



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:37 PM GMT

PDB ID : 1PXA  
Title : CRYSTAL STRUCTURES OF MUTANT PSEUDOMONAS AERUGINOSA P-HYDROXYBENZOATE HYDROXYLASE: THE TYR201PHE, TYR385PHE, AND ASN300ASP VARIANTS  
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Deposited on : 1994-09-27  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (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

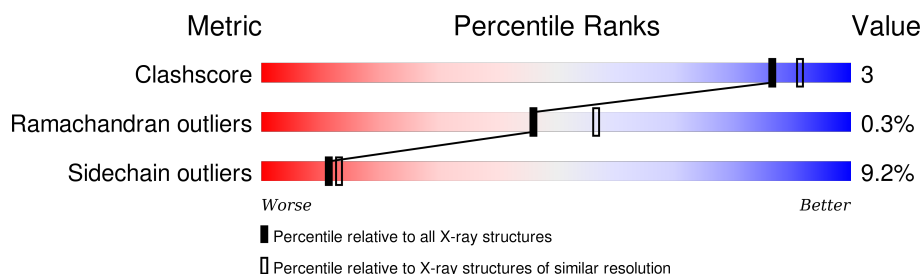
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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	A	394	 77% 19% . .

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3339 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 P-HYDROXYBENZOATE HYDROXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	394	3125	1975	562	577	11	0	0	0

There is a discrepancy between the modelled and reference sequences:

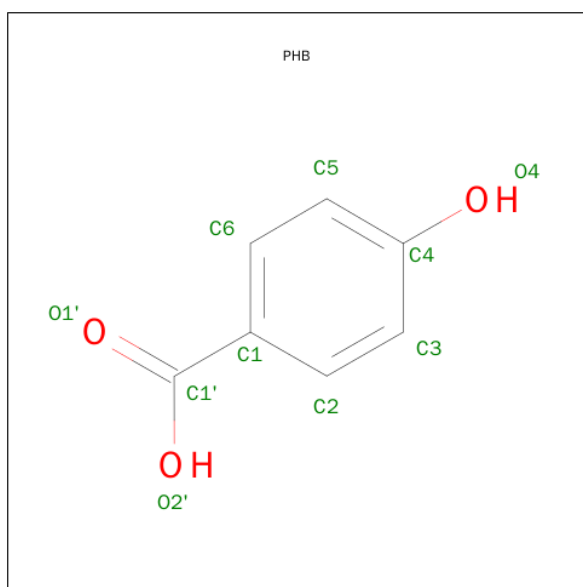
Chain	Residue	Modelled	Actual	Comment	Reference
A	300	ASP	ASN	CONFLICT	UNP P20586

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0

- Molecule 3 is P-HYDROXYBENZOIC ACID (three-letter code: PHB) (formula:  $C_7H_6O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	7	3		

- Molecule 4 is water.

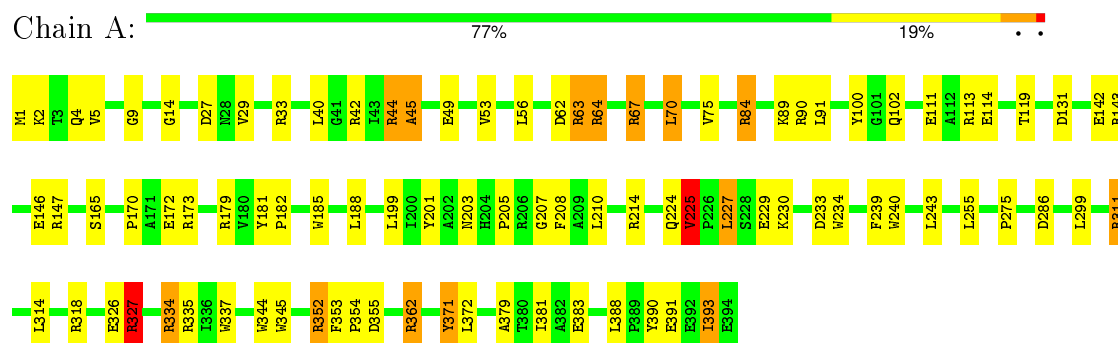
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	151	Total	O	0	0
			151	151		

### 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: P-HYDROXYBENZOATE HYDROXYLASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.88Å 146.62Å 88.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.193 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3339	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	6.0	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: PHB, FAD

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	1.01	0/3190	1.80	69/4316 (1.6%)

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	ARG	NE-CZ-NH2	-12.62	113.99	120.30
1	A	143	ARG	NE-CZ-NH1	11.99	126.29	120.30
1	A	42	ARG	NE-CZ-NH1	11.69	126.14	120.30
1	A	334	ARG	NE-CZ-NH1	9.73	125.17	120.30
1	A	234	TRP	CD1-CG-CD2	9.54	113.94	106.30
1	A	344	TRP	CD1-CG-CD2	8.79	113.33	106.30
1	A	44	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	A	33	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	A	33	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	A	214	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	A	185	TRP	CD1-CG-CD2	8.05	112.74	106.30
1	A	53	VAL	CA-CB-CG2	-7.89	99.07	110.90
1	A	344	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	A	234	TRP	CE2-CD2-CG	-7.76	101.09	107.30
1	A	179	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	A	327	ARG	CA-CB-CG	7.50	129.89	113.40
1	A	240	TRP	CE2-CD2-CG	-7.32	101.44	107.30
1	A	185	TRP	CE2-CD2-CG	-7.26	101.49	107.30
1	A	390	TYR	CB-CG-CD2	-7.09	116.75	121.00
1	A	143	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	345	TRP	CD1-CG-CD2	6.92	111.83	106.30
1	A	63	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	A	179	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	A	337	TRP	CD1-CG-CD2	6.80	111.74	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	TRP	CE2-CD2-CG	-6.73	101.91	107.30
1	A	240	TRP	CD1-CG-CD2	6.65	111.62	106.30
1	A	63	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	67	ARG	CA-CB-CG	6.50	127.69	113.40
1	A	185	TRP	CG-CD1-NE1	-6.50	103.60	110.10
1	A	64	ARG	CB-CG-CD	6.47	128.42	111.60
1	A	345	TRP	CE2-CD2-CG	-6.32	102.24	107.30
1	A	1	MET	CA-CB-CG	6.14	123.75	113.30
1	A	45	ALA	N-CA-C	6.12	127.51	111.00
1	A	64	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	199	LEU	CB-CG-CD2	-6.09	100.64	111.00
1	A	234	TRP	CG-CD1-NE1	-6.02	104.08	110.10
1	A	84	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	A	100	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	A	344	TRP	CG-CD1-NE1	-5.90	104.20	110.10
1	A	113	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	75	VAL	CG1-CB-CG2	-5.73	101.73	110.90
1	A	2	LYS	CA-CB-CG	5.72	125.98	113.40
1	A	352	ARG	CB-CG-CD	5.71	126.46	111.60
1	A	362	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	286	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	146	GLU	CA-CB-CG	5.61	125.75	113.40
1	A	165	SER	CA-C-N	5.56	129.43	117.20
1	A	111	GLU	CA-CB-CG	5.55	125.61	113.40
1	A	70	LEU	CA-CB-CG	5.51	127.97	115.30
1	A	67	ARG	CB-CA-C	-5.50	99.40	110.40
1	A	344	TRP	CB-CG-CD1	-5.49	119.86	127.00
1	A	233	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	201	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	A	311	ARG	CA-CB-CG	5.23	124.92	113.40
1	A	203	ASN	OD1-CG-ND2	-5.22	109.90	121.90
1	A	203	ASN	CB-CG-ND2	5.19	129.16	116.70
1	A	355	ASP	CA-C-N	-5.19	105.78	117.20
1	A	53	VAL	CA-CB-CG1	5.18	118.68	110.90
1	A	5	VAL	O-C-N	-5.17	114.42	122.70
1	A	225	VAL	N-CA-CB	-5.16	100.15	111.50
1	A	214	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	75	VAL	CB-CA-C	-5.13	101.66	111.40
1	A	181	TYR	CB-CG-CD2	-5.11	117.94	121.00
1	A	371	TYR	CB-CG-CD1	-5.11	117.94	121.00
1	A	337	TRP	CG-CD1-NE1	-5.10	105.00	110.10
1	A	275	PRO	N-CA-C	5.09	125.33	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	64	ARG	CD-NE-CZ	5.08	130.71	123.60
1	A	337	TRP	CA-C-N	5.05	128.32	117.20
1	A	62	ASP	N-CA-C	5.01	124.54	111.00

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	3125	0	3118	17	0
2	A	53	0	31	0	0
3	A	10	0	4	0	0
4	A	151	0	0	0	0
All	All	3339	0	3153	17	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 3.

All (17) 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:A:327:ARG:HH12	1:A:334:ARG:HH22	1.42	0.65
1:A:208:PHE:HB3	1:A:224:GLN:HB2	1.87	0.56
1:A:142:GLU:HG3	1:A:147:ARG:HH11	1.71	0.55
1:A:45:ALA:HB3	1:A:102:GLN:HB2	1.88	0.54
1:A:182:PRO:HA	1:A:227:LEU:HD22	1.90	0.53
1:A:64:ARG:HE	1:A:67:ARG:HH12	1.56	0.52
1:A:170:PRO:HB2	1:A:173:ARG:HG2	1.92	0.52
1:A:371:TYR:HB3	1:A:381:ILE:HD11	1.94	0.50
1:A:29:VAL:HG22	1:A:119:THR:HB	1.93	0.50
1:A:379:ALA:O	1:A:383:GLU:HG2	2.14	0.46
1:A:9:GLY:O	1:A:14:GLY:HA3	2.16	0.46
1:A:393:ILE:H	1:A:393:ILE:HD12	1.80	0.46
1:A:225:VAL:HG13	1:A:229:GLU:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:PHE:HA	1:A:354:PRO:HD3	1.81	0.43
1:A:4:GLN:HB2	1:A:27:ASP:O	2.20	0.42
1:A:207:GLY:HA2	1:A:352:ARG:HB3	2.03	0.41
1:A:188:LEU:HD13	1:A:239:PHE:CD2	2.55	0.41

There are no symmetry-related clashes.

## 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	392/394 (100%)	377 (96%)	14 (4%)	1 (0%)	46 57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	ARG

### 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	325/325 (100%)	295 (91%)	30 (9%)	11 13

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	49	GLU
1	A	56	LEU
1	A	63	ARG
1	A	70	LEU
1	A	84	ARG
1	A	89	LYS
1	A	91	LEU
1	A	114	GLU
1	A	131	ASP
1	A	172	GLU
1	A	205	PRO
1	A	210	LEU
1	A	225	VAL
1	A	227	LEU
1	A	230	LYS
1	A	243	LEU
1	A	255	LEU
1	A	299	LEU
1	A	311	ARG
1	A	314	LEU
1	A	318	ARG
1	A	326	GLU
1	A	327	ARG
1	A	335	ARG
1	A	362	ARG
1	A	372	LEU
1	A	388	LEU
1	A	391	GLU
1	A	393	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

2 ligands 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	$\# Z  > 2$
2	FAD	A	395	-	48,58,58	1.36	6 (12%)	54,89,89	2.75	14 (25%)
3	PHB	A	396	-	7,10,10	0.58	0	10,13,13	1.49	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
2	FAD	A	395	-	-	0/30/50/50	0/6/6/6
3	PHB	A	396	-	-	0/0/4/4	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	395	FAD	C9A-C5X	-3.55	1.35	1.42
2	A	395	FAD	C8A-N7A	-2.33	1.30	1.34
2	A	395	FAD	C4-N3	2.11	1.37	1.33
2	A	395	FAD	O2B-C2B	2.27	1.48	1.43
2	A	395	FAD	C5'-C4'	2.85	1.56	1.51
2	A	395	FAD	C4-C4X	3.15	1.47	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	395	FAD	C4X-C4-N3	-6.81	114.28	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	395	FAD	C4X-C10-N10	-5.65	117.19	120.52
2	A	395	FAD	C4-C4X-C10	-5.59	116.36	119.94
2	A	395	FAD	C4X-N5-C5X	-3.69	112.52	116.76
2	A	395	FAD	C6-C5X-N5	-3.04	115.06	118.96
2	A	395	FAD	O3B-C3B-C4B	-2.77	102.75	111.05
2	A	395	FAD	P-O3P-PA	-2.48	125.78	132.73
3	A	396	PHB	C6-C1-C1'	-2.23	117.45	120.45
2	A	395	FAD	O4'-C4'-C3'	2.13	114.36	109.02
3	A	396	PHB	C2-C1-C1'	2.21	123.42	120.45
2	A	395	FAD	N3A-C2A-N1A	2.31	130.66	128.89
2	A	395	FAD	C1'-N10-C9A	2.44	121.59	118.86
2	A	395	FAD	C4B-O4B-C1B	2.44	112.40	109.72
2	A	395	FAD	O2B-C2B-C3B	2.54	120.08	111.83
2	A	395	FAD	C9A-C5X-N5	3.73	127.87	122.36
2	A	395	FAD	C4-N3-C2	13.19	126.65	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 will therefore be empty.

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

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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