



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 24, 2026 – 10:44 AM UTC

PDB ID : 1GRL / pdb_00001grl
Title : THE CRYSTAL STRUCTURE OF THE BACTERIAL CHAPERONIN
GROEL AT 2.8 ANGSTROMS
Authors : Braig, K.; Otwinowski, Z.; Hegde, R.; Boisvert, D.C.; Joachimiak, A.; Horwich,
A.L.; Sigler, P.B.
Deposited on : 1995-03-07
Resolution : 2.80 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

<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
Xtriage (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

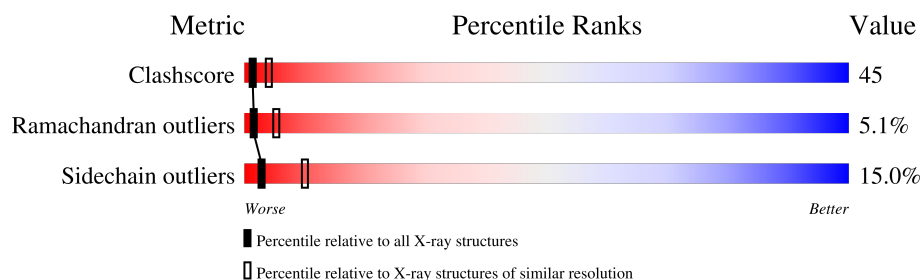
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	548	37% 45% 10% • 5%
1	B	548	37% 46% 10% • 5%
1	C	548	36% 46% 10% • 5%
1	D	548	36% 47% 10% • 5%
1	E	548	36% 46% 10% • 5%
1	F	548	37% 45% 10% • 5%
1	G	548	36% 46% 9% • 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 29274 atoms, of which 5278 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 GROEL (HSP60 CLASS).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			
1	B	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			
1	C	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			
1	D	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			
1	E	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			
1	F	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			
1	G	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	ARG	conflict	UNP P06139
A	126	VAL	ALA	conflict	UNP P06139
A	267	MET	ILE	conflict	UNP P06139
B	13	GLY	ARG	conflict	UNP P06139
B	126	VAL	ALA	conflict	UNP P06139
B	267	MET	ILE	conflict	UNP P06139
C	13	GLY	ARG	conflict	UNP P06139
C	126	VAL	ALA	conflict	UNP P06139
C	267	MET	ILE	conflict	UNP P06139
D	13	GLY	ARG	conflict	UNP P06139
D	126	VAL	ALA	conflict	UNP P06139
D	267	MET	ILE	conflict	UNP P06139
E	13	GLY	ARG	conflict	UNP P06139
E	126	VAL	ALA	conflict	UNP P06139
E	267	MET	ILE	conflict	UNP P06139

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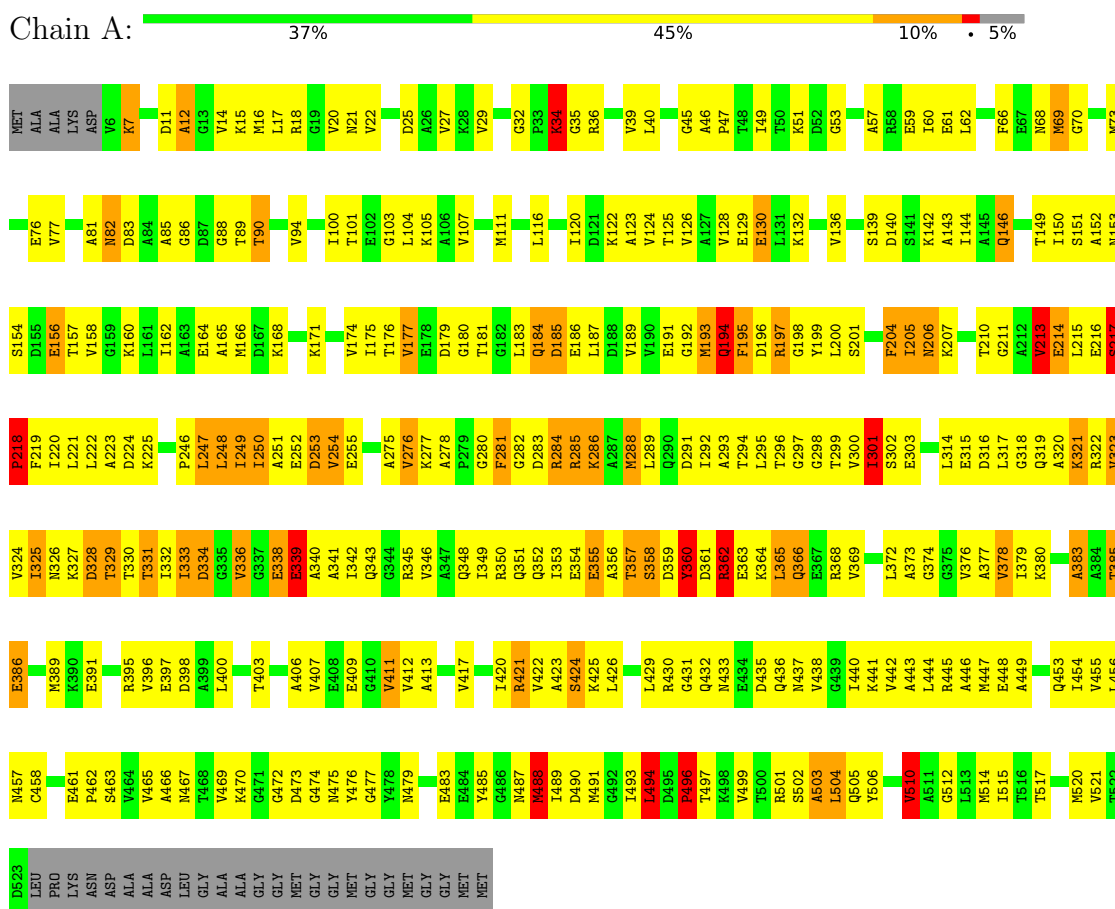
Chain	Residue	Modelled	Actual	Comment	Reference
F	13	GLY	ARG	conflict	UNP P06139
F	126	VAL	ALA	conflict	UNP P06139
F	267	MET	ILE	conflict	UNP P06139
G	13	GLY	ARG	conflict	UNP P06139
G	126	VAL	ALA	conflict	UNP P06139
G	267	MET	ILE	conflict	UNP P06139

3 Residue-property plots

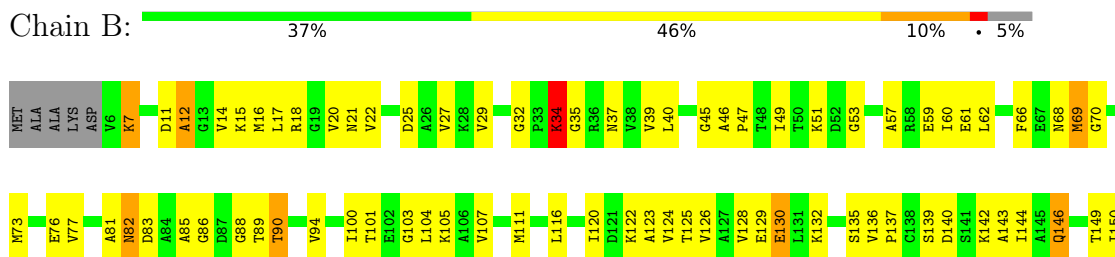
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

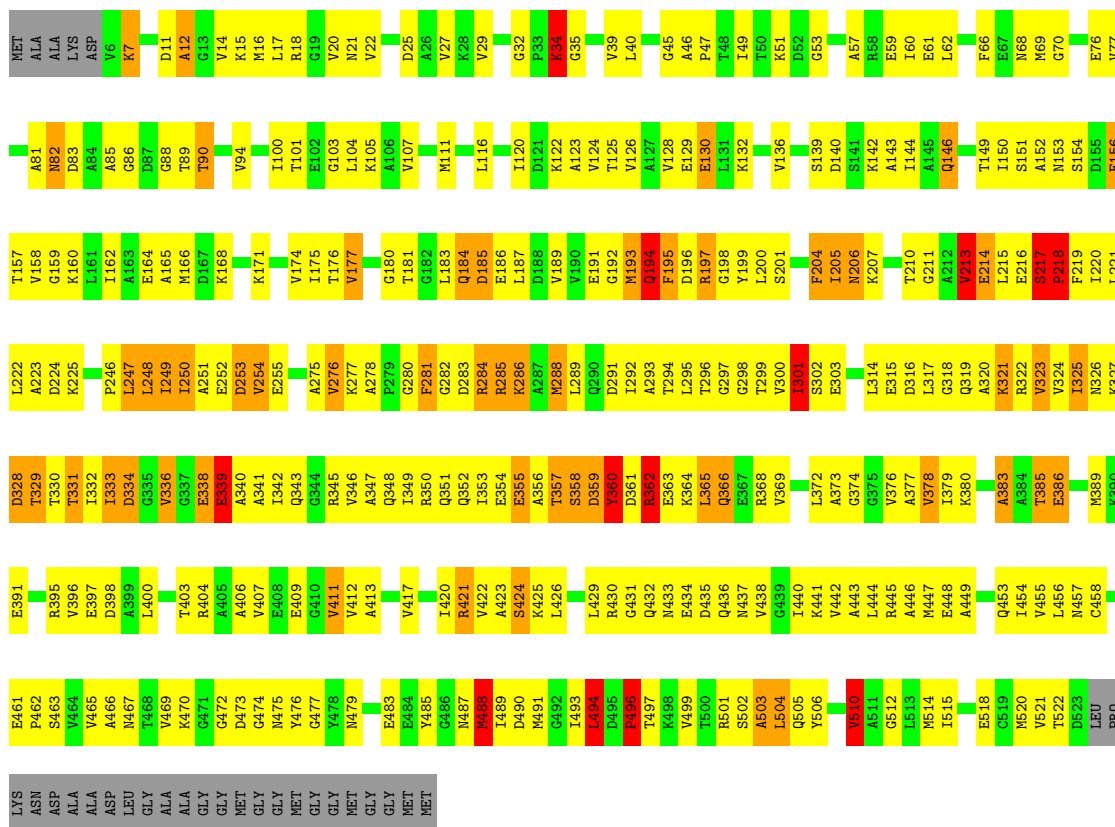
Note EDS was not executed.

• Molecule 1: GROEL (HSP60 CLASS)

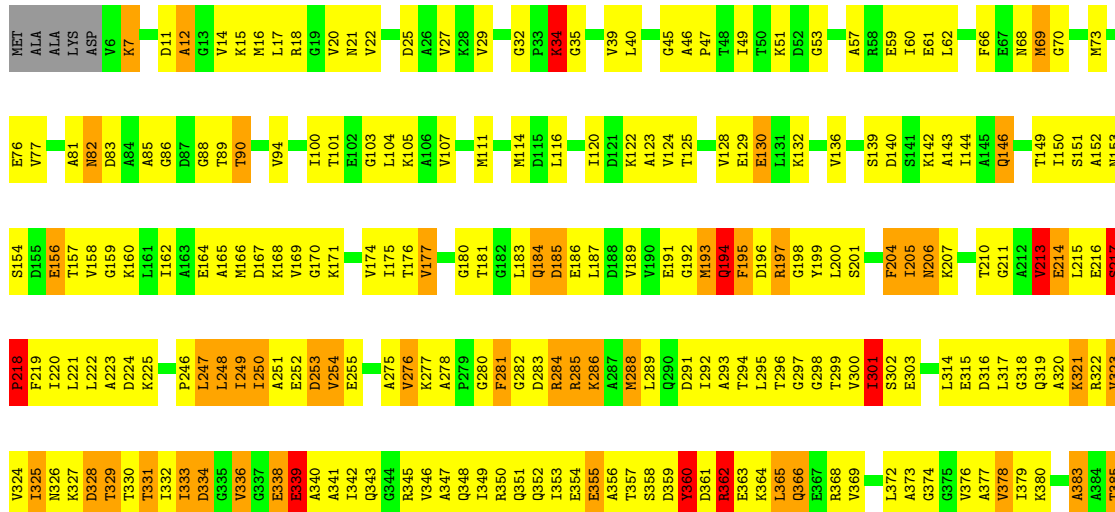


• Molecule 1: GROEL (HSP60 CLASS)





[illegible]





4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	178.00Å 203.00Å 278.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.326 , 0.368	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	29274	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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	0.77	1/3389 (0.0%)	1.27	32/4571 (0.7%)
1	B	0.77	1/3389 (0.0%)	1.27	32/4571 (0.7%)
1	C	0.77	0/3389	1.27	33/4571 (0.7%)
1	D	0.77	1/3389 (0.0%)	1.27	32/4571 (0.7%)
1	E	0.77	1/3389 (0.0%)	1.27	33/4571 (0.7%)
1	F	0.77	0/3389	1.27	32/4571 (0.7%)
1	G	0.77	1/3389 (0.0%)	1.27	33/4571 (0.7%)
All	All	0.77	5/23723 (0.0%)	1.27	227/31997 (0.7%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	69	MET	SD-CE	-5.02	1.67	1.79
1	E	69	MET	SD-CE	-5.01	1.67	1.79
1	B	69	MET	SD-CE	-5.01	1.67	1.79
1	G	69	MET	SD-CE	-5.01	1.67	1.79
1	A	69	MET	SD-CE	-5.00	1.67	1.79

The worst 5 of 227 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	461	GLU	CA-C-N	9.37	129.02	119.56
1	G	461	GLU	C-N-CA	9.37	129.02	119.56
1	C	461	GLU	CA-C-N	9.36	129.02	119.56
1	C	461	GLU	C-N-CA	9.36	129.02	119.56
1	B	461	GLU	CA-C-N	9.36	129.01	119.56

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	3428	754	3441	328	1
1	B	3428	754	3441	337	9
1	C	3428	754	3440	347	54
1	D	3428	754	3441	337	0
1	E	3428	754	3441	343	18
1	F	3428	754	3440	337	1
1	G	3428	754	3441	327	55
All	All	23996	5278	24085	2180	75

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 45.

The worst 5 of 2180 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:181:THR:O	1:G:282:GLY:CA	1.65	1.39
1:D:282:GLY:CA	1:E:181:THR:O	1.69	1.37
1:F:282:GLY:CA	1:G:181:THR:O	1.72	1.36
1:A:282:GLY:HA3	1:B:181:THR:O	1.28	1.30
1:C:281:PHE:HE2	1:D:385:THR:C	1.41	1.26

The worst 5 of 75 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:C:358:SER:OG	1:G:169:VAL:CB[5_455]	0.65	1.55
1:C:358:SER:CB	1:G:169:VAL:CA[5_455]	0.74	1.46
1:C:358:SER:CA	1:G:169:VAL:CA[5_455]	0.89	1.31
1:C:359:ASP:N	1:G:170:GLY:H[5_455]	0.31	1.29
1:C:359:ASP:CB	1:G:167:ASP:CA[5_455]	0.97	1.23

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	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	1	5
1	B	449/548 (82%)	359 (80%)	67 (15%)	23 (5%)	1	5
1	C	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	1	5
1	D	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	1	5
1	E	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	1	5
1	F	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	1	5
1	G	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	1	5
All	All	3143/3836 (82%)	2507 (80%)	475 (15%)	161 (5%)	1	5

5 of 161 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	A	185	ASP
1	A	214	GLU
1	A	253	ASP
1	A	301	ILE

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	353/414 (85%)	300 (85%)	53 (15%)	3	10
1	B	353/414 (85%)	300 (85%)	53 (15%)	3	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	353/414 (85%)	300 (85%)	53 (15%)	3	10
1	D	353/414 (85%)	300 (85%)	53 (15%)	3	10
1	E	353/414 (85%)	300 (85%)	53 (15%)	3	10
1	F	353/414 (85%)	300 (85%)	53 (15%)	3	10
1	G	353/414 (85%)	300 (85%)	53 (15%)	3	10
All	All	2471/2898 (85%)	2100 (85%)	371 (15%)	3	10

5 of 371 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	206	ASN
1	F	217	SER
1	E	254	VAL
1	E	488	MET
1	F	329	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	68	ASN
1	G	146	GLN
1	F	82	ASN
1	F	453	GLN
1	G	437	ASN

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 oligosaccharides 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.