



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:06 AM UTC

PDB ID : 8SLV / pdb_00008slv
Title : Structure of a salivary alpha-glucosidase from the mosquito vector *Aedes aegypti*.
Authors : Gittis, A.G.; Williams, A.E.; Garboczi, D.; Calvo, E.
Deposited on : 2023-04-24
Resolution : 2.32 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

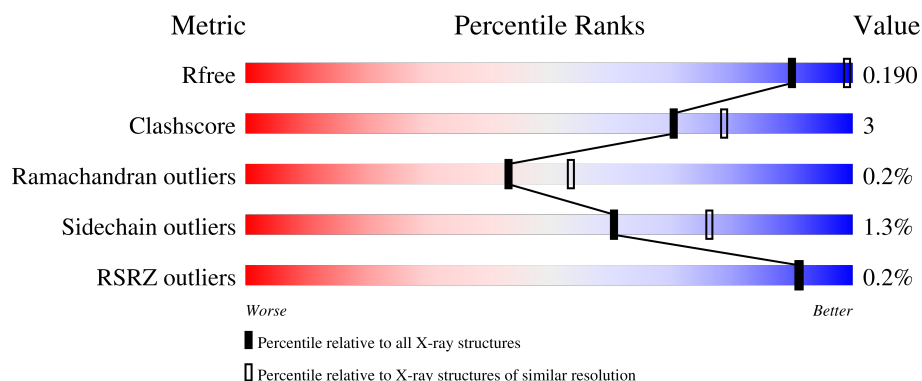
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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 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 $\leq 5\%$. 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	579	 87% 9% . .

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	GOL	A	606	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 4913 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 Salivary alpha-glucosidase.

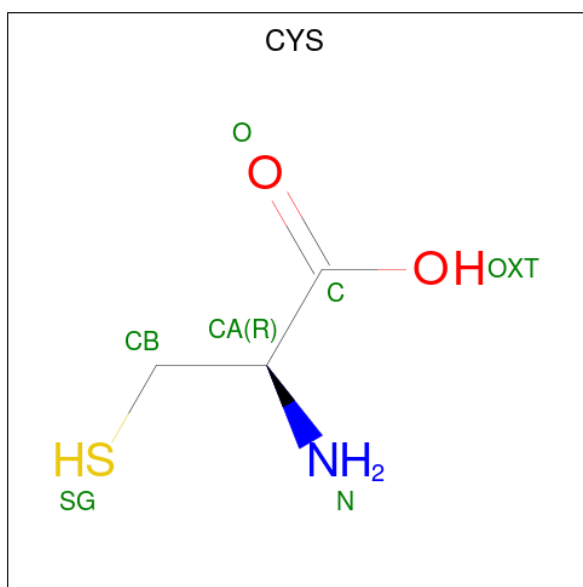
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	562	Total	C	N	O	S	0	1	0
			4508	2880	757	859	12			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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		

- Molecule 3 is CYSTEINE (CCD ID: CYS) (formula: $C_3H_7NO_2S$).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



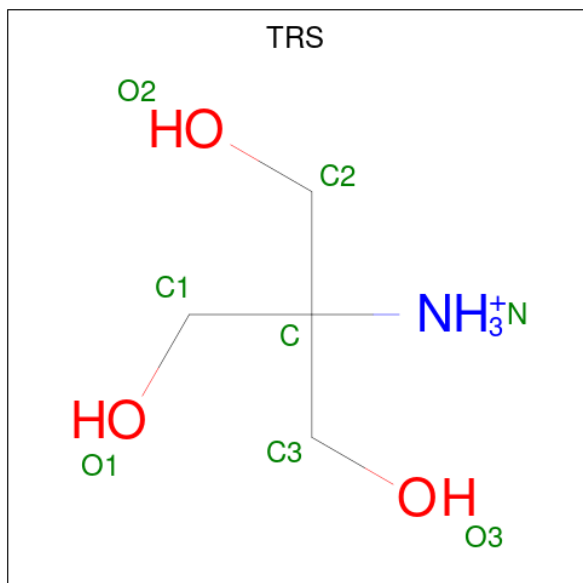
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



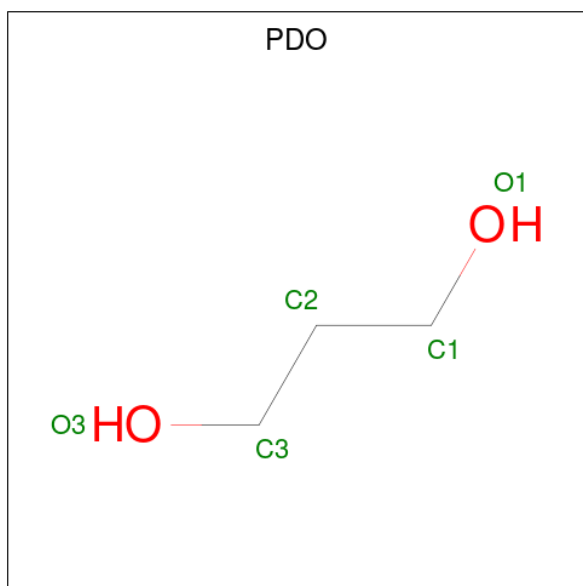
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O).



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

- Molecule 7 is 1,3-PROPANDIOL (CCD ID: PDO) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			5	3	2		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	Ca	0	0
			2	2		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	4	Total	Cl	0	0
			4	4		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	327	Total	O	0	4
			331	331		

- Molecule 1: Salivary alpha-glucosidase

P576	D259	LYS	MET
S579	1267	ILE	
	P296	PHE	
	K297	VAL	
		PRO	
	F301	LEU	
		LEU	
	F316	SER	
	F317	PHE	
	V318	LEU	
	I319	ALA	
		GLY	
	L352	LEU	
		THR	
	D356	THR	G18
	D381		Y28
	I391		M61
	N401		
	A407	S67	
		P68	
	P427	I69	F70
		S71	S72
	F438		
	I459	E86	
	Q460	Q106	
	S466	E135	
	H467	T136	
	L468		V147
		H148	
	L483	G149	
		P150	
	K491	N151	
		N152	
	P520	V155	
	V521		S158
	A522		N159
		L526	W160
	L528	F529	H181
	D530		Q182
	R531		
	A532	Q187	
	D533	P188	
		D189	
	V555		V221
			P222

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.76Å 51.03Å 70.75Å 101.82° 94.66° 95.76°	Depositor
Resolution (Å)	22.55 – 2.32 22.55 – 2.32	Depositor EDS
% Data completeness (in resolution range)	94.8 (22.55-2.32) 94.8 (22.55-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.31Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874, PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.146 , 0.188 0.147 , 0.190	Depositor DCC
R_{free} test set	2000 reflections (7.39%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtrriage
Anisotropy	0.164	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4913	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.71% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, NAG, CL, GOL, CA, PDO, IPA

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	0.73	13/4634 (0.3%)	0.79	15/6309 (0.2%)

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	PRO	N-CA	16.31	1.68	1.47
1	A	72	SER	C-N	14.35	1.48	1.34
1	A	187	GLN	C-N	13.24	1.49	1.33
1	A	68	PRO	C-O	-6.87	1.15	1.24
1	A	70	PHE	C-O	-6.67	1.14	1.23

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	SER	CA-C-N	12.56	135.55	119.84
1	A	67	SER	C-N-CA	12.56	135.55	119.84
1	A	187	GLN	CA-C-N	9.00	129.55	119.83
1	A	187	GLN	C-N-CA	9.00	129.55	119.83
1	A	187	GLN	O-C-N	-8.53	113.66	121.42

There are no chirality outliers.

There are no planarity outliers.

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	4508	0	4244	28	0
2	A	14	0	13	0	0
3	A	7	0	3	0	0
4	A	30	0	40	8	0
5	A	8	0	12	0	0
6	A	4	0	8	0	0
7	A	5	0	8	1	0
8	A	2	0	0	0	0
9	A	4	0	0	0	0
10	A	331	0	0	4	0
All	All	4913	0	4328	30	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 3.

The worst 5 of 30 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:68:PRO:N	1:A:68:PRO:CA	1.68	1.48
1:A:480:ARG:HH12	4:A:607:GOL:H2	1.13	1.07
1:A:356:ASP:HB3	4:A:606:GOL:H11	1.45	0.98
1:A:480:ARG:NH1	4:A:607:GOL:H2	1.98	0.69
1:A:356:ASP:CB	4:A:606:GOL:H11	2.23	0.66

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	561/579 (97%)	542 (97%)	18 (3%)	1 (0%)	43 53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	381	ASP

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	475/513 (93%)	469 (99%)	6 (1%)	61 76

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	ASP
1	A	401	ASN
1	A	459	ILE
1	A	148	HIS
1	A	72	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	282	ASN
1	A	357	ASN
1	A	550	ASN
1	A	460	GLN
1	A	256	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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	603	-	5,5,5	0.77	0	5,5,5	1.23	1 (20%)
4	GOL	A	607	-	5,5,5	0.15	0	5,5,5	0.63	0
7	PDO	A	610	-	4,4,4	0.17	0	3,3,3	0.46	0
2	NAG	A	601	1	14,14,15	0.69	0	17,19,21	0.37	0
3	CYS	A	602	1	5,6,6	1.12	1 (20%)	3,7,7	1.66	1 (33%)
6	IPA	A	609	-	3,3,3	0.28	0	3,3,3	0.13	0
4	GOL	A	605	-	5,5,5	0.13	0	5,5,5	0.42	0
4	GOL	A	606	-	5,5,5	0.11	0	5,5,5	0.47	0
5	TRS	A	608	-	7,7,7	0.27	0	9,9,9	0.70	0
4	GOL	A	604	-	5,5,5	0.11	0	5,5,5	0.51	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	603	-	-	3/4/4/4	-
4	GOL	A	607	-	-	2/4/4/4	-
7	PDO	A	610	-	-	2/2/2/2	-
2	NAG	A	601	1	-	2/6/23/26	0/1/1/1
3	CYS	A	602	1	-	0/6/6/6	-
4	GOL	A	605	-	-	0/4/4/4	-
4	GOL	A	606	-	-	4/4/4/4	-
5	TRS	A	608	-	-	0/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	604	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	CYS	OXT-C	-2.23	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	CYS	OXT-C-O	-2.42	118.59	124.08
4	A	603	GOL	C3-C2-C1	-2.05	104.29	111.80

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	604	GOL	O1-C1-C2-O2
4	A	604	GOL	O1-C1-C2-C3
4	A	606	GOL	C1-C2-C3-O3
7	A	610	PDO	O1-C1-C2-C3
7	A	610	PDO	C1-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	GOL	1	0
4	A	607	GOL	3	0
7	A	610	PDO	1	0
4	A	606	GOL	4	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 [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	562/579 (97%)	-0.69	1 (0%) 91 91	12, 19, 36, 66	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	531	ARG	3.6

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 oligosaccharides 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(Å ²)	Q<0.9
4	GOL	A	604	6/6	0.57	0.16	62,63,67,67	0
2	NAG	A	601	14/15	0.72	0.12	49,59,65,70	0
7	PDO	A	610	5/5	0.77	0.17	33,34,37,37	5
6	IPA	A	609	4/4	0.81	0.14	33,33,35,40	0
4	GOL	A	605	6/6	0.81	0.15	42,44,46,46	6
4	GOL	A	603	6/6	0.84	0.12	29,33,39,44	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	606	6/6	0.86	0.15	22,25,28,31	6
9	CL	A	614	1/1	0.89	0.09	51,51,51,51	0
4	GOL	A	607	6/6	0.90	0.10	29,39,45,48	6
5	TRS	A	608	8/8	0.98	0.05	10,15,16,17	0
8	CA	A	611	1/1	0.98	0.05	31,31,31,31	0
3	CYS	A	602	7/7	0.98	0.08	25,29,42,49	0
9	CL	A	616	1/1	0.98	0.08	27,27,27,27	0
8	CA	A	612	1/1	0.99	0.01	14,14,14,14	0
9	CL	A	615	1/1	0.99	0.06	23,23,23,23	0
9	CL	A	613	1/1	0.99	0.04	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.