



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 17, 2018 – 04:24 pm GMT

PDB ID : 2Q0Q  
Title : Structure of the Native M. Smegmatis Aryl Esterase  
Authors : Mathews, I.I.; Soltis, M.; Saldajeno, M.; Ganshaw, G.; Sala, R.; Weyler, W.;  
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Deposited on : 2007-05-22  
Resolution : 1.50 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

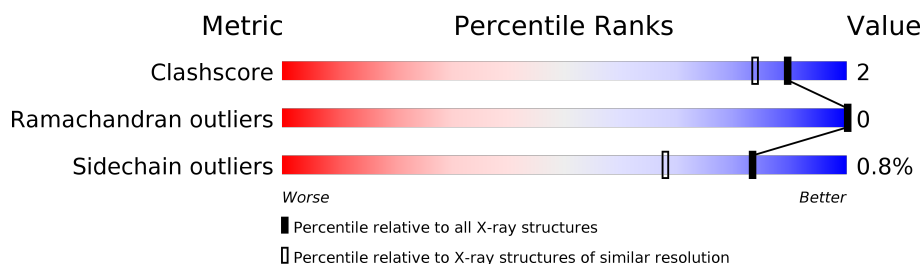
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	122078	2726 (1.50-1.50)
Ramachandran outliers	120005	2660 (1.50-1.50)
Sidechain outliers	119972	2658 (1.50-1.50)


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  $\geq 3$ , 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	216	 91% 8%
1	B	216	 94% 5%
1	C	216	 93% 6%
1	D	216	 93% 6% .
1	E	216	 94% 6%
1	F	216	 92% 7%
1	G	216	 93% 6%

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Mol	Chain	Length	Quality of chain
1	H	216	 92% 7%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14768 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 aryl esterase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	Se	0	0	0
			1634	1048	271	309	2	4			
1	B	215	Total	C	N	O	S	Se	0	0	0
			1634	1048	271	309	2	4			
1	C	215	Total	C	N	O	S	Se	0	0	0
			1634	1048	271	309	2	4			
1	D	215	Total	C	N	O	S	Se	0	0	0
			1634	1048	271	309	2	4			
1	E	215	Total	C	N	O	S	Se	0	0	0
			1634	1048	271	309	2	4			
1	F	215	Total	C	N	O	S	Se	0	0	0
			1634	1048	271	309	2	4			
1	G	215	Total	C	N	O	S	Se	0	0	0
			1634	1048	271	309	2	4			
1	H	215	Total	C	N	O	S	Se	0	0	0
			1634	1048	271	309	2	4			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
A	111	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
A	145	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
A	175	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
B	90	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
B	111	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
B	145	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
B	175	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
C	90	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
C	111	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
C	145	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
C	175	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
D	90	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	111	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
D	145	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
D	175	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
E	90	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
E	111	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
E	145	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
E	175	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
F	90	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
F	111	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
F	145	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
F	175	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
G	90	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
G	111	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
G	145	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
G	175	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
H	90	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
H	111	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
H	145	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7
H	175	MSE	MET	MODIFIED RESIDUE	UNP A0R5U7

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	260	Total	O	0	0
			260	260		
4	B	227	Total	O	0	0
			227	227		
4	C	150	Total	O	0	0
			150	150		
4	D	227	Total	O	0	0
			227	227		
4	E	184	Total	O	0	0
			184	184		
4	F	242	Total	O	0	0
			242	242		
4	G	155	Total	O	0	0
			155	155		
4	H	163	Total	O	0	0
			163	163		

### 3 Residue-property plots [i](#)

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.

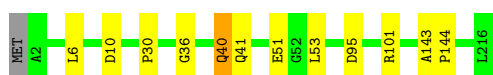
- Molecule 1: aryl esterase

Chain A: 



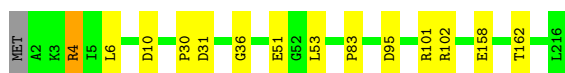
- Molecule 1: aryl esterase

Chain B: 



- Molecule 1: aryl esterase

Chain C: 



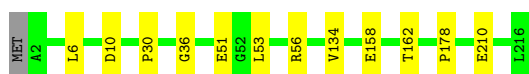
- Molecule 1: aryl esterase

Chain D: 



- Molecule 1: aryl esterase

Chain E: 



- Molecule 1: aryl esterase



Chain F:  92% 7%



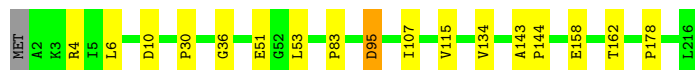
- Molecule 1: aryl esterase

Chain G:  93% 6%



- Molecule 1: aryl esterase

Chain H:  92% 7%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.16Å 98.16Å 229.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.50	Depositor
% Data completeness (in resolution range)	94.7 (30.00-1.50)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.175 , 0.196	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14768	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	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: GOL, SO4

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	0.82	0/1671	0.95	12/2280 (0.5%)
1	B	0.73	0/1671	0.80	1/2280 (0.0%)
1	C	0.59	0/1671	0.73	4/2280 (0.2%)
1	D	0.73	0/1671	0.90	6/2280 (0.3%)
1	E	0.68	0/1671	0.77	1/2280 (0.0%)
1	F	0.83	0/1671	0.91	3/2280 (0.1%)
1	G	0.57	0/1671	0.70	1/2280 (0.0%)
1	H	0.60	0/1671	0.68	0/2280
All	All	0.70	0/13368	0.81	28/18240 (0.2%)

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4	ARG	NE-CZ-NH1	12.01	126.30	120.30
1	A	4	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	D	4	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	F	101	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	E	56	ARG	NE-CZ-NH2	-7.06	116.77	120.30

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	1634	0	1625	7	0
1	B	1634	0	1625	5	0
1	C	1634	0	1625	5	0
1	D	1634	0	1625	6	0
1	E	1634	0	1625	5	0
1	F	1634	0	1625	9	0
1	G	1634	0	1625	6	0
1	H	1634	0	1625	9	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0
3	F	6	0	8	0	0
3	G	6	0	8	0	0
3	H	6	0	8	0	0
4	A	260	0	0	0	0
4	B	227	0	0	0	0
4	C	150	0	0	0	0
4	D	227	0	0	0	0
4	E	184	0	0	0	0
4	F	242	0	0	1	0
4	G	155	0	0	0	0
4	H	163	0	0	0	0
All	All	14768	0	13064	52	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 2.

The worst 5 of 52 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:D:40:GLN:HE22	1:D:41:GLN:HE21	1.15	0.94
1:A:20:GLU:OE2	1:A:191:VAL:HG21	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:ILE:HD12	1:F:86:LEU:HB3	1.71	0.72
1:D:40:GLN:NE2	1:D:41:GLN:HE21	1.92	0.68
1:A:20:GLU:OE2	1:A:191:VAL:CG2	2.42	0.67

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	213/216 (99%)	206 (97%)	7 (3%)	0	100	100
1	B	213/216 (99%)	206 (97%)	7 (3%)	0	100	100
1	C	213/216 (99%)	208 (98%)	5 (2%)	0	100	100
1	D	213/216 (99%)	206 (97%)	7 (3%)	0	100	100
1	E	213/216 (99%)	205 (96%)	8 (4%)	0	100	100
1	F	213/216 (99%)	206 (97%)	7 (3%)	0	100	100
1	G	213/216 (99%)	208 (98%)	5 (2%)	0	100	100
1	H	213/216 (99%)	206 (97%)	7 (3%)	0	100	100
All	All	1704/1728 (99%)	1651 (97%)	53 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	177/174 (102%)	177 (100%)	0	100	100
1	B	177/174 (102%)	175 (99%)	2 (1%)	76	55
1	C	177/174 (102%)	175 (99%)	2 (1%)	76	55
1	D	177/174 (102%)	174 (98%)	3 (2%)	63	35
1	E	177/174 (102%)	176 (99%)	1 (1%)	87	75
1	F	177/174 (102%)	176 (99%)	1 (1%)	87	75
1	G	177/174 (102%)	176 (99%)	1 (1%)	87	75
1	H	177/174 (102%)	176 (99%)	1 (1%)	87	75
All	All	1416/1392 (102%)	1405 (99%)	11 (1%)	83	68

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	31	ASP
1	D	95	ASP
1	F	31	ASP
1	C	95	ASP
1	E	210	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	40	GLN
1	F	40	GLN
1	H	40	GLN

### 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

16 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
3	GOL	A	1730	-	5,5,5	0.38	0	5,5,5	0.41	0
2	SO4	A	1800	-	4,4,4	0.96	0	6,6,6	0.58	0
3	GOL	B	1735	-	5,5,5	0.74	0	5,5,5	0.54	0
2	SO4	B	1805	-	4,4,4	0.97	0	6,6,6	0.75	0
3	GOL	C	1740	-	5,5,5	0.60	0	5,5,5	0.52	0
2	SO4	C	1810	-	4,4,4	0.71	0	6,6,6	0.59	0
3	GOL	D	1745	-	5,5,5	0.58	0	5,5,5	0.47	0
2	SO4	D	1815	-	4,4,4	1.00	0	6,6,6	0.65	0
3	GOL	E	1750	-	5,5,5	0.52	0	5,5,5	0.44	0
2	SO4	E	1820	-	4,4,4	0.79	0	6,6,6	0.71	0
3	GOL	F	1755	-	5,5,5	0.81	0	5,5,5	0.56	0
2	SO4	F	1825	-	4,4,4	1.28	0	6,6,6	0.59	0
3	GOL	G	1760	-	5,5,5	0.41	0	5,5,5	0.49	0
2	SO4	G	1830	-	4,4,4	0.64	0	6,6,6	0.74	0
3	GOL	H	1765	-	5,5,5	0.43	0	5,5,5	0.46	0
2	SO4	H	1835	-	4,4,4	0.68	0	6,6,6	0.64	0

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
3	GOL	A	1730	-	-	0/4/4/4	0/0/0/0
2	SO4	A	1800	-	-	0/0/0/0	0/0/0/0
3	GOL	B	1735	-	-	0/4/4/4	0/0/0/0
2	SO4	B	1805	-	-	0/0/0/0	0/0/0/0
3	GOL	C	1740	-	-	0/4/4/4	0/0/0/0
2	SO4	C	1810	-	-	0/0/0/0	0/0/0/0
3	GOL	D	1745	-	-	0/4/4/4	0/0/0/0
2	SO4	D	1815	-	-	0/0/0/0	0/0/0/0
3	GOL	E	1750	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	E	1820	-	-	0/0/0/0	0/0/0/0
3	GOL	F	1755	-	-	0/4/4/4	0/0/0/0
2	SO4	F	1825	-	-	0/0/0/0	0/0/0/0
3	GOL	G	1760	-	-	0/4/4/4	0/0/0/0
2	SO4	G	1830	-	-	0/0/0/0	0/0/0/0
3	GOL	H	1765	-	-	0/4/4/4	0/0/0/0
2	SO4	H	1835	-	-	0/0/0/0	0/0/0/0

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.

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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.