



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:57 AM UTC

PDB ID : 1FP7 / pdb_00001fp7
Title : MONOVALENT CATION BINDING SITES IN N10-FORMYLTETRAHYDROFOLATE SYNTHETASE FROM MOORELLA THERMOACETICA
Authors : Radfar, R.; Leapart, A.; Brewer, J.M.; Minor, W.; Odom, J.D.
Deposited on : 2000-08-30
Resolution : 3.20 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

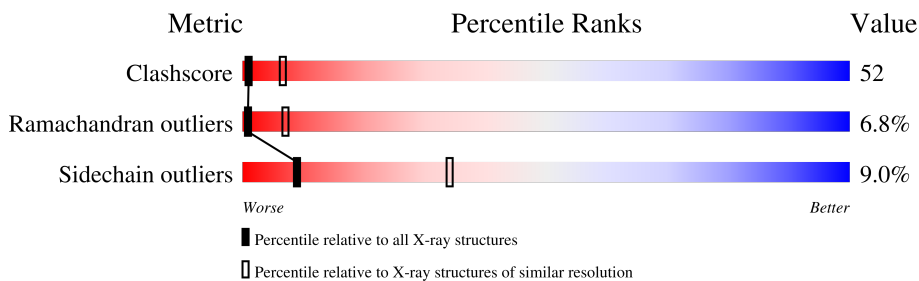
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	557	
1	B	557	

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
2	SO4	A	273	-	-	X	-
2	SO4	A	274	-	-	X	-
2	SO4	A	275	-	-	X	-
2	SO4	A	277	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	278	-	-	X	-
2	SO4	B	279	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8585 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.

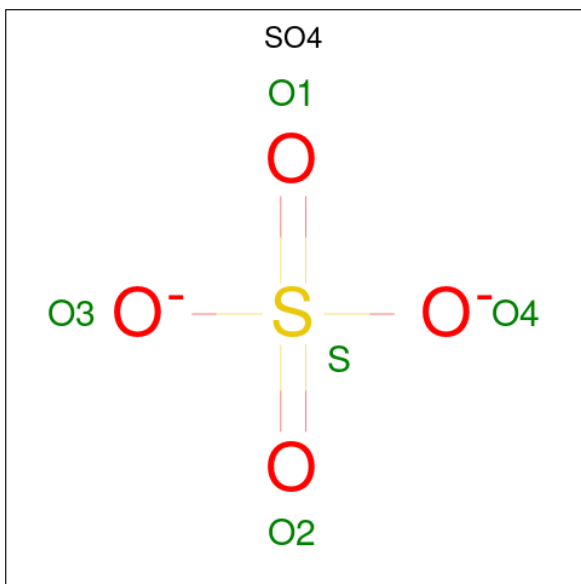
- Molecule 1 is a protein called FORMATE--TETRAHYDROFOLATE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	549	4133	2617	715	780	21	0	0	0
1	B	548	4125	2613	714	777	21	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP P21164
A	?	-	VAL	deletion	UNP P21164
B	?	-	GLU	deletion	UNP P21164
B	?	-	VAL	deletion	UNP P21164

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total K 2 2	0	1

- Molecule 4 is water.

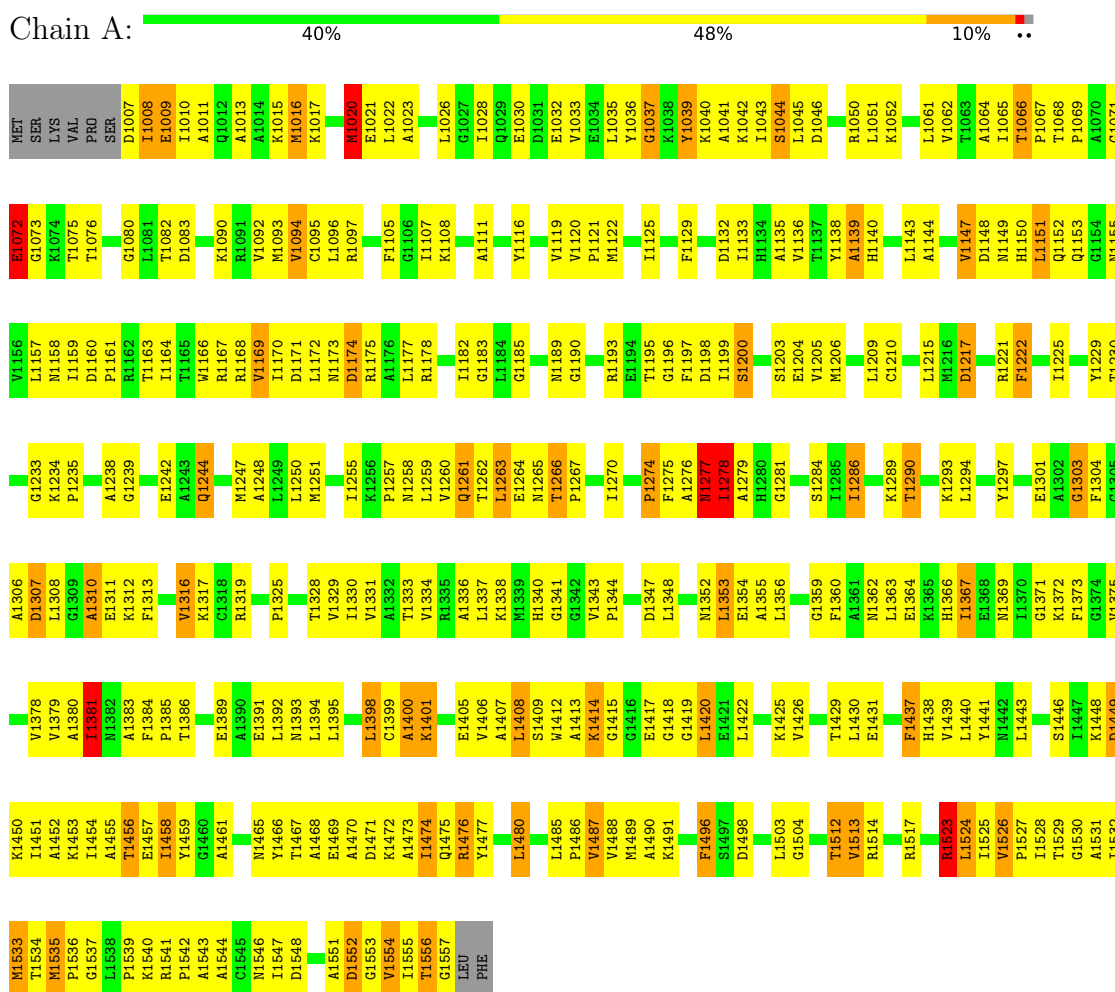
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	199	Total O 199 199	0	0
4	B	71	Total O 71 71	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: FORMATE--TETRAHYDROFOLATE LIGASE



P1527	Y1459	E1391	V1329	T1266	A1202	G1131	T1066
I1528	G1460	L1392	I1380	P1267	S1203	D1132	P1067
T1529	A1461	N1393	A1331	A1268	E1204	I1133	T1068
	D1462	L1394	A1332	F1269	V1205	H1134	P1069
	M1465	L1395	T1333	I1270	M1206	A1135	A1070
M1533	Y1466	Y1396	V1334	H1271	L1209	V1136	G1071
T1534	Y1466	L1397	R1335	G1272	C1210	E1072	
M1535	Y1466	L1398	A1336	G1273	L1211	H1140	
T1536	K1472	C1399	L1337	P1274	L1143	K1073	
	A1473	A1400	M1338	F1275	A1144	T1075	
A1543	I1474	K1401	M1339	A1276	D1214	T1076	
A1544	Q1475	A1402	H1340	M1277	L1215	T1077	
G1545	R1476	G1403	G1341	I1278	M1216	S1078	
M1546	Y1477		G1342	A1279	D1217	V1079	
I1547	E1478	L1408	V1343	H1280	E1220	G1080	
D1548	S1479	S1409	P1344	G1281	R1221	L1081	
L1480	L1480	W1412	P1344	C1282	F1222	D1082	
		A1413	D1347		S1223	Q1152	
G1483	G1483	K1414	L1348	I1285	R1224	Q1153	A1084
M1484	M1484	E1417	L1348	I1286	I1225	G1154	L1085
L1485	L1485	E1351	E1351	A1287	V1226	M1155	A1086
P1486	P1486	M1352	M1352	T1288	V1227	V1156	R1087
V1487	V1487	L1420	L1353	K1289	V1227	L1157	L1088
Y1494	Y1494	E1421	E1354	T1290	G1228	M1158	G1089
S1495	S1495	L1422	A1355	A1291	Y1229	I1159	K1090
F1496	F1496	L1430	L1356	L1292	T1230	D1160	R1091
S1497	S1497	E1431	R1357	L1293	Y1231	P1161	R1092
D1498	D1498	K1425	R1357	K1293	D1232	M1093	M1093
D1499	D1499	V1426	E1358	L1294	G1233	W1166	V1094
M1500	M1500	L1427	L1359	A1295	K1234	R1167	C1095
T1501	T1501	Q1428	F1360	I1295	P1235	R1168	L1096
M1508	M1508	T1429	A1361	Y1297	V1236	V1169	R1097
F1509	F1509	L1430	M1362	V1299	T1237	I1170	E1098
T1510	T1510	E1431	L1363	T1300	A1238	D1171	P1103
I1511	I1511	F1437	L1363	G1303	G1239	L1172	S1104
T1512	T1512	H1438	E1364	F1304	D1240	M1173	F1105
V1513	V1513	V1439	K1365	G1305		R1175	G1106
R1514	R1514	L1440	H1366	A1306	A1243	A1176	I1107
E1515	E1515	Y1441	H1366	D1307	Q1244	G1186	K1108
V1516	V1516	M1442	E1368	L1308	S1246	K1187	G1109
R1517	R1517	N1442	M1369	G1309	M1247	R1178	G1110
L1518	L1518	L1443	I1370	A1310	A1248	I1182	A1111
S1519	S1519	D1444	P1376	E1311	L1249	G1183	A1112
A1520	A1520	L1445	A1377	K1312	L1250		G1113
		S1446	A1377	F1313	M1251	G1186	G1114
		I1447	V1378	Y1314	K1252	K1187	G1115
		K1448	V1379	K1253	D1253	A1188	Y1116
		D1449	A1380	V1316	I1255	V1191	A1117
		K1450	I1381	K1317	K1256	Q1118	Q1118
		I1451	M1382	C1318	K1257	V1119	V1119
		A1452	A1383	R1319	N1257	P1192	V1120
		K1453	F1384	Y1320	N1258	E1194	P1121
		L1454	P1385	F1323	L1259	T1195	M1122
		A1455	P1386	K1324	V1260	G1196	G1123
		T1456	D1387	P1325	Q1261	F1197	D1124
		E1457	T1388	P1326	T1262	D1198	I1125
		I1458	A1390	A1327	L1263	I1199	F1129
				T1328	N1265	S1200	F1129
						V1201	T1130

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	160.88Å 160.88Å 256.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 3.20	Depositor
% Data completeness (in resolution range)	87.2 (19.99-3.20)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.285 , 0.355	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8585	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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: SO4, K

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	A	0.58	0/4201	1.11	31/5690 (0.5%)
1	B	0.52	0/4193	1.08	38/5679 (0.7%)
All	All	0.55	0/8394	1.10	69/11369 (0.6%)

There are no bond length outliers.

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1476	ARG	N-CA-C	-10.22	99.95	111.71
1	A	1524	LEU	N-CA-C	10.08	125.44	108.20
1	B	1523	ARG	N-CA-C	8.61	118.39	108.49
1	B	1324	LYS	CA-C-N	8.04	129.88	119.84
1	B	1324	LYS	C-N-CA	8.04	129.88	119.84

There are no chirality outliers.

There are no planarity outliers.

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	A	4133	0	4219	372	1
1	B	4125	0	4211	492	0
2	A	35	0	0	15	1
2	B	20	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2	0	0	1	0
4	A	199	0	0	29	0
4	B	71	0	0	17	0
All	All	8585	0	8430	865	1

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 52.

The worst 5 of 865 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:B:1175:ARG:NH1	2:B:279:SO4:O3	1.58	1.33
1:A:1175:ARG:HD3	2:A:275:SO4:O3	1.40	1.22
1:B:1222:PHE:O	1:B:1225:ILE:HG22	1.40	1.19
1:A:1007:ASP:OD2	4:A:32:HOH:O	1.68	1.11
1:B:1079:VAL:HB	1:B:1117:ALA:HB1	1.34	1.08

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:ASP:OD1	2:A:278:SO4:O3[3_665]	1.60	0.60

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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
1	A	547/557 (98%)	437 (80%)	90 (16%)	20 (4%)	2 18
1	B	546/557 (98%)	385 (70%)	107 (20%)	54 (10%)	0 2
All	All	1093/1114 (98%)	822 (75%)	197 (18%)	74 (7%)	1 7

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1015	LYS
1	A	1304	PHE
1	A	1533	MET
1	A	1556	THR
1	B	1056	ASP

5.3.2 Protein sidechains [i](#)

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	
1	A	432/440 (98%)	394 (91%)	38 (9%)	9	35
1	B	431/440 (98%)	391 (91%)	40 (9%)	8	33
All	All	863/880 (98%)	785 (91%)	78 (9%)	9	34

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1270	ILE
1	B	1503	LEU
1	B	1280	HIS
1	B	1353	LEU
1	B	1535	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1140	HIS
1	B	1189	ASN
1	B	1153	GLN
1	B	1244	GLN
1	A	1265	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 for Mogul analysis.

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	SO4	A	271	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	B	272	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	278	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	B	279	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	275	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	276	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	A	277	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	B	280	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	B	281	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	273	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	A	274	-	4,4,4	0.69	0	6,6,6	0.49	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	272	SO4	1	0
2	A	278	SO4	2	1
2	B	279	SO4	2	0
2	A	275	SO4	4	0
2	A	277	SO4	2	0
2	B	280	SO4	1	0
2	A	273	SO4	4	0
2	A	274	SO4	3	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 [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.