



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:53 am GMT

PDB ID : 1K3F
Title : Uridine Phosphorylase from E. coli, Refined in the Monoclinic Crystal Lattice
Authors : Morgunova, E.Yu.; Mikhailov, A.M.; Popov, A.N.; Blagova, E.V.; Smirnova, E.A.; Vainshtein, B.K.; Mao, C.; Armstrong, S.R.; Ealick, S.E.; Komissarov, A.A.; Linkova, E.V.; Burlakova, A.A.; Mironov, A.S.; Debabov, V.G.
Deposited on : 2001-10-02
Resolution : 2.50 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
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

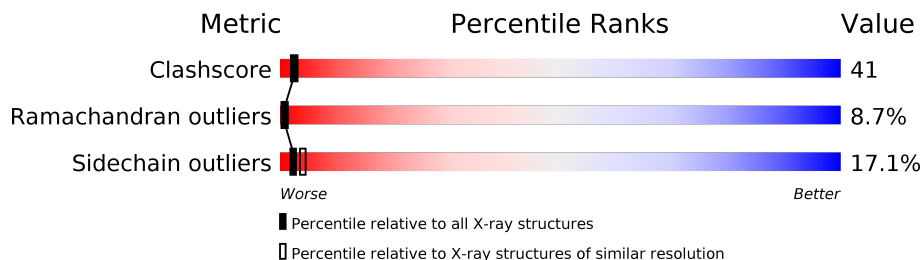
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)

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	A	253	<div> <div style="width: 45%; background-color: green;"></div> <div style="width: 41%; background-color: yellow;"></div> <div style="width: 11%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> </div> <div>45% 41% 11% .</div>
1	B	253	<div> <div style="width: 39%; background-color: green;"></div> <div style="width: 48%; background-color: yellow;"></div> <div style="width: 13%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> </div> <div>39% 48% 13% .</div>
1	C	253	<div> <div style="width: 37%; background-color: green;"></div> <div style="width: 50%; background-color: yellow;"></div> <div style="width: 11%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> </div> <div>37% 50% 11% .</div>
1	D	253	<div> <div style="width: 38%; background-color: green;"></div> <div style="width: 48%; background-color: yellow;"></div> <div style="width: 14%; background-color: orange;"></div> </div> <div>38% 48% 14%</div>
1	E	253	<div> <div style="width: 37%; background-color: green;"></div> <div style="width: 46%; background-color: yellow;"></div> <div style="width: 16%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> </div> <div>37% 46% 16% .</div>
1	F	253	<div> <div style="width: 33%; background-color: green;"></div> <div style="width: 51%; background-color: yellow;"></div> <div style="width: 14%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> </div> <div>33% 51% 14% .</div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11286 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 uridine phosphorylase.

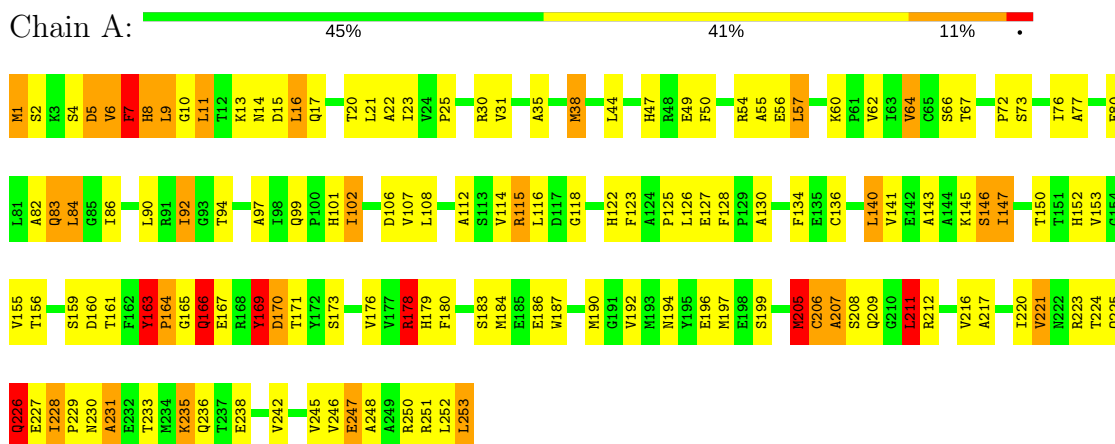
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1881	1180	322	367	12			
1	B	253	Total	C	N	O	S	0	0	0
			1881	1180	322	367	12			
1	C	253	Total	C	N	O	S	0	0	0
			1881	1180	322	367	12			
1	D	253	Total	C	N	O	S	0	0	0
			1881	1180	322	367	12			
1	E	253	Total	C	N	O	S	0	0	0
			1881	1180	322	367	12			
1	F	253	Total	C	N	O	S	0	0	0
			1881	1180	322	367	12			

3 Residue-property plots

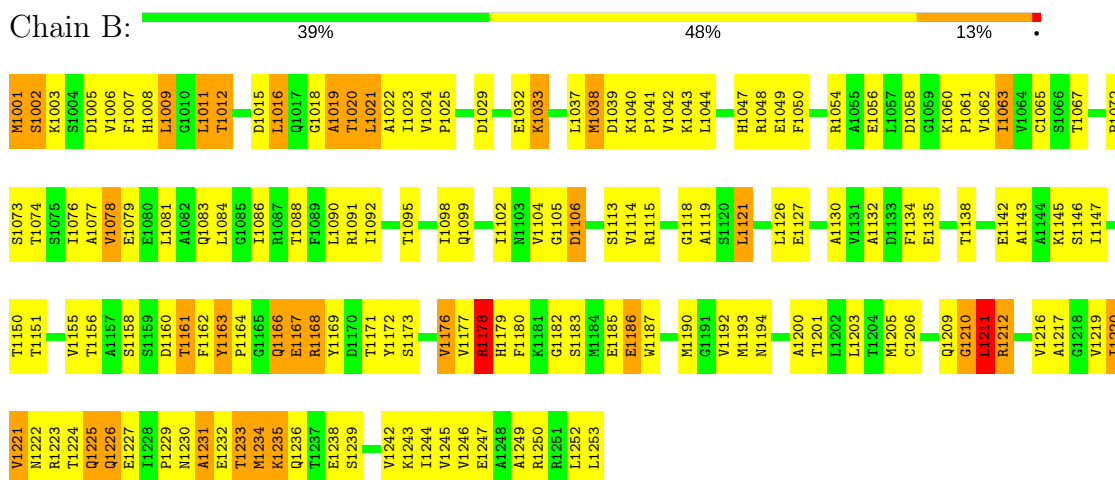
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: uridine phosphorylase

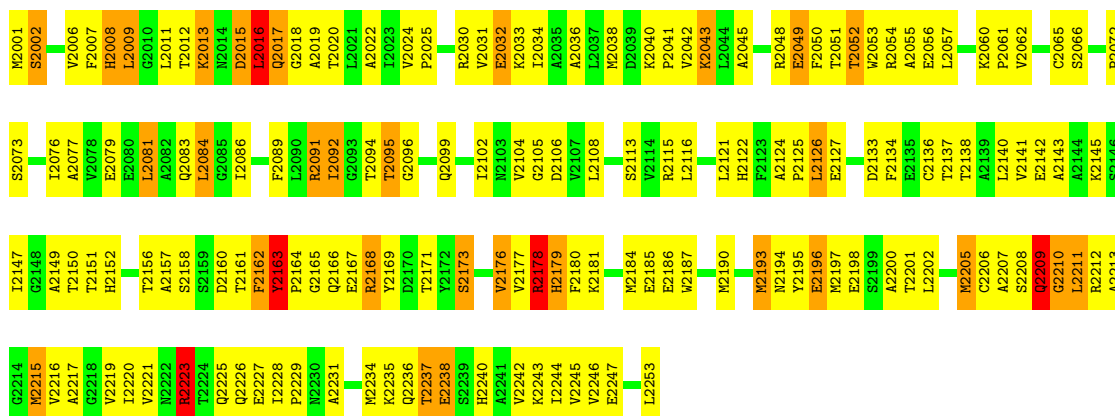


- Molecule 1: uridine phosphorylase



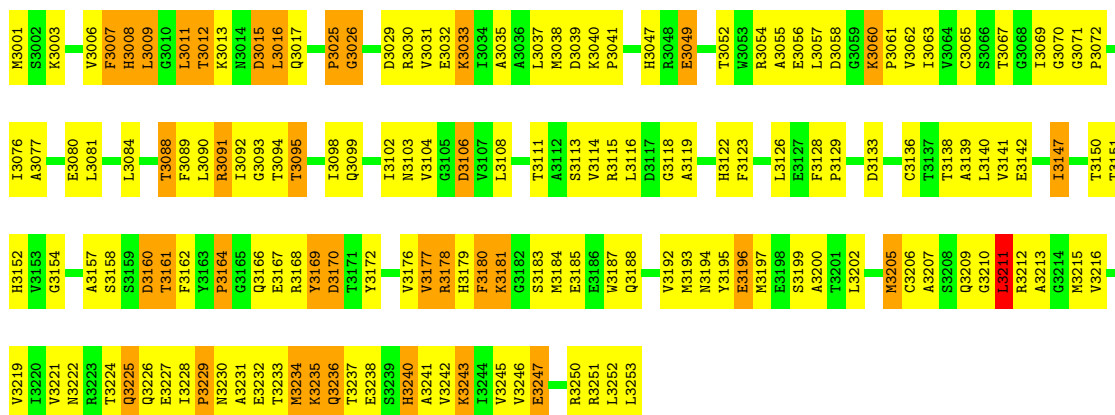
- Molecule 1: uridine phosphorylase





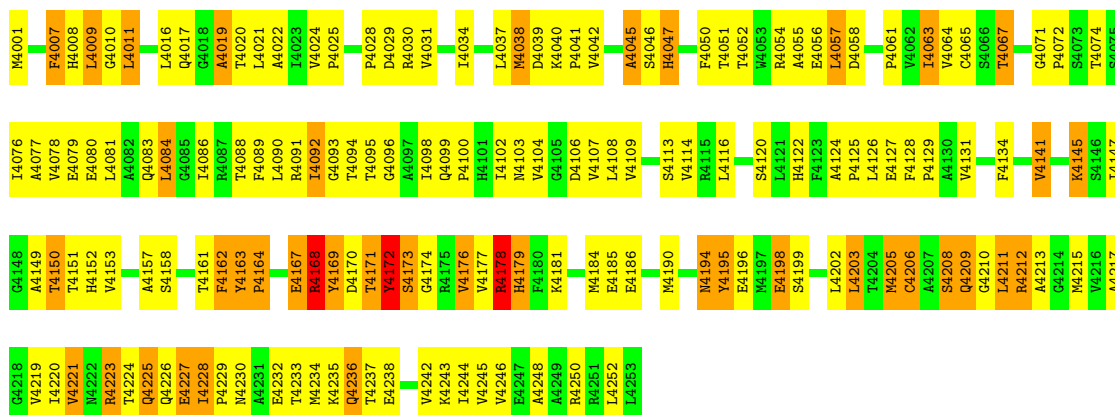
• Molecule 1: uridine phosphorylase

Chain D: 38% 48% 14%



• Molecule 1: uridine phosphorylase

Chain E: 37% 46% 16%



• Molecule 1: uridine phosphorylase

Chain F: 33% 51% 14%



M5001	S5002	K5003	S5004	D5005	V5006	F5007	H5008	L5009	G5010	L5011	T5012	K5013	L5014	D5015	L5016	Q5017	G5018	A5019	T5020	L5021	A5022	I5023	V5024	P5025	G5026	D5027	P5028	D5029	R5030	V5031	F5032	K5033	I5034	L5037	M5038	D5039	K5040	P5041	V5042	K5043	L5044	H5047	R5048	F5049	F5050	R5054	A5055	E5056	L5057	K5060	P5061	V5062	I5063	V5064	C5065
S5066	I5067	S5073	T5074	S5075	I5076	E5079	E5080	Q5083	L5084	G5085	L5086	R5087	T5088	F5089	L5090	R5091	I5092	G5093	T5094	T5095	G5096	Q5099	P5100	H5101	I5102	D5106	V5107	L5108	V5109	T5110	T5111	A5112	S5113	V5114	R5115	L5116	D5117	G5118	A5119	S5120	L5121	H5122	F5123	A5124	P5125	L5126	E5127	F5128	P5129	A5130	D5133	F5134			
T5137	T5138	A5139	L5140	V5141	E5142	K5145	S5146	I5147	H5152	V5153	G5154	V5155	T5156	A5157	S5158	S5159	F5162	V5163	T5171	Y5172	S5173	G5174	R5175	V5176	V5177	R5178	H5179	F5180	K5181	G5182	S5183	M5184	F5185	E5186	W5187	V5192	M5193	N5194	Y5195	E5196	S5199	A5200	T5201	L5202	L5203	T5204	R5205	C5206	A5207	S5208	Q5209	G5210	L5211		
R5212	A5213	G5214	M5215	V5216	A5217	I5220	V5221	N5222	R5223	T5224	Q5225	Q5226	E5227	I5228	P5229	N5230	A5231	E5232	T5233	M5234	K5235	Q5236	S5239	H5240	A5241	V5242	K5243	V5246	R5250	R5251	L5252	L5253																							

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.60Å 98.80Å 93.70Å 90.00° 120.20° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.50)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11286	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.68	1/1913 (0.1%)	0.95	3/2599 (0.1%)
1	B	0.62	0/1913	0.92	2/2599 (0.1%)
1	C	0.69	1/1913 (0.1%)	0.91	0/2599
1	D	0.65	0/1913	0.94	1/2599 (0.0%)
1	E	0.67	0/1913	0.92	5/2599 (0.2%)
1	F	2.39	8/1913 (0.4%)	1.02	5/2599 (0.2%)
All	All	1.15	10/11478 (0.1%)	0.94	16/15594 (0.1%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	5007	PHE	CE1-CZ	45.72	2.24	1.37
1	F	5007	PHE	CE2-CZ	45.69	2.24	1.37
1	F	5007	PHE	CD2-CE2	44.49	2.28	1.39
1	F	5007	PHE	CD1-CE1	44.03	2.27	1.39
1	F	5007	PHE	CG-CD2	29.57	1.83	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	5001	MET	C-N-CA	15.24	159.80	121.70
1	F	5007	PHE	CB-CG-CD1	-9.44	114.19	120.80
1	A	211	LEU	CA-CB-CG	6.32	129.84	115.30
1	E	4170	ASP	N-CA-C	6.25	127.87	111.00
1	A	16	LEU	CA-CB-CG	6.14	129.42	115.30

There are no chirality outliers.

There are no planarity outliers.

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	A	1881	0	1871	155	0
1	B	1881	0	1868	145	0
1	C	1881	0	1868	180	0
1	D	1881	0	1868	151	0
1	E	1881	0	1868	154	0
1	F	1881	0	1868	214	0
All	All	11286	0	11211	929	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 41.

The worst 5 of 929 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:F:5007:PHE:CG	1:F:5007:PHE:CD1	1.82	1.67
1:F:5007:PHE:CD2	1:F:5007:PHE:CG	1.83	1.60
1:F:5002:SER:CA	1:F:5002:SER:N	1.75	1.48
1:F:5007:PHE:CZ	1:F:5007:PHE:CE1	2.24	1.26
1:F:5007:PHE:CE2	1:F:5007:PHE:CZ	2.24	1.25

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
1	A	251/253 (99%)	189 (75%)	37 (15%)	25 (10%)	1 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	251/253 (99%)	180 (72%)	47 (19%)	24 (10%)	1	0
1	C	251/253 (99%)	193 (77%)	35 (14%)	23 (9%)	1	1
1	D	251/253 (99%)	194 (77%)	40 (16%)	17 (7%)	1	1
1	E	251/253 (99%)	187 (74%)	41 (16%)	23 (9%)	1	1
1	F	251/253 (99%)	193 (77%)	39 (16%)	19 (8%)	1	1
All	All	1506/1518 (99%)	1136 (75%)	239 (16%)	131 (9%)	1	1

5 of 131 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	7	PHE
1	A	13	LYS
1	A	30	ARG
1	A	163	TYR

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	
1	A	200/204 (98%)	170 (85%)	30 (15%)	3	6
1	B	200/204 (98%)	166 (83%)	34 (17%)	2	4
1	C	200/204 (98%)	168 (84%)	32 (16%)	3	5
1	D	200/204 (98%)	158 (79%)	42 (21%)	1	2
1	E	200/204 (98%)	165 (82%)	35 (18%)	2	4
1	F	200/204 (98%)	168 (84%)	32 (16%)	3	5
All	All	1200/1224 (98%)	995 (83%)	205 (17%)	2	4

5 of 205 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2215	MET

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Mol	Chain	Res	Type
1	D	3113	SER
1	F	5137	THR
1	C	2238	GLU
1	D	3052	THR

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

Mol	Chain	Res	Type
1	C	2240	HIS
1	D	3194	ASN
1	F	5152	HIS
1	D	3099	GLN
1	D	3166	GLN

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 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.