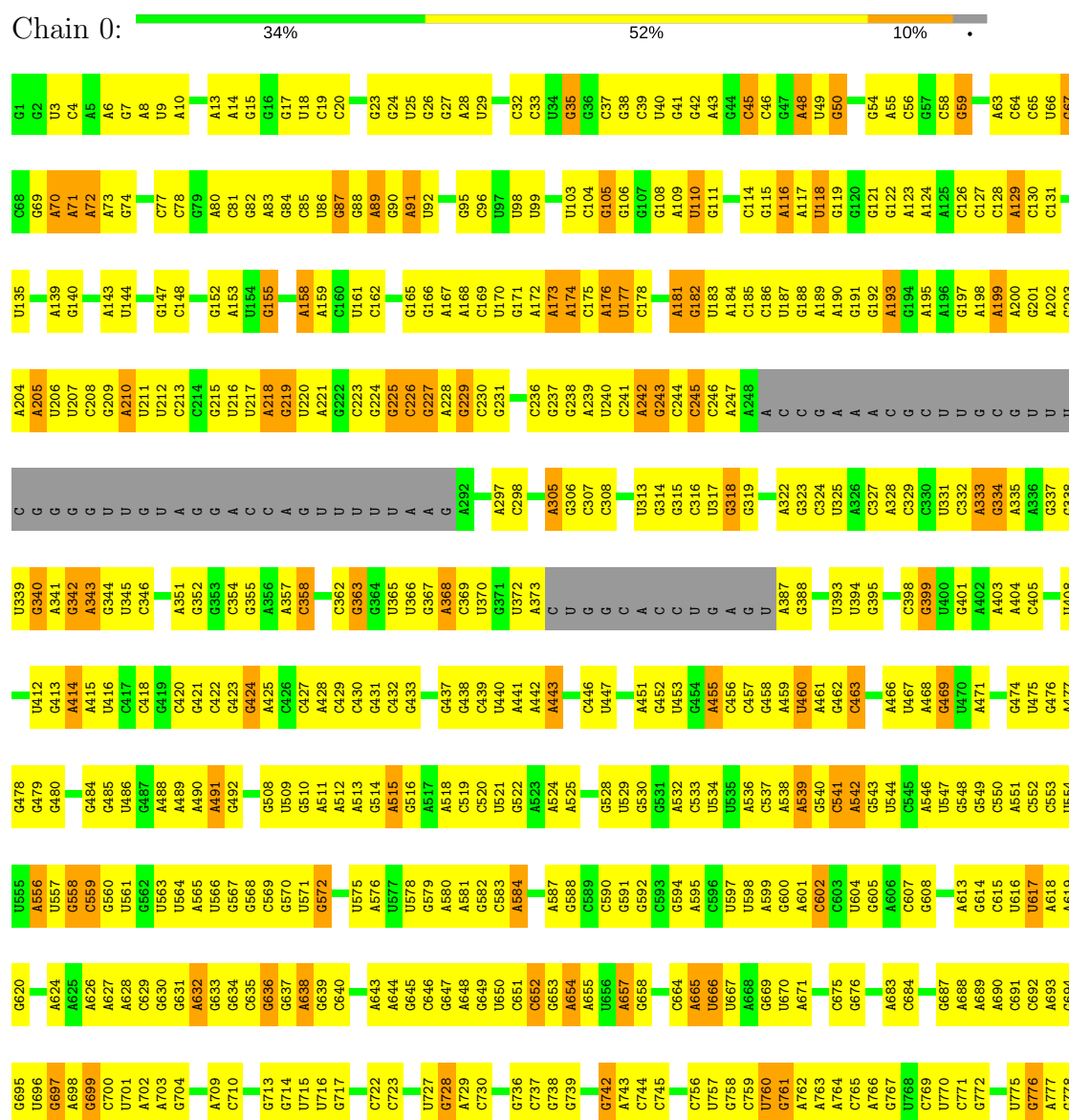
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	5	4	Total	C	N	O	P	0	0	0
			96	50	18	25	3			

### 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	G1818	U1732	C1655	A1582	G1504	G1436	U1357	A1290	U1144	G1047	G980	A913	G841	U779
A1910	U1819	U1733	U1656	A1583	U1505	A1437	C1358	A1291	C1145	C1052	C981	U916	A842	U780
G1912	A1820	A1657	A1657	G1594	G1508	A1441	G1359	A1292	G1146	G1052	A984	U917	G843	G781
G1913	C1822	G1742	G1658	A1585	A1509	C1442	U1365	A1293	G1147	C1052	A984	U918	G844	G782
G1914	G1743	C1743	G1659	A1586	A1510	C1443	A1366	G1221	G1148	C1054	G985	U919	U845	G783
A1915	C1825	C1744	G1660	A1587	A1511	C1444	A1367	G1222	G1149	A1055	A986	U920	U846	G784
G1916	U1826	C1745	C1661	U1591	A1512	C1445	A1368	A1224	C1150	U1056	G987	G921	C847	U785
C1917	G1662	A1746	G1663	U1592	U1513	A1446	G1369	G1225	U1151	A1057	G988	A921	U852	U786
C1829	G1663	G1747	C1664	U1593	U1514	A1447	G1370	A1226	A1154	A991	G989	A922	G853	A787
C1830	G1664	U1748	C1665	U1594	U1515	A1448	G1371	A1227	G1155	A991	G990	U925	G854	G788
G1831	A1750	A1750	G1666	A1595	A1516	C1449	A1372	A1231	U1156	A994	G991	U926	G855	G789
C1835	G1754	G1754	G1667	A1596	A1517	C1450	G1373	U1232	U1157	A995	G992	C926	G856	A790
C1836	G1755	G1755	G1668	A1597	C1518	C1451	G1374	U1233	A1162	C996	G993	G928	U857	U792
G1837	U1756	U1756	A1669	U1598	G1519	U1452	G1377	C1234	C1163	C997	G994	A929	U858	U793
A1838	G1670	G1670	G1671	U1599	G1520	C1455	C1380	C1235	C1164	C998	G995	A930	U859	A794
A1839	A1671	A1671	U1600	U1601	C1524	C1456	C1381	A1242	G1165	G1073	G1000	G932	U860	A795
A1840	U1672	U1672	G1602	G1602	G1527	A1457	G1382	G1243	U1172	C1074	A1001	G933	U861	A796
G1841	U1676	U1676	A1603	A1603	G1528	A1458	G1383	U1244	G1167	C1075	A1002	G934	U862	A797
A1841	A1763	A1763	A1604	A1604	C1529	U1459	G1384	U1245	G1168	C1076	C1003	G935	U863	G798
U1842	U1764	U1764	U1605	A1605	U1530	C1463	A1386	G1248	U1173	A1081	A1004	A936	U864	U800
U1843	U1765	U1765	U1606	A1606	U1531	G1464	G1387	G1249	G1179	C1087	U1005	G939	U865	C803
U1844	U1766	U1766	U1607	A1607	A1532	G1465	G1388	G1250	U1179	C1088	U1006	C940	U866	C804
A1845	U1767	U1767	U1608	U1608	A1533	G1466	G1389	G1251	U1179	C1089	U1007	C941	U867	C805
G1855	U1770	U1770	U1609	G1609	G1533	U1467	U1392	C1252	U1179	C1090	U1008	U942	U868	A806
U1856	A1771	A1771	U1610	A1610	U1539	A1468	G1393	C1253	A1179	C1091	U1009	U943	U869	A807
C1944	U1772	U1772	U1611	U1611	C1540	A1469	U1394	U1257	G1180	C1092	U1010	G945	U870	C808
C1945	A1773	A1773	U1612	A1612	G1541	G1470	U1395	U1258	C1181	C1093	U1011	G946	U871	C809
U1946	U1774	U1774	U1613	G1613	G1542	C1471	G1396	G1259	C1182	C1094	U1012	G947	U872	U810
C1947	A1775	A1775	U1614	C1614	U1543	C1472	G1397	A1259	C1183	G1091	U1013	G948	U873	G811
A1948	U1776	U1776	U1615	C1615	A1544	C1473	U1398	U1260	G1184	C1092	U1014	G949	U874	G812
A1949	U1777	U1777	U1616	C1616	U1545	U1474	G1399	G1261	C1185	U1093	U1015	G950	U875	G813
C1950	U1778	U1778	U1617	U1617	C1546	U1475	U1403	G1262	G1186	C1094	U1016	G951	U876	G814
G1951	C1779	C1779	U1618	U1618	U1547	U1476	U1404	G1263	A1187	G1098	U1017	G952	U877	A813
A1952	U1780	U1780	U1619	A1619	U1548	U1477	U1405	G1264	A1188	C1099	U1018	G953	U878	A814
C1953	A1785	A1785	U1620	C1620	U1549	U1478	G1407	C1265	A1189	G1100	U1019	G954	U879	A815
U1954	C1786	C1786	U1621	C1621	G1552	U1479	U1410	G1266	G1190	A1114	U1020	G955	U880	A816
G1955	U1787	U1787	U1622	G1622	U1557	U1480	U1411	U1267	C1191	C1023	U1021	G956	U881	A817
G1956	U1788	U1788	U1623	A1623	G1558	U1481	C1412	U1268	A1192	A1025	U1022	G957	U882	G818
C1957	U1789	U1789	U1624	A1624	C1558	U1482	G1413	U1269	G1193	C1026	U1023	G958	U883	C819
G1958	C1708	C1708	U1625	A1625	U1561	A1486	G1414	C1270	U1194	C1120	U1024	G959	U884	A821
A1961	U1709	U1709	A1626	C1626	G1562	C1487	C1415	C1271	U1195	G1121	U1025	U960	U885	G822
C1962	U1710	U1710	U1627	C1627	U1562	C1488	C1416	C1272	G1196	A1122	C1026	U961	U886	U823
G1963	C1711	C1711	U1628	C1628	G1566	U1489	C1417	G1273	G1197	C1122	U1027	U962	U887	U824
A1964	G1712	G1712	U1629	G1629	U1567	U1490	G1418	G1274	U1198	A1123	C1028	U963	U888	C825
G1965	U1713	U1713	U1630	C1630	U1568	C1491	C1419	G1275	U1199	G1124	U1029	G964	U889	C826
C1966	A1714	A1714	U1631	C1631	A1568	C1492	U1424	A1278	G1200	C1127	U1030	A964	U890	G827
U1967	U1715	U1715	U1632	C1632	U1569	U1493	G1425	U1279	A1203	G1128	U1031	A965	U891	C828
G1968	G1716	G1716	A1633	C1633	U1570	U1494	U1426	U1280	G1204	A1129	A1032	G966	U892	C829
C1969	A1717	A1717	U1634	A1634	U1571	U1495	U1427	U1281	G1205	G1130	G1033	C967	U893	C830
U1970	U1718	U1718	U1635	G1635	U1572	U1496	C1428	A1281	U1206	G1131	G1034	C968	U894	C831
C1971	G1722	G1722	U1643	A1643	C1573	U1497	G1429	U1282	A1137	C1132	U1035	U969	U895	C832
G1972	U1723	U1723	U1644	C1644	U1574	U1498	U1430	A1283	A1138	G1133	G1036	U970	U896	C833
A1973	C1724	C1724	U1645	A1645	C1575	U1499	U1431	U1284	A1139	A1137	G1037	A971	U897	A833
U1974	U1810	U1810	U1646	C1646	U1576	U1500	G1432	U1285	A1140	C1138	U1038	C972	U898	A834
A1975	A1811	A1811	U1647	C1647	U1577	U1501	U1433	U1286	U1211	A1139	A1039	G973	U899	U837
C1976	C1727	C1727	U1648	C1648	U1578	U1502	U1434	U1287	A1141	U1140	A1040	U974	U900	A838
U1977	U1728	U1728	U1649	C1649	U1579	U1503	U1435	A1288	U1214	U1141	G1041	C975	U901	U839
U1978	C1729	C1729	U1650	C1650	U1580	U1504	U1436	A1289	U1217	U1142	U1042	U976	U902	U840
C1979	U1812	U1812	U1651	C1651	U1581	U1505	U1437				U1043	U977	U903	
A1980	A1813	A1813	U1652	C1652	U1582	U1506	U1438				U1044	U978	U904	
C1981	G1814	G1814	U1653	C1653	U1583	U1507	U1439				U1045	U979	U905	
U1982	C1731	C1731	U1654	A1654	C1581	U1508	U1440				U1046	U980	U906	



Frequency	Percentage
Daily	50%
Weekly	25%
Monthly	25%



## 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, $\alpha$ , $\beta$ , $\gamma$	169.90Å 410.40Å 697.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.70	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.70)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.283 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	59455	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	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	0.21	0/65	0.56	0/99
All	All	0.14	0/66532	0.63	0/103772

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	1732	0
2	5	96	0	62	1	0
All	All	59455	0	29979	1732	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 1732 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	1.05
1:0:1073:G:H2'	1:0:1074:G:H4'	1.40	1.00
1:0:2769:C:H2'	1:0:2867:G:H22	1.21	0.99
1:0:2668:U:H4'	1:0:2669:C:H5'	1.45	0.97

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2757/2880 (95%)	411 (14%)	0
2	5	2/4 (50%)	2 (100%)	0
All	All	2759/2884 (95%)	413 (14%)	0

5 of 413 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	15	G

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Mol	Chain	Res	Type
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	2.71	5 (16%)	34,57,60	1.15	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	-5.00	1.27	1.42
2	5	35	PPU	CE2-CZ	2.59	1.44	1.38
2	5	35	PPU	CD2-CG	2.74	1.44	1.38
2	5	35	PPU	CE1-CZ	3.64	1.46	1.38
2	5	35	PPU	C-N3'	12.17	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	2.16	117.83	109.10
2	5	35	PPU	C9-N6-C6	2.24	126.28	119.51
2	5	35	PPU	CM-OC-CZ	2.97	123.99	117.50
2	5	35	PPU	C2-N1-C6	3.31	119.95	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.