Full wwPDB X-ray Structure Validation Report (i)

Mar 10, 2018 – 04:45 am GMT

PDB ID	:	2OKK
Title	:	The X-ray crystal structure of the 65kDa isoform of Glutamic Acid Decarboxylase (GAD65)
Authors	:	Buckle, A.M.; Fenalti, G.; Law, R.H.P.; Whisstock, J.C.
Deposited on	:	2007-01-17
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

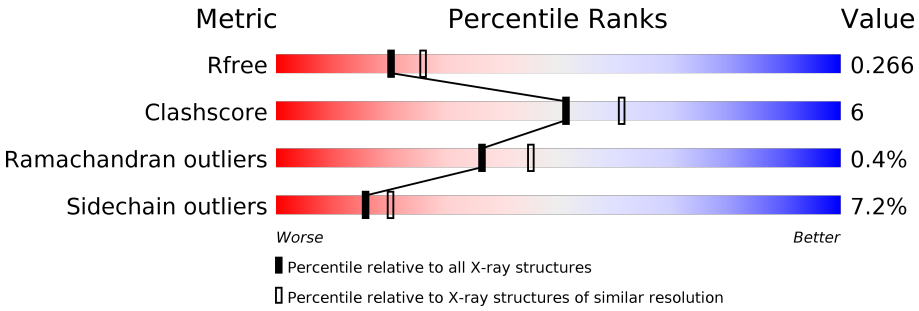
MolProbity	:	4.02b-467
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

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 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))
R_{free}	111664	4477 (2.30-2.30)
Clashscore	122126	5072 (2.30-2.30)
Ramachandran outliers	120053	5022 (2.30-2.30)
Sidechain outliers	120020	5021 (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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	497	81% 14%

2 Entry composition

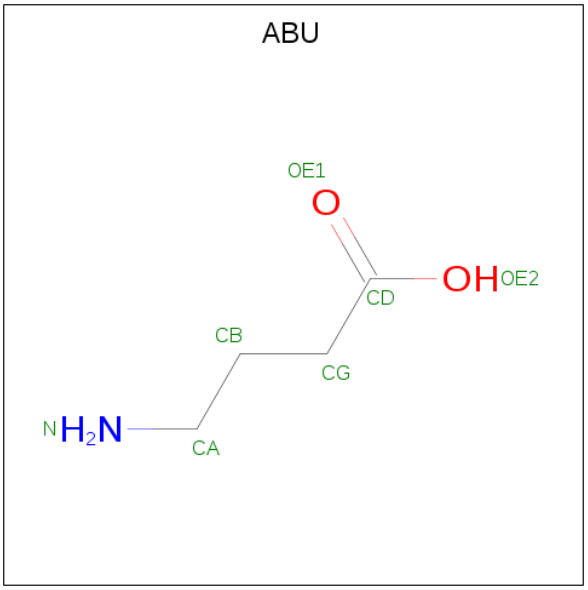
There are 4 unique types of molecules in this entry. The entry contains 3882 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamate decarboxylase 2.

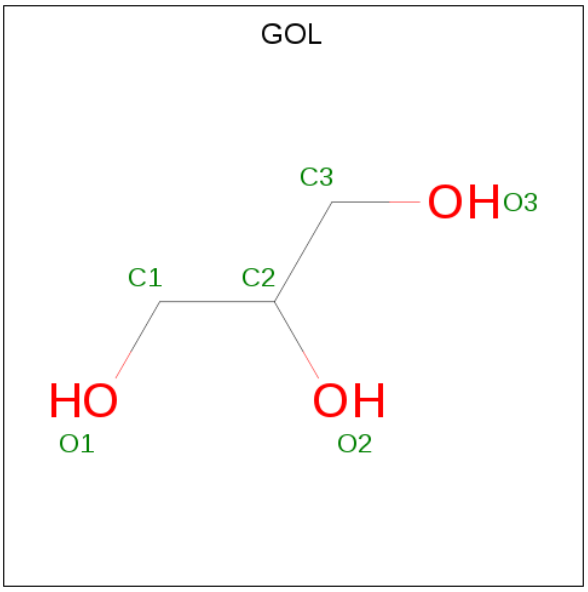
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	483	3770	2430	628	679	1	32	0	0	0

- Molecule 2 is GAMMA-AMINO-BUTANOIC ACID (three-letter code: ABU) (formula: $C_4H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	7	4	1	2	0	1
			Total	C	N	O		
2	A	1	7	4	1	2	0	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 6 3 3	0	0

- Molecule 4 is water.

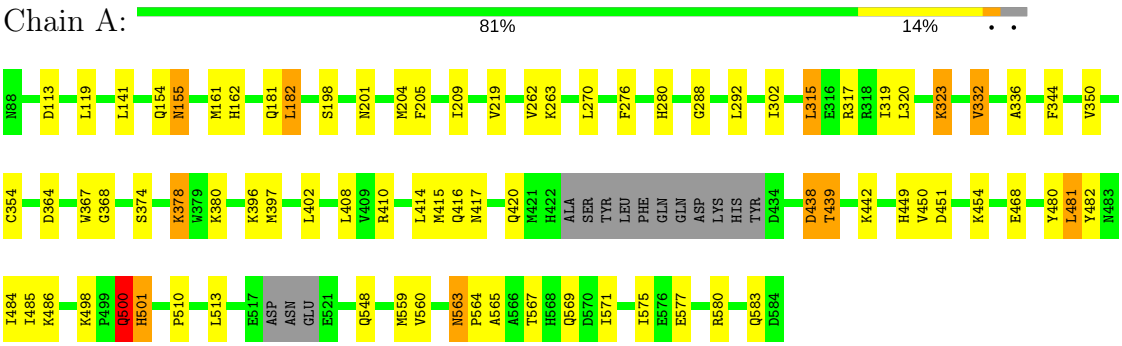
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	92	Total O 92 92	0	0

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. 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: Glutamate decarboxylase 2

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	78.25Å 99.06Å 120.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.19 – 2.30 37.20 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (37.19-2.30) 93.0 (37.20-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.256 0.212 , 0.266	Depositor DCC
R_{free} test set	1500 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	27.7	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 53.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	3882	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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: GOL, LLP, ABU

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	0.46	0/3834	0.63	3/5191 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	500	GLN	N-CA-C	5.94	127.05	111.00
1	A	501	HIS	N-CA-C	5.44	125.70	111.00
1	A	500	GLN	C-N-CA	5.37	135.11	121.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	501	HIS	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	500	GLN	Peptide

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	3770	0	3697	46	0
2	A	14	0	10	3	0
3	A	6	0	8	0	0
4	A	92	0	0	3	0
All	All	3882	0	3715	46	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 6.

All (46) 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:438:ASP:HA	1:A:439:THR:OG1	1.52	1.08
1:A:481:LEU:HD11	1:A:559:MET:HG2	1.66	0.77
1:A:449:HIS:HE1	4:A:649:HOH:O	1.67	0.76
1:A:454:LYS:NZ	4:A:664:HOH:O	2.21	0.71
1:A:449:HIS:HD2	1:A:451:ASP:OD1	1.76	0.67
1:A:563:ASN:HD22	1:A:564:PRO:HD2	1.63	0.63
1:A:276:PHE:HB3	1:A:302:ILE:HD11	1.81	0.62
1:A:181:GLN:HE21	2:A:585[A]:ABU:HB1	1.64	0.62
1:A:276:PHE:HB3	1:A:302:ILE:CD1	2.30	0.61
1:A:563:ASN:HD22	1:A:564:PRO:CD	2.16	0.58
1:A:336:ALA:O	1:A:368:GLY:HA3	2.04	0.58
1:A:481:LEU:CD1	1:A:559:MET:HG2	2.35	0.57
1:A:563:ASN:ND2	1:A:565:ALA:H	2.04	0.56
1:A:482:TYR:CZ	1:A:486:LYS:HD3	2.43	0.54
1:A:571:ILE:O	1:A:575:ILE:HG12	2.09	0.53
1:A:319:ILE:O	1:A:323:LYS:HG2	2.09	0.53
1:A:280:HIS:HD2	4:A:605:HOH:O	1.91	0.53
1:A:154:GLN:OE1	1:A:162:HIS:HE1	1.91	0.52
1:A:374:SER:HA	1:A:468:GLU:HG3	1.91	0.52
1:A:396:LLP:NZ	1:A:396:LLP:O3	2.43	0.52
1:A:380:LYS:HD3	1:A:500:GLN:O	2.11	0.51
1:A:332:VAL:HG13	1:A:354:CYS:SG	2.50	0.50
1:A:364:ASP:OD2	1:A:396:LLP:N1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:GLN:HE21	1:A:420:GLN:HE21	1.60	0.48
1:A:567:THR:OG1	1:A:569:GLN:HG2	2.13	0.48
1:A:367:TRP:CZ3	1:A:397:MET:HG2	2.49	0.47
1:A:480:TYR:CZ	1:A:484:ILE:HD11	2.50	0.46
1:A:182:LEU:HD22	2:A:585[A]:ABU:HE2	1.98	0.46
1:A:482:TYR:O	1:A:486:LYS:HB2	2.16	0.46
1:A:262:VAL:HB	1:A:270:LEU:HD11	1.99	0.45
1:A:510:PRO:HD2	1:A:513:LEU:HD12	1.98	0.45
1:A:563:ASN:HD22	1:A:564:PRO:N	2.15	0.45
1:A:182:LEU:HD22	2:A:586[B]:ABU:HB2	2.00	0.44
1:A:263:LYS:NZ	1:A:420:GLN:O	2.40	0.44
1:A:577:GLU:OE2	1:A:580:ARG:NH1	2.51	0.44
1:A:416:GLN:HE21	1:A:420:GLN:NE2	2.16	0.44
1:A:204:MET:SD	1:A:450:VAL:HG22	2.58	0.43
1:A:288:GLY:O	1:A:292:LEU:HG	2.18	0.43
1:A:315:LEU:HD22	1:A:319:ILE:HD11	2.00	0.43
1:A:438:ASP:CA	1:A:439:THR:OG1	2.44	0.42
1:A:415:MET:HB3	1:A:442:LYS:HG2	2.01	0.42
1:A:198:SER:O	1:A:201:ASN:HB2	2.20	0.42
1:A:155:ASN:HD22	1:A:155:ASN:C	2.23	0.41
1:A:344:PHE:H	1:A:500:GLN:NE2	2.19	0.41
1:A:378:LYS:HE3	1:A:378:LYS:HB2	1.89	0.41
1:A:481:LEU:O	1:A:485:ILE:HG12	2.22	0.40

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	476/497 (96%)	462 (97%)	12 (2%)	2 (0%)	36 45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	HIS
1	A	439	THR

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	387/424 (91%)	359 (93%)	28 (7%)	16 20

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	ASP
1	A	119	LEU
1	A	141	LEU
1	A	155	ASN
1	A	161	MET
1	A	182	LEU
1	A	205	PHE
1	A	209	ILE
1	A	219	VAL
1	A	315	LEU
1	A	317	ARG
1	A	320	LEU
1	A	323	LYS
1	A	332	VAL
1	A	350	VAL
1	A	378	LYS
1	A	402	LEU
1	A	408	LEU
1	A	410	ARG
1	A	414	LEU
1	A	417	ASN
1	A	438	ASP
1	A	481	LEU
1	A	498	LYS
1	A	548	GLN

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Mol	Chain	Res	Type
1	A	560	VAL
1	A	563	ASN
1	A	583	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	155	ASN
1	A	162	HIS
1	A	181	GLN
1	A	247	ASN
1	A	417	ASN
1	A	420	GLN
1	A	449	HIS
1	A	470	HIS
1	A	483	ASN
1	A	500	GLN
1	A	555	ASN
1	A	563	ASN
1	A	568	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
1	LLP	A	396	1	24,24,25	1.83	5 (20%)	28,32,34	1.71	4 (14%)

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
1	LLP	A	396	1	-	0/15/17/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	396	LLP	O3-C3	-5.54	1.24	1.37
1	A	396	LLP	C4'-NZ	2.16	1.34	1.27
1	A	396	LLP	C2-N1	2.34	1.38	1.33
1	A	396	LLP	C4-C4'	2.74	1.51	1.46
1	A	396	LLP	CA-C	3.97	1.55	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	396	LLP	OP4-P-OP1	-3.82	95.76	106.47
1	A	396	LLP	C4-C4'-NZ	-3.06	109.80	124.66
1	A	396	LLP	C5-C6-N1	-2.76	119.15	123.83
1	A	396	LLP	OP4-C5'-C5	5.11	119.21	109.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	396	LLP	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

3 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	ABU	A	585[A]	-	3,6,6	0.21	0	2,6,6	0.34	0
2	ABU	A	586[B]	-	3,6,6	0.17	0	2,6,6	0.41	0
3	GOL	A	587	-	5,5,5	0.35	0	5,5,5	0.16	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
2	ABU	A	585[A]	-	-	0/2/4/4	0/0/0/0
2	ABU	A	586[B]	-	-	0/2/4/4	0/0/0/0
3	GOL	A	587	-	-	0/4/4/4	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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	585[A]	ABU	2	0
2	A	586[B]	ABU	1	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.