



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 28, 2018 – 11:04 AM EST

PDB ID : 5ONU
Title : Trimeric OmpU structure
Authors : Li, H.Y.; Dong, C.J.
Deposited on : 2017-08-04
Resolution : 2.22 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

<http://wwpdb.org/validation/2016/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 : **FAILED**
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

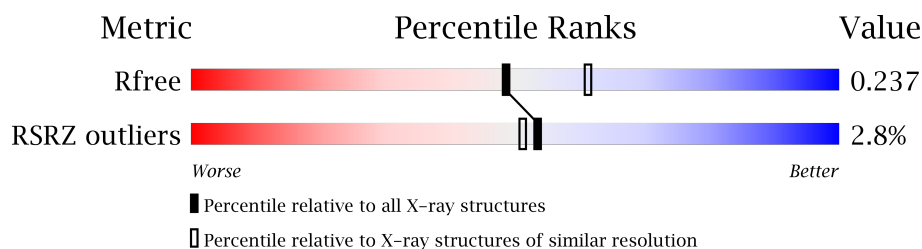
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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}	100719	4744 (2.24-2.20)
RSRZ outliers	101464	4776 (2.24-2.20)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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
2	C8E	C	401	-	-	-	X
3	GOL	B	402	-	-	-	X
4	LDA	A	404	-	-	-	X
4	LDA	A	405	-	-	-	X
4	LDA	A	406	-	-	-	X
4	LDA	B	407	-	-	-	X
4	LDA	C	406	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8240 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.

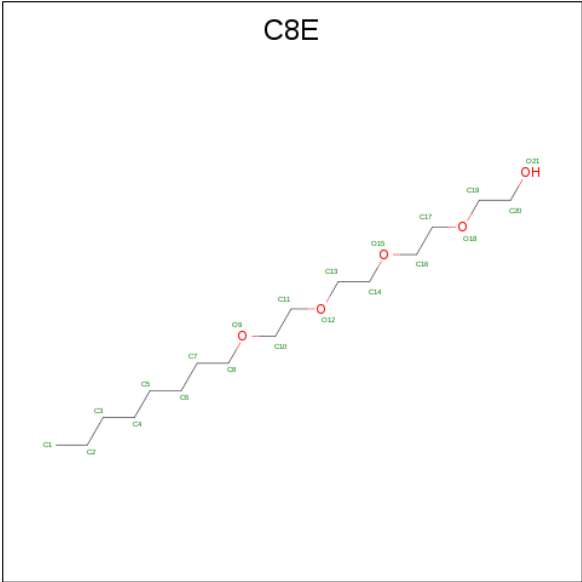
- Molecule 1 is a protein called Outer membrane protein OmpU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2448	1526	406	511	5			
1	B	320	Total	C	N	O	S	0	0	0
			2448	1526	406	511	5			
1	C	320	Total	C	N	O	S	0	0	0
			2448	1526	406	511	5			

There are 18 discrepancies between the modelled and reference sequences:

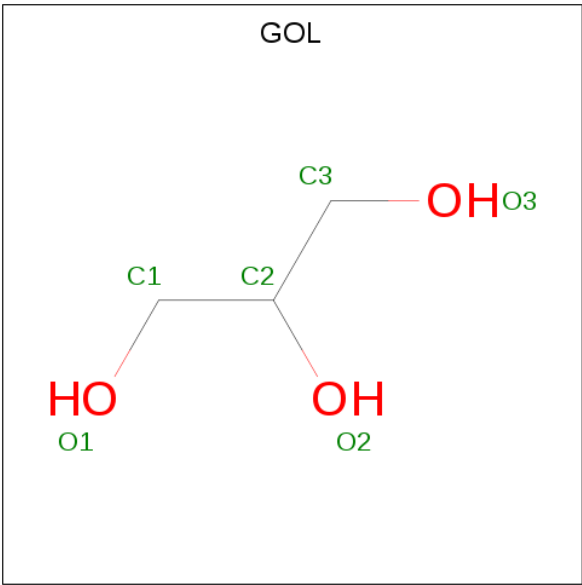
Chain	Residue	Modelled	Actual	Comment	Reference
A	351	HIS	-	expression tag	UNP A0A1V9N7P1
A	352	HIS	-	expression tag	UNP A0A1V9N7P1
A	353	HIS	-	expression tag	UNP A0A1V9N7P1
A	354	HIS	-	expression tag	UNP A0A1V9N7P1
A	355	HIS	-	expression tag	UNP A0A1V9N7P1
A	356	HIS	-	expression tag	UNP A0A1V9N7P1
B	351	HIS	-	expression tag	UNP A0A1V9N7P1
B	352	HIS	-	expression tag	UNP A0A1V9N7P1
B	353	HIS	-	expression tag	UNP A0A1V9N7P1
B	354	HIS	-	expression tag	UNP A0A1V9N7P1
B	355	HIS	-	expression tag	UNP A0A1V9N7P1
B	356	HIS	-	expression tag	UNP A0A1V9N7P1
C	351	HIS	-	expression tag	UNP A0A1V9N7P1
C	352	HIS	-	expression tag	UNP A0A1V9N7P1
C	353	HIS	-	expression tag	UNP A0A1V9N7P1
C	354	HIS	-	expression tag	UNP A0A1V9N7P1
C	355	HIS	-	expression tag	UNP A0A1V9N7P1
C	356	HIS	-	expression tag	UNP A0A1V9N7P1

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			21	16	5		
2	B	1	Total	C	O	0	0
			21	16	5		
2	C	1	Total	C	O	0	0
			21	16	5		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



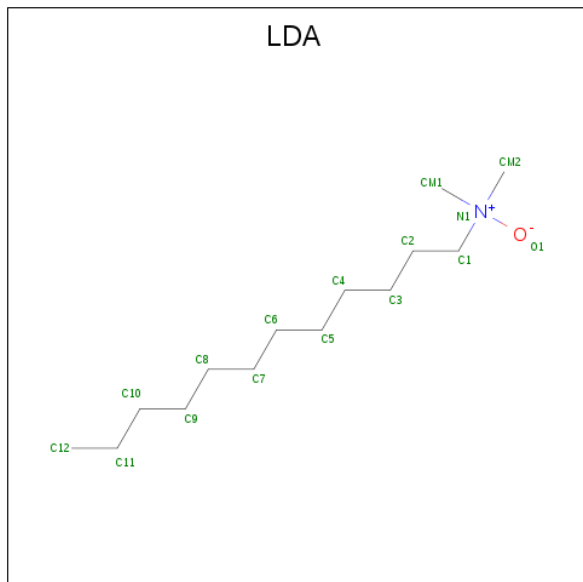
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	B	1	Total	C	N	O	0	0
			16	14	1	1		
4	B	1	Total	C	N	O	0	0
			16	14	1	1		
4	B	1	Total	C	N	O	0	0
			16	14	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			16	14	1	1		
4	C	1	Total	C	N	O	0	0
			16	14	1	1		
4	C	1	Total	C	N	O	0	0
			16	14	1	1		
4	C	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	204	Total	O	0	0
			204	204		
5	B	208	Total	O	0	0
			208	208		
5	C	225	Total	O	0	0
			225	225		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	129.88Å 153.47Å 81.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.73 – 2.22 64.94 – 2.22	Depositor EDS
% Data completeness (in resolution range)	99.7 (62.73-2.22) 99.8 (64.94-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.208 , 0.236 0.209 , 0.237	Depositor DCC
R_{free} test set	4016 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8240	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

4.6 Ligand geometry [i](#)

19 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	C8E	A	401	-	20,20,20	0.38	0	19,19,19	0.40	0
3	GOL	A	402	-	5,5,5	0.35	0	5,5,5	0.26	0
3	GOL	A	403	-	5,5,5	0.36	0	5,5,5	0.24	0
4	LDA	A	404	-	13,15,15	2.44	2 (15%)	14,17,17	0.64	0
4	LDA	A	405	-	13,15,15	2.45	2 (15%)	14,17,17	0.62	0
4	LDA	A	406	-	13,15,15	2.45	2 (15%)	14,17,17	0.52	0
2	C8E	B	401	-	20,20,20	0.38	0	19,19,19	0.42	0
3	GOL	B	402	-	5,5,5	0.35	0	5,5,5	0.25	0
3	GOL	B	403	-	5,5,5	0.35	0	5,5,5	0.30	0
4	LDA	B	404	-	13,15,15	2.45	2 (15%)	14,17,17	0.69	0
4	LDA	B	405	4	13,15,15	2.48	2 (15%)	14,17,17	1.14	2 (14%)
4	LDA	B	406	4	13,15,15	2.56	2 (15%)	14,17,17	0.69	0
4	LDA	B	407	-	13,15,15	2.43	2 (15%)	14,17,17	0.75	0
2	C8E	C	401	-	20,20,20	0.37	0	19,19,19	0.53	0
3	GOL	C	402	-	5,5,5	0.36	0	5,5,5	0.29	0
3	GOL	C	403	-	5,5,5	0.35	0	5,5,5	0.18	0
4	LDA	C	404	4	13,15,15	2.72	1 (7%)	14,17,17	0.55	0
4	LDA	C	405	4	13,15,15	2.51	1 (7%)	14,17,17	0.96	1 (7%)
4	LDA	C	406	-	13,15,15	2.45	2 (15%)	14,17,17	0.64	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	C8E	A	401	-	-	0/18/18/18	0/0/0/0
3	GOL	A	402	-	-	0/4/4/4	0/0/0/0
3	GOL	A	403	-	-	0/4/4/4	0/0/0/0
4	LDA	A	404	-	-	0/13/13/13	0/0/0/0
4	LDA	A	405	-	-	0/13/13/13	0/0/0/0
4	LDA	A	406	-	-	0/13/13/13	0/0/0/0
2	C8E	B	401	-	-	0/18/18/18	0/0/0/0
3	GOL	B	402	-	-	0/4/4/4	0/0/0/0
3	GOL	B	403	-	-	0/4/4/4	0/0/0/0
4	LDA	B	404	-	-	0/13/13/13	0/0/0/0
4	LDA	B	405	4	-	0/13/13/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LDA	B	406	4	-	0/13/13/13	0/0/0/0
4	LDA	B	407	-	-	0/13/13/13	0/0/0/0
2	C8E	C	401	-	-	0/18/18/18	0/0/0/0
3	GOL	C	402	-	-	0/4/4/4	0/0/0/0
3	GOL	C	403	-	-	0/4/4/4	0/0/0/0
4	LDA	C	404	4	-	0/13/13/13	0/0/0/0
4	LDA	C	405	4	-	0/13/13/13	0/0/0/0
4	LDA	C	406	-	-	0/13/13/13	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	404	LDA	O1-N1	-9.61	1.23	1.42
4	B	406	LDA	O1-N1	-8.99	1.24	1.42
4	C	405	LDA	O1-N1	-8.95	1.24	1.42
4	B	405	LDA	O1-N1	-8.65	1.25	1.42
4	A	405	LDA	O1-N1	-8.48	1.25	1.42
4	A	406	LDA	O1-N1	-8.46	1.25	1.42
4	B	404	LDA	O1-N1	-8.46	1.25	1.42
4	C	406	LDA	O1-N1	-8.46	1.25	1.42
4	B	407	LDA	O1-N1	-8.43	1.25	1.42
4	A	404	LDA	O1-N1	-8.42	1.25	1.42
4	B	404	LDA	C1-N1	-2.47	1.45	1.51
4	A	406	LDA	C1-N1	-2.42	1.45	1.51
4	C	406	LDA	C1-N1	-2.39	1.45	1.51
4	A	404	LDA	C1-N1	-2.38	1.46	1.51
4	A	405	LDA	C1-N1	-2.28	1.46	1.51
4	B	405	LDA	C1-N1	-2.24	1.46	1.51
4	B	407	LDA	C1-N1	-2.24	1.46	1.51
4	B	406	LDA	C1-N1	-2.07	1.46	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	405	LDA	CM1-N1-C1	-2.59	104.80	110.23
4	C	405	LDA	CM2-N1-CM1	-2.01	107.15	110.99
4	B	405	LDA	O1-N1-C1	2.03	114.26	109.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	405	LDA	0	31
4	B	406	LDA	0	42
4	C	404	LDA	0	31
4	C	405	LDA	0	42

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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	320/356 (89%)	-0.01	7 (2%) 62 60	27, 38, 76, 102	0
1	B	320/356 (89%)	0.03	8 (2%) 58 55	25, 37, 75, 136	0
1	C	320/356 (89%)	0.01	12 (3%) 41 39	26, 37, 69, 95	0
All	All	960/1068 (89%)	0.01	27 (2%) 53 51	25, 37, 73, 136	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	267	LYS	5.2
1	A	126	TYR	4.3
1	A	47	ALA	4.2
1	C	45	TYR	3.9
1	C	44	VAL	3.7
1	C	221	TYR	3.7
1	B	269	VAL	3.5
1	B	126	TYR	3.3
1	C	41	GLY	3.3
1	C	333	VAL	3.2
1	B	351	HIS	3.1
1	B	268	ASP	3.0
1	C	268	ASP	2.9
1	B	333	VAL	2.9
1	A	268	ASP	2.9
1	C	48	LYS	2.7
1	A	44	VAL	2.7
1	C	267	LYS	2.7
1	C	46	SER	2.5
1	A	351	HIS	2.5
1	B	280	TYR	2.5
1	B	45	TYR	2.4
1	A	175	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	43	THR	2.3
1	A	45	TYR	2.2
1	C	351	HIS	2.1
1	C	175	PHE	2.1

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

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

5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.4 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	LDA	A	405	16/16	0.33	0.69	18.62	103,114,129,130	0
4	LDA	C	406	16/16	0.78	0.38	8.84	45,60,96,98	0
4	LDA	B	407	16/16	0.68	0.29	7.03	66,76,114,116	0
4	LDA	A	406	16/16	0.71	0.30	4.59	53,72,103,104	0
4	LDA	A	404	16/16	0.65	0.41	4.46	58,90,132,132	0
2	C8E	C	401	21/21	0.71	0.40	4.30	66,91,97,99	0
3	GOL	B	402	6/6	0.96	0.24	2.69	46,51,52,54	0
4	LDA	B	405	16/16	0.78	0.24	1.52	174,177,187,187	0
4	LDA	B	406	16/16	0.47	0.26	0.88	152,180,196,196	0
4	LDA	C	405	16/16	0.53	0.26	0.88	122,130,163,163	0
4	LDA	B	404	16/16	0.79	0.19	0.87	49,57,100,102	0
4	LDA	C	404	16/16	0.76	0.21	0.80	142,158,194,194	0
3	GOL	A	403	6/6	0.74	0.15	0.49	60,69,71,74	0
2	C8E	B	401	21/21	0.79	0.17	0.36	44,53,68,80	0
3	GOL	A	402	6/6	0.92	0.12	0.31	47,56,57,57	0
2	C8E	A	401	21/21	0.85	0.17	0.31	56,74,82,83	0
3	GOL	C	402	6/6	0.87	0.13	0.25	58,61,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	GOL	C	403	6/6	0.79	0.19	-	64,67,68,69	0
3	GOL	B	403	6/6	0.62	0.32	-	62,68,72,74	0

5.5 Other polymers [i](#)

There are no such residues in this entry.