wwPDB X-ray Structure Validation Summary Report (i)

Jul 4, 2022 – 04:18 pm BST

PDB ID	:	7BBV
Title	:	Pectate lyase B from Verticillium dahliae
Authors	:	Safran, J.; Habrylo, O.; Bouckaert, J.; Pau Roblot, C.; Senechal, F.; Pelloux, J.
Deposited on	:	2020-12-18
Resolution	:	1.20 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 (i) 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 (i)) were used in the production of this report:

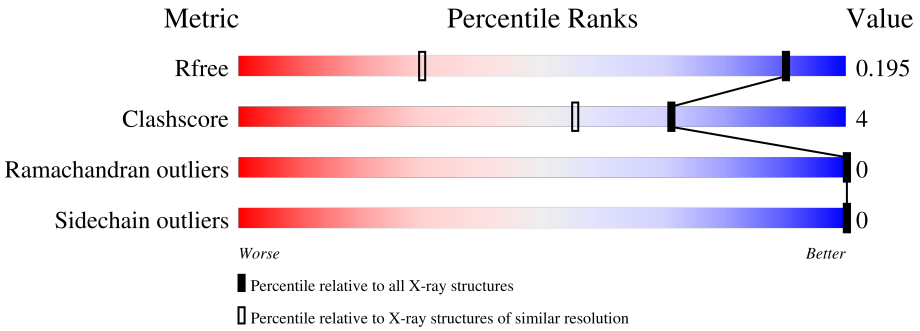
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 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))
R_{free}	130704	1223 (1.22-1.18)
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	343	83% · 13%
1	B	343	79% 8% 13%

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
4	PEG	B	402	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10384 atoms, of which 4624 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 Pectate lyase B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	298	Total	C	H	N	O	S	0	9	0
			4553	1423	2267	400	459	4			
1	B	298	Total	C	H	N	O	S	0	9	0
			4544	1420	2262	401	457	4			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	317	ALA	-	expression tag	UNP G2X3Y1
A	318	ALA	-	expression tag	UNP G2X3Y1
A	319	ALA	-	expression tag	UNP G2X3Y1
A	320	SER	-	expression tag	UNP G2X3Y1
A	321	PHE	-	expression tag	UNP G2X3Y1
A	322	LEU	-	expression tag	UNP G2X3Y1
A	323	GLU	-	expression tag	UNP G2X3Y1
A	324	GLN	-	expression tag	UNP G2X3Y1
A	325	LYS	-	expression tag	UNP G2X3Y1
A	326	LEU	-	expression tag	UNP G2X3Y1
A	327	ILE	-	expression tag	UNP G2X3Y1
A	328	SER	-	expression tag	UNP G2X3Y1
A	329	GLU	-	expression tag	UNP G2X3Y1
A	330	GLU	-	expression tag	UNP G2X3Y1
A	331	ASP	-	expression tag	UNP G2X3Y1
A	332	LEU	-	expression tag	UNP G2X3Y1
A	333	ASN	-	expression tag	UNP G2X3Y1
A	334	SER	-	expression tag	UNP G2X3Y1
A	335	ALA	-	expression tag	UNP G2X3Y1
A	336	VAL	-	expression tag	UNP G2X3Y1
A	337	ASP	-	expression tag	UNP G2X3Y1
A	338	HIS	-	expression tag	UNP G2X3Y1
A	339	HIS	-	expression tag	UNP G2X3Y1
A	340	HIS	-	expression tag	UNP G2X3Y1
A	341	HIS	-	expression tag	UNP G2X3Y1

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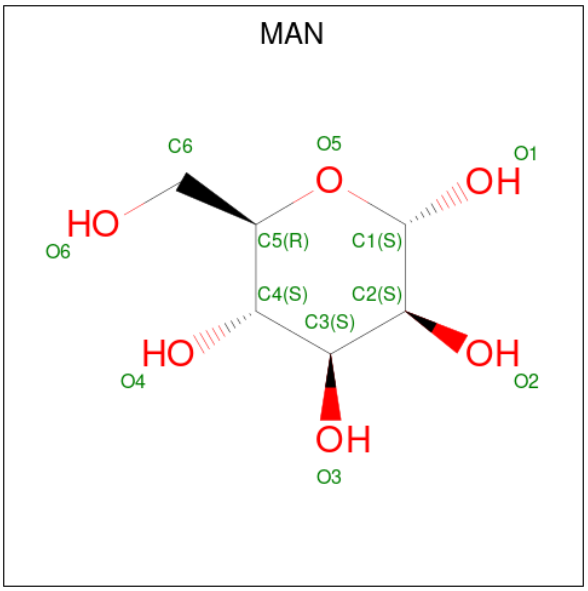
Chain	Residue	Modelled	Actual	Comment	Reference
A	342	HIS	-	expression tag	UNP G2X3Y1
A	343	HIS	-	expression tag	UNP G2X3Y1
B	317	ALA	-	expression tag	UNP G2X3Y1
B	318	ALA	-	expression tag	UNP G2X3Y1
B	319	ALA	-	expression tag	UNP G2X3Y1
B	320	SER	-	expression tag	UNP G2X3Y1
B	321	PHE	-	expression tag	UNP G2X3Y1
B	322	LEU	-	expression tag	UNP G2X3Y1
B	323	GLU	-	expression tag	UNP G2X3Y1
B	324	GLN	-	expression tag	UNP G2X3Y1
B	325	LYS	-	expression tag	UNP G2X3Y1
B	326	LEU	-	expression tag	UNP G2X3Y1
B	327	ILE	-	expression tag	UNP G2X3Y1
B	328	SER	-	expression tag	UNP G2X3Y1
B	329	GLU	-	expression tag	UNP G2X3Y1
B	330	GLU	-	expression tag	UNP G2X3Y1
B	331	ASP	-	expression tag	UNP G2X3Y1
B	332	LEU	-	expression tag	UNP G2X3Y1
B	333	ASN	-	expression tag	UNP G2X3Y1
B	334	SER	-	expression tag	UNP G2X3Y1
B	335	ALA	-	expression tag	UNP G2X3Y1
B	336	VAL	-	expression tag	UNP G2X3Y1
B	337	ASP	-	expression tag	UNP G2X3Y1
B	338	HIS	-	expression tag	UNP G2X3Y1
B	339	HIS	-	expression tag	UNP G2X3Y1
B	340	HIS	-	expression tag	UNP G2X3Y1
B	341	HIS	-	expression tag	UNP G2X3Y1
B	342	HIS	-	expression tag	UNP G2X3Y1
B	343	HIS	-	expression tag	UNP G2X3Y1

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

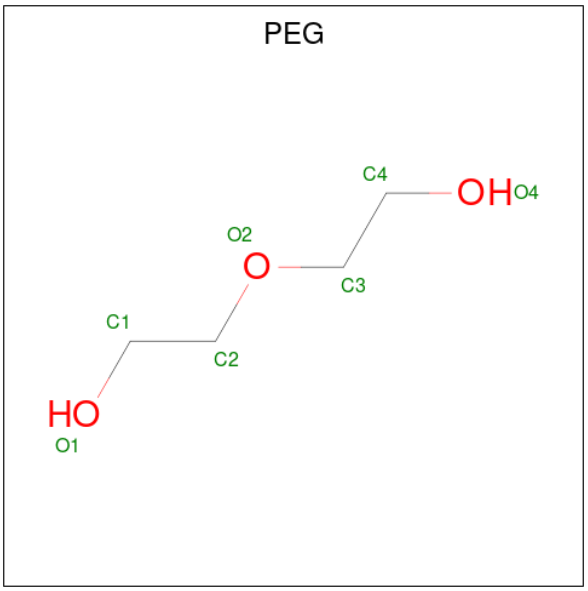
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0

- Molecule 3 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 17 6 6 5	0	0
3	A	1	Total C H O 17 6 6 5	0	0
3	A	1	Total C H O 19 6 8 5	0	0
3	A	1	Total C H O 19 6 8 5	0	0
3	A	1	Total C H O 19 6 8 5	0	0
3	A	1	Total C H O 17 6 6 5	0	0
3	B	1	Total C H O 17 6 6 5	0	0
3	B	1	Total C H O 19 6 8 5	0	0
3	B	1	Total C H O 19 6 8 5	0	0
3	B	1	Total C H O 17 6 6 5	0	0
3	B	1	Total C H O 19 6 8 5	0	0
3	B	1	Total C H O 18 6 7 5	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	543	Total	O	0	0
			543	543		
5	B	508	Total	O	0	0
			508	508		

3 Residue-property plots (i)

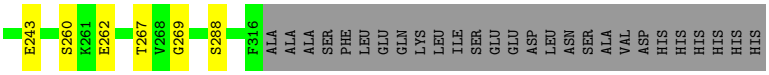
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

- Molecule 1: Pectate lyase B

Chain A:

- Molecule 1: Pectate lyase B

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.89Å 59.69Å 93.87Å 90.00° 96.35° 90.00°	Depositor
Resolution (Å)	60.52 – 1.20 60.52 – 1.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (60.52-1.20) 99.0 (60.52-1.20)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.96 (at 1.20Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.172 , 0.196 0.171 , 0.195	Depositor DCC
R_{free} test set	10378 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	23.2	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	10384	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, PEG, MAN

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	0.64	0/2349	0.81	0/3174
1	B	0.66	0/2346	0.80	0/3171
All	All	0.65	0/4695	0.81	0/6345

There are no bond length outliers.

There are no bond angle outliers.

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	2286	2267	2253	10	0
1	B	2282	2262	2245	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	66	42	60	0	0
3	B	66	43	60	0	0
4	B	7	10	10	7	0
5	A	543	0	0	2	4
5	B	508	0	0	5	4
All	All	5760	4624	4628	33	4

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 4.

The worst 5 of 33 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:122:ASP:OD2	4:B:402:PEG:H42	1.65	0.94
1:B:121:GLY:HA3	4:B:402:PEG:H12	1.54	0.88
1:B:76:LYS:HG3	4:B:402:PEG:H11	1.70	0.72
1:B:99:TYR:CD1	4:B:402:PEG:H31	2.26	0.70
1:B:147:LYS:O	1:B:175:LYS:HE2	1.96	0.65

All (4) 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)
5:A:910:HOH:O	5:B:942:HOH:O[2_454]	2.11	0.09
5:A:899:HOH:O	5:B:669:HOH:O[1_655]	2.14	0.06
5:A:1010:HOH:O	5:B:962:HOH:O[2_455]	2.18	0.02
5:A:742:HOH:O	5:B:886:HOH:O[2_455]	2.19	0.01

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	305/343 (89%)	291 (95%)	14 (5%)	0	100	100
1	B	305/343 (89%)	290 (95%)	15 (5%)	0	100	100
All	All	610/686 (89%)	581 (95%)	29 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	254/283 (90%)	254 (100%)	0	100	100
1	B	254/283 (90%)	254 (100%)	0	100	100
All	All	508/566 (90%)	508 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	253	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
3	MAN	B	406	1	11,11,12	0.27	0	15,15,17	0.64	0
3	MAN	A	404	1	11,11,12	0.26	0	15,15,17	0.64	0
3	MAN	B	405	1	11,11,12	1.21	1 (9%)	15,15,17	1.06	1 (6%)
3	MAN	B	408	1	11,11,12	1.02	1 (9%)	15,15,17	2.87	5 (33%)
4	PEG	B	402	-	6,6,6	0.39	0	5,5,5	0.28	0
3	MAN	A	403	1	11,11,12	1.68	2 (18%)	15,15,17	1.10	1 (6%)
3	MAN	A	405	1	11,11,12	0.27	0	15,15,17	0.63	0
3	MAN	A	407	1	11,11,12	1.39	1 (9%)	15,15,17	2.51	6 (40%)
3	MAN	B	404	1	11,11,12	0.26	0	15,15,17	0.62	0
3	MAN	B	407	1	11,11,12	1.31	2 (18%)	15,15,17	1.08	1 (6%)
3	MAN	A	402	1	11,11,12	1.21	1 (9%)	15,15,17	2.23	4 (26%)
3	MAN	B	403	1	11,11,12	0.27	0	15,15,17	0.63	0
3	MAN	A	406	1	11,11,12	0.27	0	15,15,17	0.65	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	MAN	B	406	1	-	2/2/19/22	0/1/1/1
3	MAN	A	404	1	-	2/2/19/22	0/1/1/1
3	MAN	B	405	1	-	0/2/19/22	0/1/1/1
3	MAN	B	408	1	-	2/2/19/22	0/1/1/1
4	PEG	B	402	-	-	3/4/4/4	-
3	MAN	A	403	1	-	1/2/19/22	0/1/1/1
3	MAN	A	405	1	-	1/2/19/22	0/1/1/1
3	MAN	A	407	1	-	0/2/19/22	0/1/1/1
3	MAN	B	404	1	-	0/2/19/22	0/1/1/1
3	MAN	B	407	1	-	0/2/19/22	0/1/1/1
3	MAN	A	402	1	-	0/2/19/22	0/1/1/1
3	MAN	B	403	1	-	0/2/19/22	0/1/1/1
3	MAN	A	406	1	-	0/2/19/22	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	405	MAN	O5-C1	-3.50	1.38	1.43
3	A	403	MAN	O5-C1	-3.43	1.38	1.43
3	A	407	MAN	O5-C1	-3.23	1.38	1.43
3	B	407	MAN	C2-C3	3.12	1.57	1.52
3	A	403	MAN	O5-C5	-2.81	1.37	1.43

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	408	MAN	O5-C5-C6	7.25	118.56	107.20
3	A	402	MAN	O5-C1-C2	-5.62	102.09	110.77
3	B	408	MAN	O5-C1-C2	-5.08	102.92	110.77
3	A	407	MAN	O5-C1-C2	-4.80	103.36	110.77
3	A	407	MAN	O5-C5-C6	4.20	113.78	107.20

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	408	MAN	O5-C5-C6-O6
3	B	408	MAN	C4-C5-C6-O6
3	B	406	MAN	C4-C5-C6-O6
4	B	402	PEG	O1-C1-C2-O2
4	B	402	PEG	O2-C3-C4-O4

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	402	PEG	7	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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.