



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 11:02 AM BST

PDB ID : 6RTV
Title : Crystal Structure of Glucuronoyl Esterase from *Cerrena unicolor* inactive S270A variant
Authors : Ernst, H.A.; Mosbech, C.; Langkilde, A.; Westh, P.; Meyer, A.; Agger, J.W.; Larsen, S.
Deposited on : 2019-05-27
Resolution : 1.46 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 ⓘ 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

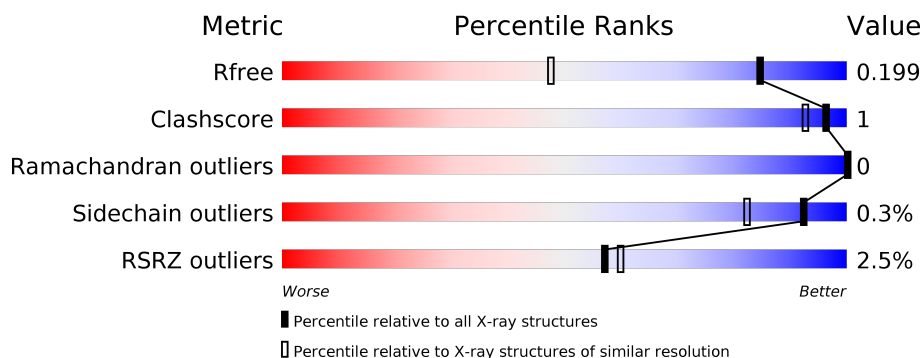
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.46 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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	401	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> % 93% • • </div> </div>
1	B	401	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 1%, green 95%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> 3% 94% • • </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6840 atoms, of which 68 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	386	Total	C	N	O	S	0	13	0
			2975	1880	505	575	15			
1	B	386	Total	C	N	O	S	0	9	0
			2961	1872	504	570	15			

There are 44 discrepancies between the modelled and reference sequences:

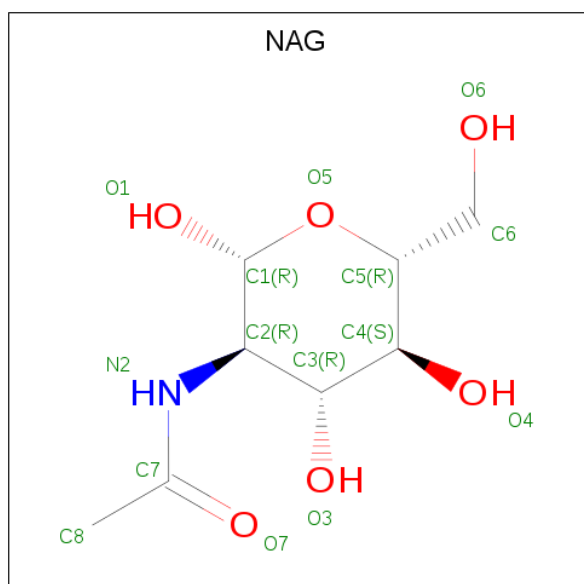
Chain	Residue	Modelled	Actual	Comment	Reference
A	73	GLU	-	expression tag	UNP A0A0A7EQR3
A	74	ALA	-	expression tag	UNP A0A0A7EQR3
A	75	GLU	-	expression tag	UNP A0A0A7EQR3
A	76	ALA	-	expression tag	UNP A0A0A7EQR3
A	77	GLU	-	expression tag	UNP A0A0A7EQR3
A	78	PHE	-	expression tag	UNP A0A0A7EQR3
A	270	ALA	SER	engineered mutation	UNP A0A0A7EQR3
A	459	GLU	-	expression tag	UNP A0A0A7EQR3
A	460	ASN	-	expression tag	UNP A0A0A7EQR3
A	461	LEU	-	expression tag	UNP A0A0A7EQR3
A	462	TYR	-	expression tag	UNP A0A0A7EQR3
A	463	PHE	-	expression tag	UNP A0A0A7EQR3
A	464	GLN	-	expression tag	UNP A0A0A7EQR3
A	465	GLY	-	expression tag	UNP A0A0A7EQR3
A	466	VAL	-	expression tag	UNP A0A0A7EQR3
A	467	ASP	-	expression tag	UNP A0A0A7EQR3
A	468	HIS	-	expression tag	UNP A0A0A7EQR3
A	469	HIS	-	expression tag	UNP A0A0A7EQR3
A	470	HIS	-	expression tag	UNP A0A0A7EQR3
A	471	HIS	-	expression tag	UNP A0A0A7EQR3
A	472	HIS	-	expression tag	UNP A0A0A7EQR3
A	473	HIS	-	expression tag	UNP A0A0A7EQR3
B	73	GLU	-	expression tag	UNP A0A0A7EQR3
B	74	ALA	-	expression tag	UNP A0A0A7EQR3
B	75	GLU	-	expression tag	UNP A0A0A7EQR3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	76	ALA	-	expression tag	UNP A0A0A7EQR3
B	77	GLU	-	expression tag	UNP A0A0A7EQR3
B	78	PHE	-	expression tag	UNP A0A0A7EQR3
B	270	ALA	SER	engineered mutation	UNP A0A0A7EQR3
B	459	GLU	-	expression tag	UNP A0A0A7EQR3
B	460	ASN	-	expression tag	UNP A0A0A7EQR3
B	461	LEU	-	expression tag	UNP A0A0A7EQR3
B	462	TYR	-	expression tag	UNP A0A0A7EQR3
B	463	PHE	-	expression tag	UNP A0A0A7EQR3
B	464	GLN	-	expression tag	UNP A0A0A7EQR3
B	465	GLY	-	expression tag	UNP A0A0A7EQR3
B	466	VAL	-	expression tag	UNP A0A0A7EQR3
B	467	ASP	-	expression tag	UNP A0A0A7EQR3
B	468	HIS	-	expression tag	UNP A0A0A7EQR3
B	469	HIS	-	expression tag	UNP A0A0A7EQR3
B	470	HIS	-	expression tag	UNP A0A0A7EQR3
B	471	HIS	-	expression tag	UNP A0A0A7EQR3
B	472	HIS	-	expression tag	UNP A0A0A7EQR3
B	473	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		

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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	382	Total	O	0	0
			382	382		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	375	Total	O	0	0
			375	375		

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 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.

- Molecule 1: 4-O-methyl-glucuronoyl methylesterase



- Molecule 1: 4-O-methyl-glucuronoyl methylesterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	84.27Å 84.27Å 261.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.39 – 1.46 49.17 – 1.46	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.39-1.46) 100.0 (49.17-1.46)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.46Å)	Xtriage
Refinement program	PHENIX 1.13 _2998	Depositor
R, R_{free}	0.182 , 0.199 0.182 , 0.199	Depositor DCC
R_{free} test set	8194 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	11.6	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6840	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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, EDO, NA, NAG

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	0.33	0/3090	0.56	0/4224
1	B	0.33	0/3065	0.56	0/4192
All	All	0.33	0/6155	0.56	0/8416

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	2975	0	2873	7	0
1	B	2961	0	2849	5	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
3	A	4	6	6	0	0
3	B	4	6	6	0	0
4	A	18	24	24	0	0
4	B	24	32	30	0	0
5	B	1	0	0	0	0
6	A	382	0	0	1	0
6	B	375	0	0	2	0
All	All	6772	68	5814	12	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.

All (12) 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:109[A]:ARG:NH2	6:B:601:HOH:O	2.12	0.68
1:A:314[A]:GLN:NE2	6:A:603:HOH:O	2.39	0.55
1:B:434[A]:THR:HG21	6:B:884:HOH:O	2.10	0.51
1:A:178:PRO:HB3	1:A:183:TRP:NE1	2.33	0.44
1:A:385:TRP:CD2	1:A:394:HIS:HB2	2.53	0.44
1:B:190:GLU:HG2	1:B:207:ASN:OD1	2.18	0.43
1:A:304:LEU:CD2	1:A:449:TRP:CD2	3.03	0.41
1:B:242:TRP:O	1:B:246:ARG:HG2	2.20	0.41
1:A:373:SER:O	1:A:377:CYS:HB2	2.21	0.41
1:A:304:LEU:HD21	1:A:449:TRP:CD2	2.57	0.40
1:B:289:THR:O	1:B:358[B]:MET:HG2	2.22	0.40
1:A:353:VAL:HG11	1:A:358[B]:MET:HB2	2.03	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	397/401 (99%)	382 (96%)	15 (4%)	0	100	100
1	B	393/401 (98%)	378 (96%)	15 (4%)	0	100	100
All	All	790/802 (98%)	760 (96%)	30 (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	319/320 (100%)	318 (100%)	1 (0%)	92	82
1	B	315/320 (98%)	314 (100%)	1 (0%)	92	82
All	All	634/640 (99%)	632 (100%)	2 (0%)	92	82

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	GOL	A	503	-	5,5,5	0.84	0	5,5,5	0.84	0
4	GOL	B	503	-	5,5,5	0.77	0	5,5,5	0.78	0
4	GOL	A	504	-	5,5,5	0.74	0	5,5,5	1.03	0
4	GOL	B	504	-	5,5,5	0.70	0	5,5,5	0.92	0
3	EDO	B	502	-	3,3,3	0.54	0	2,2,2	0.15	0
3	EDO	A	502	-	3,3,3	0.47	0	2,2,2	0.20	0
2	NAG	A	501	1	14,14,15	0.15	0	17,19,21	0.64	1 (5%)
4	GOL	B	505	5	5,5,5	0.67	0	5,5,5	0.78	0
4	GOL	B	506	-	5,5,5	0.79	0	5,5,5	1.09	0
2	NAG	B	501	1	14,14,15	0.22	0	17,19,21	0.69	1 (5%)
4	GOL	A	505	-	5,5,5	0.72	0	5,5,5	0.85	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	GOL	A	503	-	-	0/4/4/4	-
4	GOL	B	503	-	-	0/4/4/4	-
4	GOL	A	504	-	-	2/4/4/4	-
4	GOL	B	504	-	-	1/4/4/4	-
3	EDO	B	502	-	-	0/1/1/1	-
3	EDO	A	502	-	-	0/1/1/1	-
2	NAG	A	501	1	-	0/6/23/26	0/1/1/1
4	GOL	B	505	5	-	0/4/4/4	-
4	GOL	B	506	-	-	2/4/4/4	-
2	NAG	B	501	1	-	0/6/23/26	0/1/1/1
4	GOL	A	505	-	-	1/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAG	C1-O5-C5	2.26	115.26	112.19
2	A	501	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	504	GOL	C1-C2-C3-O3
4	A	504	GOL	C1-C2-C3-O3
4	A	504	GOL	O2-C2-C3-O3
4	B	506	GOL	O2-C2-C3-O3
4	A	505	GOL	O1-C1-C2-C3
4	B	506	GOL	C1-C2-C3-O3

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	386/401 (96%)	-0.41	5 (1%) 77 78	8, 12, 23, 57	0
1	B	386/401 (96%)	-0.31	14 (3%) 42 46	8, 12, 26, 53	0
All	All	772/802 (96%)	-0.36	19 (2%) 57 60	8, 12, 24, 57	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	76	ALA	6.5
1	B	76	ALA	6.5
1	B	175	SER	5.7
1	B	78	PHE	5.6
1	A	78	PHE	4.9
1	B	74	ALA	4.3
1	B	176	GLY	4.2
1	B	177	THR	4.2
1	B	198	ALA	3.3
1	B	73	GLU	2.9
1	A	74	ALA	2.9
1	A	73	GLU	2.4
1	B	77	GLU	2.3
1	B	149	ASN	2.2
1	B	79	GLY	2.2
1	B	75	GLU	2.2
1	A	79	GLY	2.2
1	B	84	ILE	2.0
1	B	163[A]	GLN	2.0

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
4	GOL	B	504	6/6	0.85	0.22	26,54,66,68	0
4	GOL	B	506	6/6	0.85	0.14	25,41,54,58	0
4	GOL	A	503	6/6	0.88	0.17	19,29,37,37	0
4	GOL	A	504	6/6	0.89	0.17	20,41,51,56	0
4	GOL	A	505	6/6	0.90	0.11	26,35,42,47	0
3	EDO	B	502	4/4	0.91	0.14	16,30,39,39	0
4	GOL	B	503	6/6	0.92	0.13	16,22,28,28	0
4	GOL	B	505	6/6	0.95	0.11	18,22,24,26	0
2	NAG	B	501	14/15	0.96	0.07	10,14,17,18	0
2	NAG	A	501	14/15	0.96	0.06	11,15,19,19	0
3	EDO	A	502	4/4	0.97	0.07	13,20,28,28	0
5	NA	B	507	1/1	0.99	0.05	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.