



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:48 am GMT

PDB ID : 5H0T  
Title : Crystal structure of proliferating cell nuclear antigen from Leishmania donovani at 2.73 Angstrom resolution  
Authors : Singh, P.K.; Yadav, S.P.; Sharma, P.S.; Kaur, P.; Sharma, S.; Singh, T.P.  
Deposited on : 2016-10-06  
Resolution : 2.73 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
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) : recalc28949

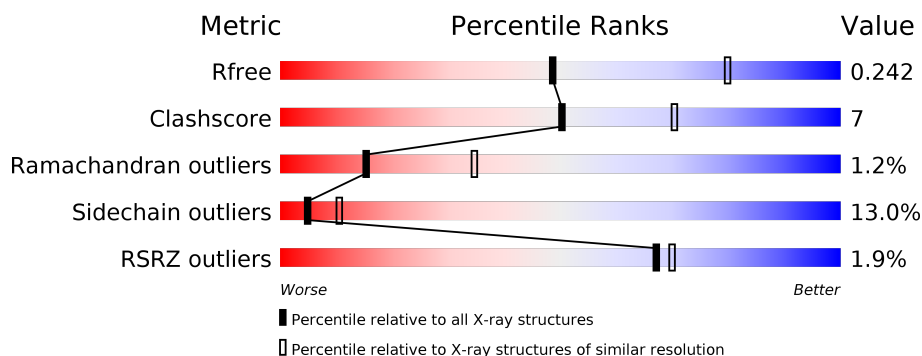
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.73 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	3342 (2.78-2.70)
Clashscore	112137	3731 (2.78-2.70)
Ramachandran outliers	110173	3670 (2.78-2.70)
Sidechain outliers	110143	3671 (2.78-2.70)
RSRZ outliers	101464	3362 (2.78-2.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	292	<div> <div>%</div> <div> <div></div> <div>65%</div> <div>14%</div> <div>5%</div> <div>15%</div> </div> </div>
1	B	292	<div> <div>2%</div> <div> <div></div> <div>66%</div> <div>16%</div> <div>•</div> <div>15%</div> </div> </div>
1	C	292	<div> <div>%</div> <div> <div></div> <div>61%</div> <div>18%</div> <div>• •</div> <div>15%</div> </div> </div>
1	D	292	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>17%</div> <div>• •</div> <div>15%</div> </div> </div>
1	E	292	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>14%</div> <div>• •</div> <div>15%</div> </div> </div>
1	F	292	<div> <div>2%</div> <div> <div></div> <div>63%</div> <div>17%</div> <div>• •</div> <div>15%</div> </div> </div>

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	PEG	A	301	-	-	-	X

## 2 Entry composition [i](#)

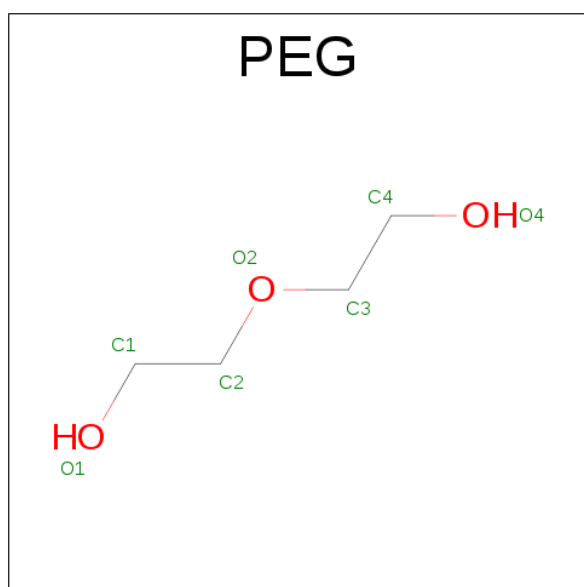
There are 3 unique types of molecules in this entry. The entry contains 11778 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1919	1210	317	377	15			
1	D	248	Total	C	N	O	S	0	0	0
			1919	1210	317	377	15			
1	E	248	Total	C	N	O	S	0	0	0
			1919	1210	317	377	15			
1	B	248	Total	C	N	O	S	0	0	0
			1919	1210	317	377	15			
1	C	248	Total	C	N	O	S	0	0	0
			1919	1210	317	377	15			
1	F	248	Total	C	N	O	S	0	0	0
			1919	1210	317	377	15			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	E	1	Total	C	O	0	0
			7	4	3		

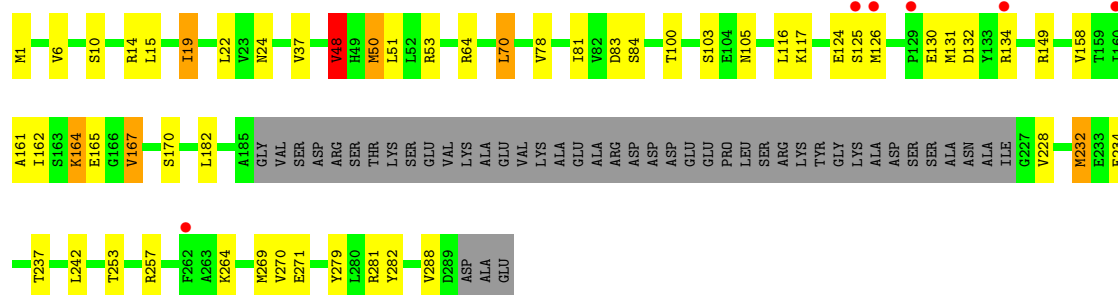
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total	O	0	0
			55	55		
3	D	59	Total	O	0	0
			59	59		
3	E	53	Total	O	0	0
			53	53		
3	B	26	Total	O	0	0
			26	26		
3	C	30	Total	O	0	0
			30	30		
3	F	27	Total	O	0	0
			27	27		

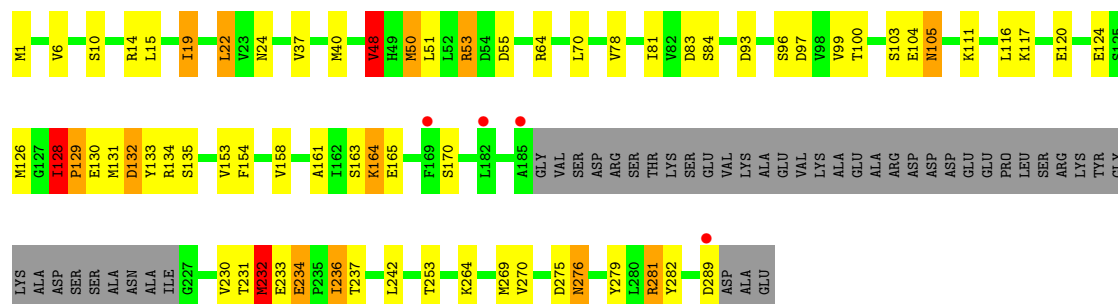




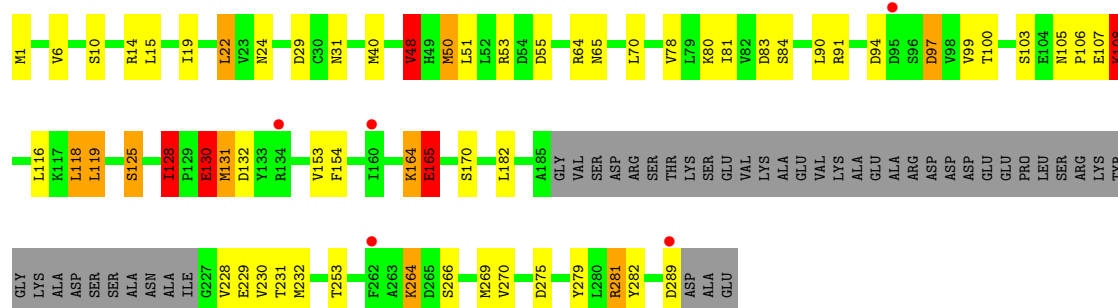
• Molecule 1: Proliferating cell nuclear antigen



• Molecule 1: Proliferating cell nuclear antigen



• Molecule 1: Proliferating cell nuclear antigen



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.80Å 149.57Å 169.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	112.08 – 2.73 43.13 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.3 (112.08-2.73) 99.3 (43.13-2.73)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.197 , 0.239 0.202 , 0.242	Depositor DCC
$R_{free}$ test set	927 reflections (1.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	80.7	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 60.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11778	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PEG

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	0.93	1/1947 (0.1%)	1.17	12/2627 (0.5%)
1	B	0.86	0/1947	1.16	10/2627 (0.4%)
1	C	0.91	0/1947	1.11	5/2627 (0.2%)
1	D	0.90	1/1947 (0.1%)	1.18	18/2627 (0.7%)
1	E	0.89	0/1947	1.14	11/2627 (0.4%)
1	F	0.85	0/1947	1.14	16/2627 (0.6%)
All	All	0.89	2/11682 (0.0%)	1.15	72/15762 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	1
1	F	0	3
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	MET	N-CA	5.74	1.57	1.46
1	D	287	LYS	C-O	-5.05	1.13	1.23

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	LEU	CB-CG-CD1	16.92	139.76	111.00
1	A	1	MET	CG-SD-CE	10.28	116.65	100.20
1	E	277	VAL	CG1-CB-CG2	9.75	126.50	110.90
1	D	277	VAL	CG1-CB-CG2	9.71	126.44	110.90
1	B	70	LEU	CB-CG-CD2	-9.09	95.55	111.00

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	GLU	Peptide
1	A	276	ASN	Sidechain
1	B	130	GLU	Peptide
1	B	288	VAL	Peptide
1	D	119	LEU	Peptide

## 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	1919	0	1914	27	0
1	B	1919	0	1914	19	0
1	C	1919	0	1914	36	0
1	D	1919	0	1914	23	0
1	E	1919	0	1914	27	0
1	F	1919	0	1914	20	0
2	A	7	0	10	0	0
2	E	7	0	10	1	0
3	A	55	0	0	3	0
3	B	26	0	0	1	0
3	C	30	0	0	2	0
3	D	59	0	0	2	0
3	E	53	0	0	0	0
3	F	27	0	0	1	0
All	All	11778	0	11504	151	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 7.

The worst 5 of 151 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:C:233:GLU:O	1:C:234:GLU:HB2	1.75	0.85
1:C:232:MET:CG	1:C:234:GLU:O	2.35	0.74
1:C:232:MET:HG3	1:C:234:GLU:O	1.91	0.70
1:C:93:ASP:HB2	1:C:96:SER:OG	1.92	0.67
1:B:124:GLU:HB2	1:B:126:MET:SD	2.35	0.65

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	244/292 (84%)	229 (94%)	13 (5%)	2 (1%)	22	47
1	B	244/292 (84%)	230 (94%)	13 (5%)	1 (0%)	38	65
1	C	244/292 (84%)	228 (93%)	12 (5%)	4 (2%)	11	26
1	D	244/292 (84%)	228 (93%)	12 (5%)	4 (2%)	11	26
1	E	244/292 (84%)	227 (93%)	14 (6%)	3 (1%)	15	34
1	F	244/292 (84%)	225 (92%)	15 (6%)	4 (2%)	11	26
All	All	1464/1752 (84%)	1367 (93%)	79 (5%)	18 (1%)	15	34

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	135	SER
1	C	129	PRO
1	C	234	GLU
1	F	130	GLU
1	C	128	ILE

### 5.3.2 Protein sidechains ⓘ

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	216/251 (86%)	190 (88%)	26 (12%)	6	13
1	B	216/251 (86%)	193 (89%)	23 (11%)	8	17
1	C	216/251 (86%)	188 (87%)	28 (13%)	5	10
1	D	216/251 (86%)	187 (87%)	29 (13%)	4	9
1	E	216/251 (86%)	186 (86%)	30 (14%)	4	8
1	F	216/251 (86%)	183 (85%)	33 (15%)	3	7
All	All	1296/1506 (86%)	1127 (87%)	169 (13%)	5	10

5 of 169 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	134	ARG
1	B	103	SER
1	F	118	LEU
1	E	170	SER
1	B	6	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	38	GLN
1	B	115	GLN
1	F	115	GLN
1	B	49	HIS
1	C	38	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 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	PEG	A	301	-	6,6,6	0.57	0	5,5,5	0.38	0
2	PEG	E	301	-	6,6,6	0.83	0	5,5,5	0.95	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	PEG	A	301	-	-	0/4/4/4	0/0/0/0
2	PEG	E	301	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	PEG	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	248/292 (84%)	0.22	2 (0%) 86 87	50, 75, 127, 177	0
1	B	248/292 (84%)	0.27	6 (2%) 59 62	59, 91, 140, 171	0
1	C	248/292 (84%)	0.29	4 (1%) 72 75	63, 92, 152, 187	0
1	D	248/292 (84%)	0.26	2 (0%) 86 87	51, 83, 139, 182	0
1	E	248/292 (84%)	0.30	10 (4%) 39 39	55, 82, 138, 160	0
1	F	248/292 (84%)	0.34	5 (2%) 65 68	64, 99, 157, 195	0
All	All	1488/1752 (84%)	0.28	29 (1%) 67 70	50, 88, 145, 195	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	289	ASP	8.0
1	D	185	ALA	4.2
1	E	289	ASP	4.1
1	E	185	ALA	4.0
1	C	169	PHE	4.0

### 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 carbohydrates 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. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	PEG	A	301	7/7	0.84	0.31	5.60	93,113,124,140	0
2	PEG	E	301	7/7	0.86	0.17	-0.30	88,99,105,111	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.