



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:50 PM UTC

PDB ID : 8U9I / pdb_00008u9i
Title : Pasteurella multocida alpha2,3/2,6 sialyltransferase D141N bound to CMP
Authors : Stubbs, H.E.; Iverson, T.M.
Deposited on : 2023-09-19
Resolution : 1.55 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

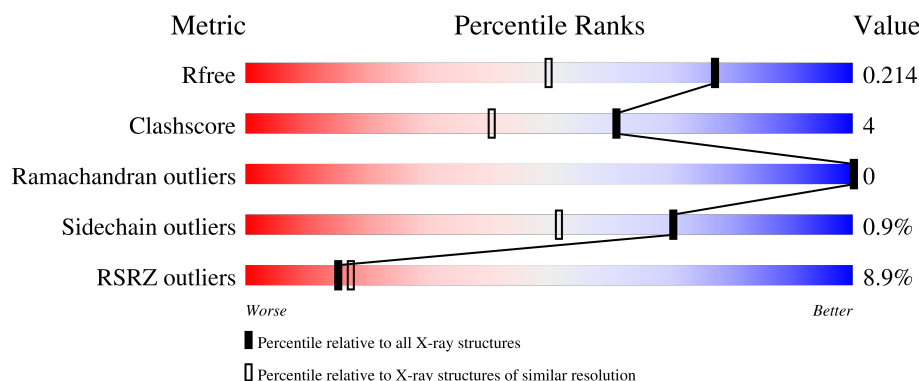
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

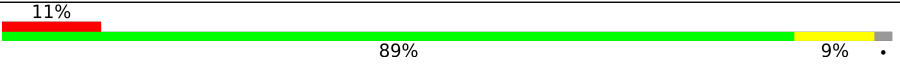
The reported resolution of this entry is 1.55 Å.

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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	399	
1	B	399	

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
3	PEG	A	502	-	-	X	-
4	GOL	B	502	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13576 atoms, of which 6237 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 Alpha-2,3/2,6-sialyltransferase/sialidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	393	Total	C	H	N	O	S	0	0	0
			6261	2051	3079	528	597	6			
1	B	391	Total	C	H	N	O	S	0	2	0
			6293	2056	3110	530	591	6			

There are 26 discrepancies between the modelled and reference sequences:

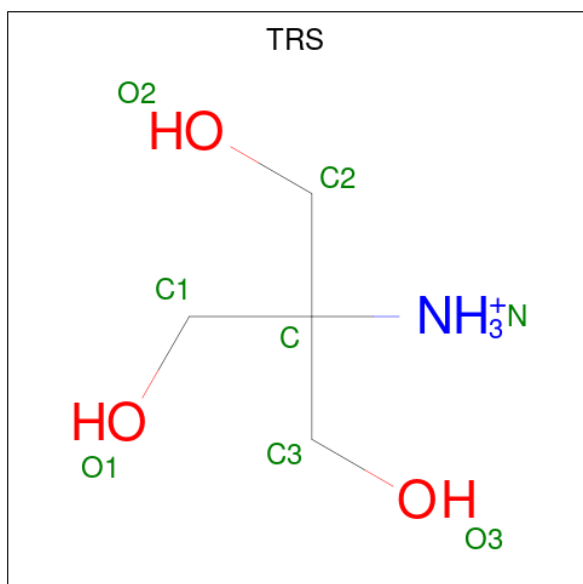
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	initiating methionine	UNP Q15KI8
A	141	ASN	ASP	engineered mutation	UNP Q15KI8
A	413	GLY	-	expression tag	UNP Q15KI8
A	414	GLY	-	expression tag	UNP Q15KI8
A	415	GLY	-	expression tag	UNP Q15KI8
A	416	LEU	-	expression tag	UNP Q15KI8
A	417	GLU	-	expression tag	UNP Q15KI8
A	418	HIS	-	expression tag	UNP Q15KI8
A	419	HIS	-	expression tag	UNP Q15KI8
A	420	HIS	-	expression tag	UNP Q15KI8
A	421	HIS	-	expression tag	UNP Q15KI8
A	422	HIS	-	expression tag	UNP Q15KI8
A	423	HIS	-	expression tag	UNP Q15KI8
B	25	MET	-	initiating methionine	UNP Q15KI8
B	141	ASN	ASP	engineered mutation	UNP Q15KI8
B	413	GLY	-	expression tag	UNP Q15KI8
B	414	GLY	-	expression tag	UNP Q15KI8
B	415	GLY	-	expression tag	UNP Q15KI8
B	416	LEU	-	expression tag	UNP Q15KI8
B	417	GLU	-	expression tag	UNP Q15KI8
B	418	HIS	-	expression tag	UNP Q15KI8
B	419	HIS	-	expression tag	UNP Q15KI8
B	420	HIS	-	expression tag	UNP Q15KI8
B	421	HIS	-	expression tag	UNP Q15KI8
B	422	HIS	-	expression tag	UNP Q15KI8

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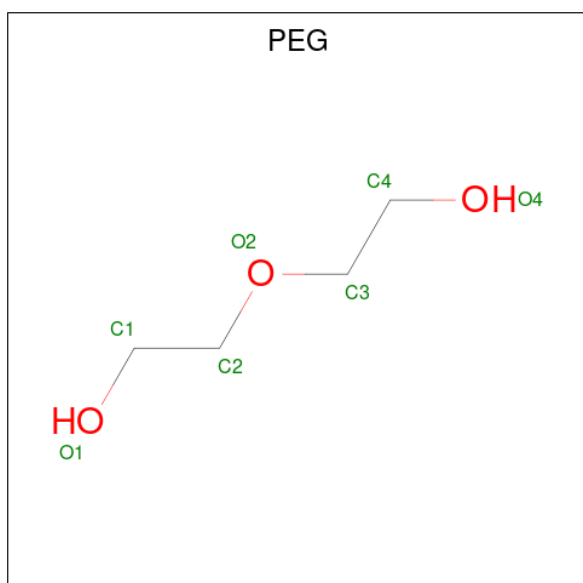
Chain	Residue	Modelled	Actual	Comment	Reference
B	423	HIS	-	expression tag	UNP Q15KI8

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			20	4	12	1	3		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 4 is GLYCEROL (CCD ID: 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	B	1	Total	C	H	O	0	0
			14	3	8	3		

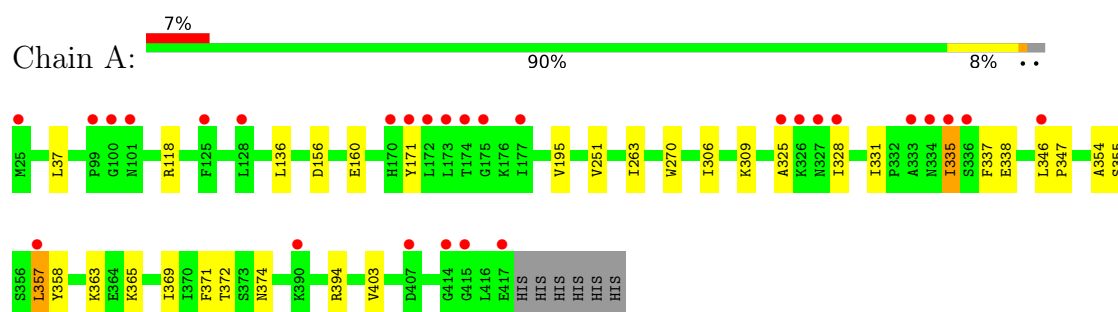
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	472	Total	O	0	0
			472	472		
5	B	468	Total	O	0	0
			468	468		

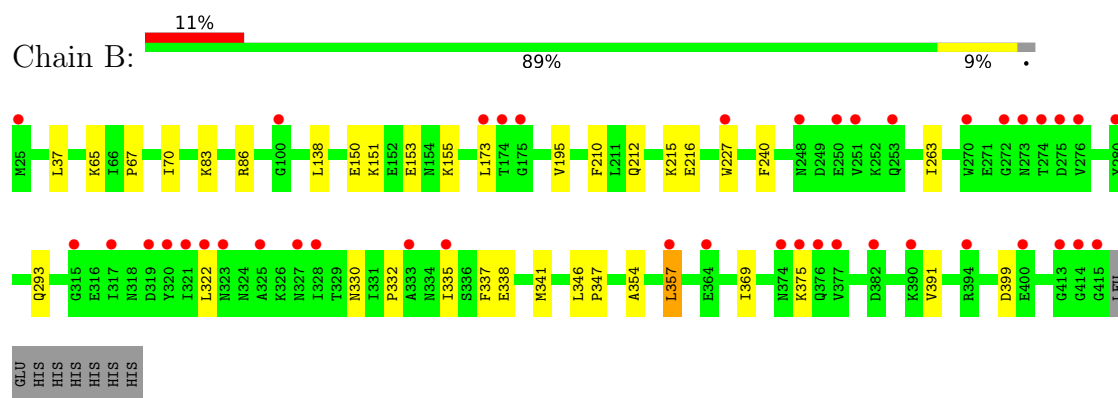
3 Residue-property plots

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: Alpha-2,3/2,6-sialyltransferase/sialidase



- Molecule 1: Alpha-2,3/2,6-sialyltransferase/sialidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.92Å 60.95Å 96.17Å 90.00° 101.63° 90.00°	Depositor
Resolution (Å)	28.99 – 1.55 28.99 – 1.55	Depositor EDS
% Data completeness (in resolution range)	85.4 (28.99-1.55) 86.1 (28.99-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 1.54Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.179 , 0.212 0.182 , 0.214	Depositor DCC
R_{free} test set	4562 reflections (4.33%)	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13576	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.9455e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL, PEG, TRS

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	0.52	0/3259	0.59	1/4424 (0.0%)
1	B	0.42	0/3260	0.55	0/4423
All	All	0.47	0/6519	0.57	1/8847 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	ALA	N-CA-C	6.07	119.06	110.50

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	3182	3079	3091	25	0
1	B	3183	3110	3115	28	0
2	A	8	12	12	0	0
3	A	7	10	10	5	0
3	B	7	10	10	0	0
4	A	6	8	8	0	0
4	B	6	8	8	5	0
5	A	472	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	468	0	0	3	0
All	All	7339	6237	6254	53	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 4.

The worst 5 of 53 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:341:MET:HE2	1:B:346:LEU:HD11	1.71	0.73
1:B:65:LYS:HE2	4:B:502:GOL:H2	1.70	0.73
1:B:332:PRO:HD2	1:B:335:ILE:HD12	1.69	0.73
1:A:346:LEU:HD23	1:A:365:LYS:CD	2.20	0.72
1:A:371:PHE:HD2	3:A:502:PEG:H31	1.59	0.67

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	391/399 (98%)	381 (97%)	10 (3%)	0	100	100
1	B	391/399 (98%)	382 (98%)	9 (2%)	0	100	100
All	All	782/798 (98%)	763 (98%)	19 (2%)	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	342/360 (95%)	339 (99%)	3 (1%)	70	51
1	B	343/360 (95%)	340 (99%)	3 (1%)	70	51
All	All	685/720 (95%)	679 (99%)	6 (1%)	70	51

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

Mol	Chain	Res	Type
1	B	357	LEU
1	B	375	LYS
1	B	399	ASP
1	A	357	LEU
1	A	335	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	330	ASN
1	B	283	GLN
1	A	323	ASN
1	B	137	ASN
1	A	293	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

5 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	$\# Z > 2$
4	GOL	A	503	-	5,5,5	1.09	0	5,5,5	0.78	0
2	TRS	A	501	-	7,7,7	0.32	0	9,9,9	0.32	0
3	PEG	A	502	-	6,6,6	0.21	0	5,5,5	0.25	0
4	GOL	B	502	-	5,5,5	0.23	0	5,5,5	0.30	0
3	PEG	B	501	-	6,6,6	0.16	0	5,5,5	0.04	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	-	-	4/4/4/4	-
2	TRS	A	501	-	-	1/9/9/9	-
3	PEG	A	502	-	-	1/4/4/4	-
4	GOL	B	502	-	-	2/4/4/4	-
3	PEG	B	501	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	GOL	C1-C2-C3-O3
4	A	503	GOL	O1-C1-C2-C3
4	B	502	GOL	O1-C1-C2-C3
4	A	503	GOL	O2-C2-C3-O3
4	B	502	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	PEG	5	0
4	B	502	GOL	5	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	393/399 (98%)	0.50	28 (7%)	22 25	9, 19, 39, 55	0
1	B	391/399 (97%)	0.59	42 (10%)	11 13	6, 19, 45, 72	2 (0%)
All	All	784/798 (98%)	0.54	70 (8%)	15 17	6, 19, 43, 72	2 (0%)

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	335	ILE	5.9
1	A	173	LEU	5.4
1	A	357	LEU	5.3
1	A	172	LEU	5.2
1	A	128	LEU	4.7

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($\text{\AA}^2$)	Q<0.9
4	GOL	A	503	6/6	0.61	0.23	27,62,74,84	0
2	TRS	A	501	8/8	0.69	0.18	31,62,83,86	0
4	GOL	B	502	6/6	0.80	0.23	20,20,20,20	0
3	PEG	B	501	7/7	0.81	0.14	37,45,53,60	0
3	PEG	A	502	7/7	0.82	0.12	29,37,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.