



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 05:24 PM BST

PDB ID : 6RU2
Title : Crystal Structure of Glucuronoyl Esterase from *Cerrena unicolor*
Authors : Ernst, H.A.; Mosbech, C.; Langkilde, A.; Westh, P.; Meyer, A.; Agger, J.W.;
Larsen, S.
Deposited on : 2019-05-27
Resolution : 1.96 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

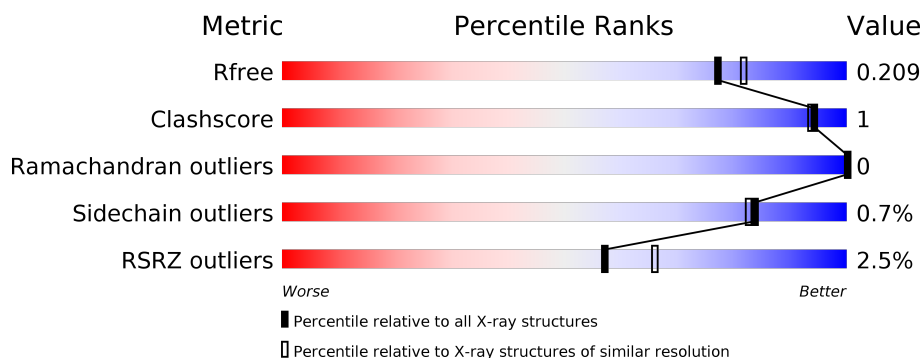
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	403	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>6%</div> </div> </div>
1	B	403	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>6%</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6457 atoms, of which 64 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 4-O-methyl-glucuronoyl methylesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	5	0
			2889	1824	496	554	15			
1	B	379	Total	C	N	O	S	0	3	0
			2875	1815	494	551	15			

There are 46 discrepancies between the modelled and reference sequences:

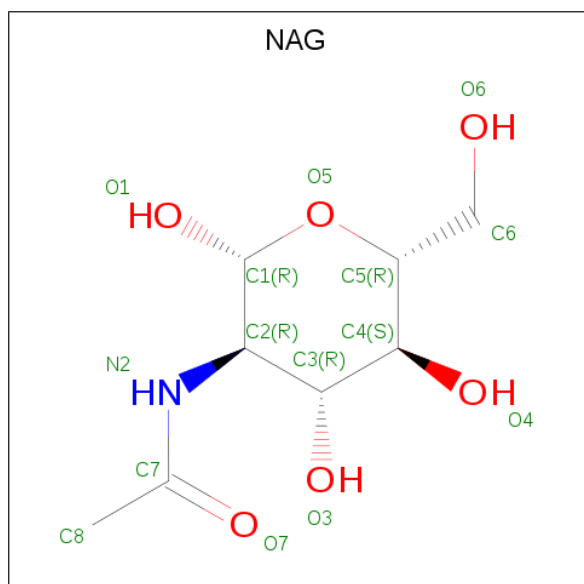
Chain	Residue	Modelled	Actual	Comment	Reference
A	459	GLY	-	expression tag	UNP A0A0A7EQR3
A	460	LEU	-	expression tag	UNP A0A0A7EQR3
A	461	GLU	-	expression tag	UNP A0A0A7EQR3
A	462	GLN	-	expression tag	UNP A0A0A7EQR3
A	463	LYS	-	expression tag	UNP A0A0A7EQR3
A	464	LEU	-	expression tag	UNP A0A0A7EQR3
A	465	ILE	-	expression tag	UNP A0A0A7EQR3
A	466	SER	-	expression tag	UNP A0A0A7EQR3
A	467	GLU	-	expression tag	UNP A0A0A7EQR3
A	468	GLU	-	expression tag	UNP A0A0A7EQR3
A	469	ASP	-	expression tag	UNP A0A0A7EQR3
A	470	LEU	-	expression tag	UNP A0A0A7EQR3
A	471	ASN	-	expression tag	UNP A0A0A7EQR3
A	472	SER	-	expression tag	UNP A0A0A7EQR3
A	473	ALA	-	expression tag	UNP A0A0A7EQR3
A	474	VAL	-	expression tag	UNP A0A0A7EQR3
A	475	ASP	-	expression tag	UNP A0A0A7EQR3
A	476	HIS	-	expression tag	UNP A0A0A7EQR3
A	477	HIS	-	expression tag	UNP A0A0A7EQR3
A	478	HIS	-	expression tag	UNP A0A0A7EQR3
A	479	HIS	-	expression tag	UNP A0A0A7EQR3
A	480	HIS	-	expression tag	UNP A0A0A7EQR3
A	481	HIS	-	expression tag	UNP A0A0A7EQR3
B	459	GLY	-	expression tag	UNP A0A0A7EQR3
B	460	LEU	-	expression tag	UNP A0A0A7EQR3

Continued on next page...

Continued from previous page...

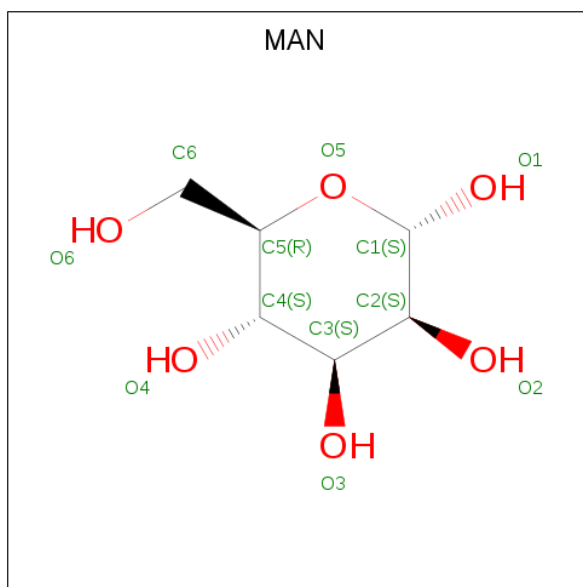
Chain	Residue	Modelled	Actual	Comment	Reference
B	461	GLU	-	expression tag	UNP A0A0A7EQR3
B	462	GLN	-	expression tag	UNP A0A0A7EQR3
B	463	LYS	-	expression tag	UNP A0A0A7EQR3
B	464	LEU	-	expression tag	UNP A0A0A7EQR3
B	465	ILE	-	expression tag	UNP A0A0A7EQR3
B	466	SER	-	expression tag	UNP A0A0A7EQR3
B	467	GLU	-	expression tag	UNP A0A0A7EQR3
B	468	GLU	-	expression tag	UNP A0A0A7EQR3
B	469	ASP	-	expression tag	UNP A0A0A7EQR3
B	470	LEU	-	expression tag	UNP A0A0A7EQR3
B	471	ASN	-	expression tag	UNP A0A0A7EQR3
B	472	SER	-	expression tag	UNP A0A0A7EQR3
B	473	ALA	-	expression tag	UNP A0A0A7EQR3
B	474	VAL	-	expression tag	UNP A0A0A7EQR3
B	475	ASP	-	expression tag	UNP A0A0A7EQR3
B	476	HIS	-	expression tag	UNP A0A0A7EQR3
B	477	HIS	-	expression tag	UNP A0A0A7EQR3
B	478	HIS	-	expression tag	UNP A0A0A7EQR3
B	479	HIS	-	expression tag	UNP A0A0A7EQR3
B	480	HIS	-	expression tag	UNP A0A0A7EQR3
B	481	HIS	-	expression tag	UNP A0A0A7EQR3

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



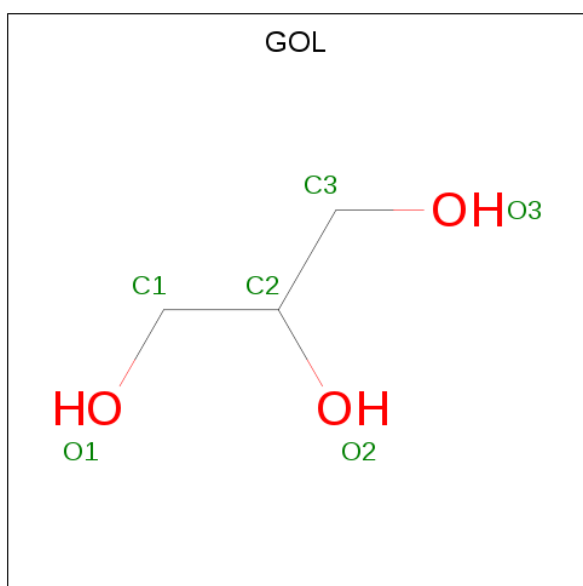
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			22	6	11	5		
3	A	1	Total	C	H	O	0	0
			22	6	11	5		
3	B	1	Total	C	H	O	0	0
			22	6	11	5		
3	B	1	Total	C	H	O	0	0
			22	6	11	5		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	Na 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	293	Total 293	O 293	0	0
7	B	249	Total 249	O 249	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	84.45Å 84.45Å 262.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.55 – 1.96 44.55 – 1.97	Depositor EDS
% Data completeness (in resolution range)	98.2 (44.55-1.96) 97.3 (44.55-1.97)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.85 (at 1.97Å)	Xtriage
Refinement program	PHENIX 1.13 _2998	Depositor
R, R_{free}	0.178 , 0.204 0.185 , 0.209	Depositor DCC
R_{free} test set	3288 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6457	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, MAN, EDO, NAG, NA

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	0.32	0/2979	0.51	0/4074
1	B	0.31	0/2962	0.50	0/4052
All	All	0.32	0/5941	0.51	0/8126

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	2889	0	2780	8	0
1	B	2875	0	2764	7	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
3	A	22	22	20	0	0
3	B	22	22	20	0	0
4	A	4	6	6	0	0
4	B	4	6	6	0	0
5	B	6	8	8	0	0
6	B	1	0	0	0	0
7	A	293	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	249	0	0	1	0
All	All	6393	64	5630	15	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 1.

The worst 5 of 15 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:178:PRO:HB3	1:B:183:TRP:NE1	2.26	0.50
1:B:253:MET:HE2	7:B:795:HOH:O	2.11	0.49
1:B:242:TRP:O	1:B:246:ARG:HG2	2.12	0.49
1:A:178:PRO:HB3	1:A:183:TRP:CE2	2.49	0.47
1:A:178:PRO:HB3	1:A:183:TRP:NE1	2.29	0.47

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	382/403 (95%)	365 (96%)	17 (4%)	0	100	100
1	B	380/403 (94%)	365 (96%)	15 (4%)	0	100	100
All	All	762/806 (94%)	730 (96%)	32 (4%)	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	308/324 (95%)	306 (99%)	2 (1%)	86	85
1	B	306/324 (94%)	304 (99%)	2 (1%)	84	82
All	All	614/648 (95%)	610 (99%)	4 (1%)	84	82

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	370	SER
1	A	427	SER
1	B	370	SER
1	B	433	PHE

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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	$\# Z > 2$
4	EDO	B	503	-	3,3,3	0.52	0	2,2,2	0.11	0
3	MAN	B	502	1	11,11,12	0.85	1 (9%)	15,15,17	1.29	3 (20%)
2	NAG	A	501	1	14,14,15	0.21	0	17,19,21	0.61	0
3	MAN	A	502	1	11,11,12	0.95	0	15,15,17	1.15	2 (13%)
4	EDO	A	503	-	3,3,3	0.49	0	2,2,2	0.32	0
3	MAN	A	504	1	11,11,12	0.80	0	15,15,17	0.89	0
3	MAN	B	504	1	11,11,12	0.89	1 (9%)	15,15,17	0.89	0
2	NAG	B	501	1	14,14,15	0.41	0	17,19,21	0.50	0
5	GOL	B	505	6	5,5,5	0.76	0	5,5,5	0.88	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
4	EDO	B	503	-	-	1/1/1/1	-
3	MAN	B	502	1	-	0/2/19/22	0/1/1/1
2	NAG	A	501	1	-	0/6/23/26	0/1/1/1
3	MAN	A	502	1	-	0/2/19/22	0/1/1/1
4	EDO	A	503	-	-	1/1/1/1	-
3	MAN	A	504	1	-	0/2/19/22	0/1/1/1
3	MAN	B	504	1	-	0/2/19/22	0/1/1/1
2	NAG	B	501	1	-	0/6/23/26	0/1/1/1
5	GOL	B	505	6	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	MAN	C1-C2	2.13	1.57	1.52
3	B	504	MAN	O5-C1	-2.08	1.40	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	MAN	C1-O5-C5	3.21	116.55	112.19
3	A	502	MAN	O2-C2-C3	-2.46	105.22	110.14
3	A	502	MAN	C1-O5-C5	2.35	115.37	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	MAN	O2-C2-C3	-2.20	105.74	110.14
3	B	502	MAN	O5-C1-C2	2.19	114.16	110.77

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	503	EDO	O1-C1-C2-O2
4	A	503	EDO	O1-C1-C2-O2

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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	379/403 (94%)	0.04	7 (1%) 68 76	12, 18, 31, 49	0
1	B	379/403 (94%)	0.13	12 (3%) 47 57	13, 19, 37, 62	0
All	All	758/806 (94%)	0.08	19 (2%) 57 66	12, 18, 33, 62	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	175	SER	6.2
1	B	177	THR	3.6
1	B	84	ILE	3.5
1	B	176	GLY	3.4
1	A	198	ALA	3.4

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MAN	B	502	11/12	0.67	0.29	39,50,59,62	0
3	MAN	A	502	11/12	0.67	0.32	38,51,60,63	0
5	GOL	B	505	6/6	0.69	0.24	64,77,79,79	0
3	MAN	B	504	11/12	0.73	0.25	38,49,59,60	0
3	MAN	A	504	11/12	0.75	0.30	40,52,62,63	0
4	EDO	B	503	4/4	0.84	0.16	27,33,34,34	0
2	NAG	A	501	14/15	0.93	0.11	16,20,24,24	0
4	EDO	A	503	4/4	0.94	0.17	24,28,31,31	0
6	NA	B	506	1/1	0.94	0.24	54,54,54,54	0
2	NAG	B	501	14/15	0.95	0.14	17,24,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.