



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 9, 2017 – 11:17 AM EST

PDB ID : 5G22  
Title : Plasmodium vivax N-myristoyltransferase in complex with a quinoline inhibitor (compound 26)  
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Deposited on : 2016-04-06  
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](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	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20028442

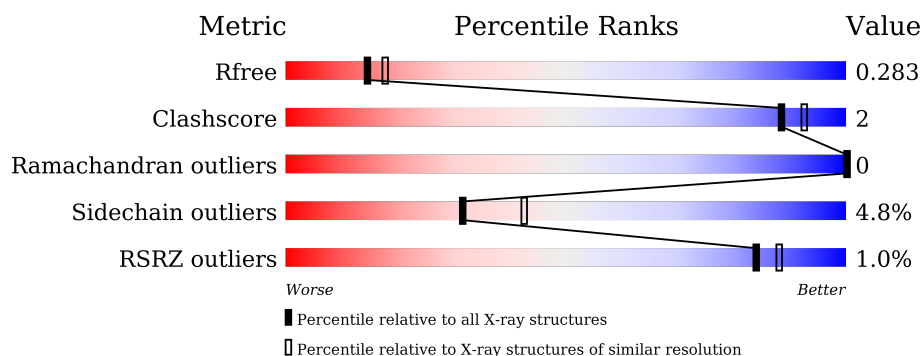
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	91344	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (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 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	385	<div> <div></div> <div>91%</div> <div>9%</div> </div>
1	B	385	<div> <div></div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	C	385	<div> <div></div> <div>86%</div> <div>9%</div> <div>.</div> <div>.</div> </div>

## 2 Entry composition [i](#)

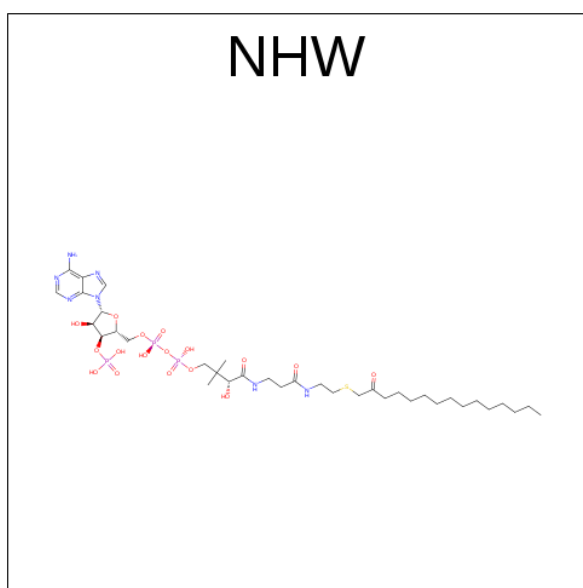
There are 7 unique types of molecules in this entry. The entry contains 10381 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE.

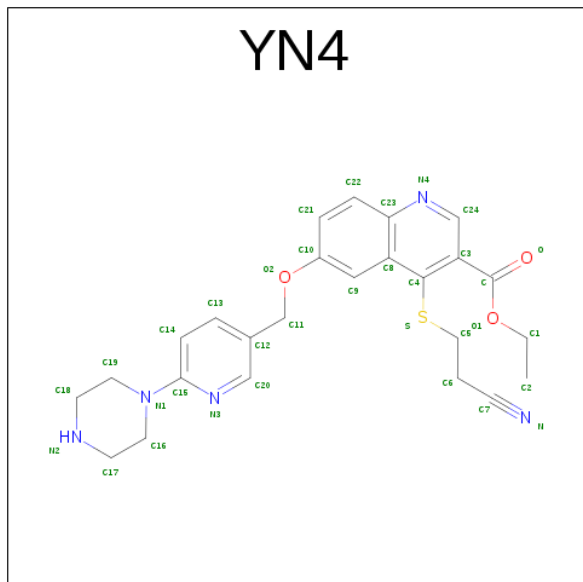
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	9	0
			3232	2103	529	589	11			
1	B	385	Total	C	N	O	S	0	12	0
			3258	2120	537	590	11			
1	C	369	Total	C	N	O	S	0	15	0
			3147	2055	504	577	11			

- Molecule 2 is 2-OXOPENTADECYL-COA (three-letter code: NHW) (formula:  $C_{36}H_{64}N_7O_{17}P_3S$ ).



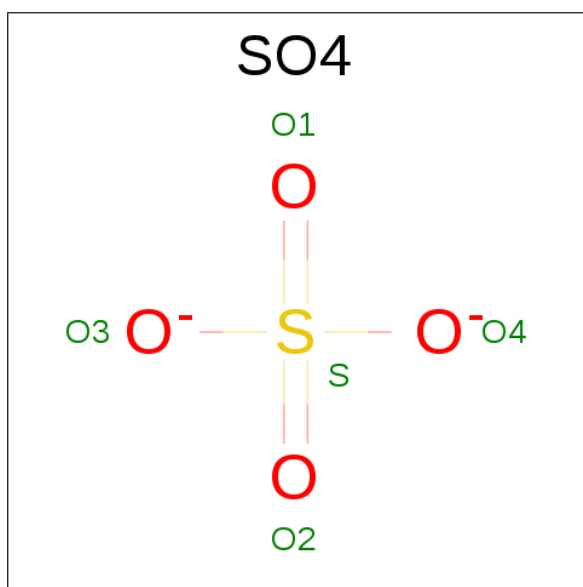
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P S	0	0
			64	36	7	17	3 1		
2	B	1	Total	C	N	O	P S	0	0
			64	36	7	17	3 1		
2	C	1	Total	C	N	O	P S	0	0
			64	36	7	17	3 1		

- Molecule 3 is ETHYL 4-[(2-CYANOETHYL)SULFANYL]-6-{[6-(PIPERAZIN-1-YL) (three-letter code: YN4) (formula: C<sub>25</sub>H<sub>27</sub>N<sub>5</sub>O<sub>3</sub>S)].



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			34	25	5	3	1		
3	B	1	Total	C	N	O	S	0	0
			34	25	5	3	1		
3	C	1	Total	C	N	O	S	0	0
			34	25	5	3	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	A	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	123	Total O 123 123	0	0
7	B	138	Total O 138 138	0	0
7	C	178	Total O 178 178	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.97Å 123.36Å 179.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	101.64 – 2.32 42.24 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.1 (101.64-2.32) 99.2 (42.24-2.32)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.220 , 0.283 0.220 , 0.283	Depositor DCC
$R_{free}$ test set	2827 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.6	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 28.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	10381	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: YN4, SO4, MG, NHW, CL

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	0.70	0/3337	0.81	2/4518 (0.0%)
1	B	0.70	0/3372	0.79	1/4561 (0.0%)
1	C	0.70	0/3263	0.80	2/4418 (0.0%)
All	All	0.70	0/9972	0.80	5/13497 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	409	LEU	CA-CB-CG	5.87	128.81	115.30
1	A	104	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	104	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	B	77	ASP	CB-CG-OD1	5.13	122.92	118.30
1	C	225	GLY	N-CA-C	5.04	125.71	113.10

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	3232	0	3243	11	0
1	B	3258	0	3285	24	0
1	C	3147	0	3145	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	64	0	60	0	0
2	B	64	0	60	0	0
2	C	64	0	60	3	0
3	A	34	0	0	1	0
3	B	34	0	0	0	0
3	C	34	0	0	0	0
4	A	5	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	123	0	0	0	0
7	B	138	0	0	2	0
7	C	178	0	0	1	0
All	All	10381	0	9853	49	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 2.

The worst 5 of 49 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:153[A]:ARG:HB2	1:B:153[A]:ARG:HH11	1.22	1.04
1:B:153[A]:ARG:CB	1:B:153[A]:ARG:HH11	1.87	0.88
1:C:208:ASP:O	1:C:402[A]:PRO:HG3	1.84	0.77
1:A:42:GLU:OE2	1:B:346[A]:LYS:HE2	1.90	0.71
1:B:39:ILE:HD11	1:B:201:TYR:HE2	1.62	0.64

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	392/385 (102%)	372 (95%)	20 (5%)	0	100	100
1	B	395/385 (103%)	381 (96%)	14 (4%)	0	100	100
1	C	380/385 (99%)	363 (96%)	17 (4%)	0	100	100
All	All	1167/1155 (101%)	1116 (96%)	51 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	360/351 (103%)	341 (95%)	19 (5%)	28	37
1	B	363/351 (103%)	345 (95%)	18 (5%)	30	41
1	C	351/351 (100%)	335 (95%)	16 (5%)	33	44
All	All	1074/1053 (102%)	1021 (95%)	53 (5%)	31	41

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	122	LEU
1	B	211	TYR
1	C	244	VAL
1	B	123	LYS
1	B	153[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	106	ASN
1	B	187	ASN
1	B	350	GLN

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Mol	Chain	Res	Type
1	B	34	GLN
1	B	230	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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$
2	NHW	A	1000	-	57,66,66	0.94	2 (3%)	67,92,92	1.82	11 (16%)
3	YN4	A	1001	-	37,37,37	2.11	7 (18%)	43,49,49	2.19	14 (32%)
4	SO4	A	1411	-	4,4,4	0.21	0	6,6,6	0.28	0
2	NHW	B	1000	5	57,66,66	0.99	3 (5%)	67,92,92	1.69	8 (11%)
3	YN4	B	1001	-	37,37,37	2.11	8 (21%)	43,49,49	2.17	14 (32%)
2	NHW	C	1000	5	57,66,66	0.84	1 (1%)	67,92,92	1.81	5 (7%)
3	YN4	C	1001	-	37,37,37	2.16	7 (18%)	43,49,49	2.01	11 (25%)

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	NHW	A	1000	-	-	0/61/81/81	0/3/3/3
3	YN4	A	1001	-	-	0/21/29/29	0/4/4/4
4	SO4	A	1411	-	-	0/0/0/0	0/0/0/0
2	NHW	B	1000	5	-	0/61/81/81	0/3/3/3
3	YN4	B	1001	-	-	0/21/29/29	0/4/4/4
2	NHW	C	1000	5	-	0/61/81/81	0/3/3/3
3	YN4	C	1001	-	-	0/21/29/29	0/4/4/4

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	YN4	C4-S	-6.90	1.68	1.77
3	B	1001	YN4	C4-S	-5.75	1.70	1.77
3	C	1001	YN4	C4-S	-4.66	1.71	1.77
2	B	1000	NHW	P2A-O4A	-2.09	1.46	1.55
3	B	1001	YN4	C24-N4	2.04	1.35	1.31

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1000	NHW	N3A-C2A-N1A	-11.25	120.04	128.87
2	A	1000	NHW	N3A-C2A-N1A	-9.70	121.25	128.87
2	B	1000	NHW	N3A-C2A-N1A	-9.50	121.41	128.87
2	A	1000	NHW	C13-C11-C12	-4.13	103.15	108.50
3	B	1001	YN4	C5-C6-C7	-3.85	101.01	112.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	YN4	1	0
2	C	1000	NHW	3	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	385/385 (100%)	-0.12	2 (0%) 91 94	11, 20, 36, 55	19 (4%)
1	B	385/385 (100%)	-0.17	4 (1%) 84 88	9, 18, 35, 63	16 (4%)
1	C	369/385 (95%)	-0.10	5 (1%) 78 83	9, 20, 39, 69	14 (3%)
All	All	1139/1155 (98%)	-0.13	11 (0%) 84 88	9, 20, 38, 69	49 (4%)

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	ASP	3.4
1	B	26	ILE	3.3
1	A	232	ARG	3.3
1	B	39	ILE	2.8
1	C	32	TYR	2.6

### 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 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( $\text{\AA}^2$ )	Q<0.9
4	SO4	A	1411	5/5	0.97	0.15	1.23	39,40,42,43	0
3	YN4	A	1001	34/34	0.88	0.17	0.70	26,27,37,38	0
3	YN4	C	1001	34/34	0.90	0.15	0.41	25,29,34,38	0
3	YN4	B	1001	34/34	0.92	0.14	0.38	26,28,41,46	0
5	MG	A	1412	1/1	0.96	0.14	0.18	36,36,36,36	0
5	MG	C	1411	1/1	0.95	0.12	-0.13	29,29,29,29	0
2	NHW	C	1000	64/64	0.94	0.12	-0.28	11,16,23,25	0
2	NHW	B	1000	64/64	0.96	0.12	-0.30	12,14,16,18	0
5	MG	B	1411	1/1	0.97	0.12	-0.67	33,33,33,33	0
2	NHW	A	1000	64/64	0.96	0.11	-0.81	8,15,18,20	0
6	CL	B	1412	1/1	0.99	0.08	-2.42	29,29,29,29	0
6	CL	A	1413	1/1	0.99	0.07	-2.59	26,26,26,26	0
6	CL	C	1412	1/1	0.99	0.07	-4.98	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.