



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:46 PM GMT

PDB ID : 1H71  
Title : PSYCHROPHILIC PROTEASE FROM PSEUDOALTEROMONAS 'TAC II 18'  
Authors : Villeret, V.; Van Petegem, F.; Aghajari, N.; Chessa, J.-P.; Gerday, C.; Haser, R.; Van Beeumen, J.  
Deposited on : 2001-07-02  
Resolution : 2.10 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](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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

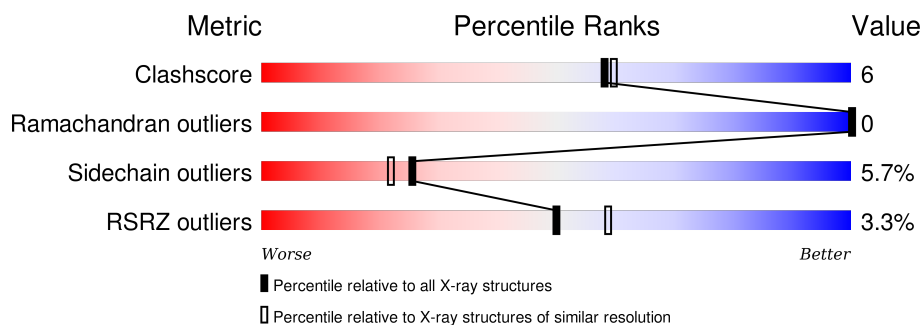
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	P	463	

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	CA	P	502	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3696 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 SERRALYSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	456	Total	C	N	O	S	0	1	0
			3403	2131	569	701	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	22	ASP	GLU	CONFLICT	UNP O69771
P	117	GLN	MET	CONFLICT	UNP O69771

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	Zn	0	0
			1	1		

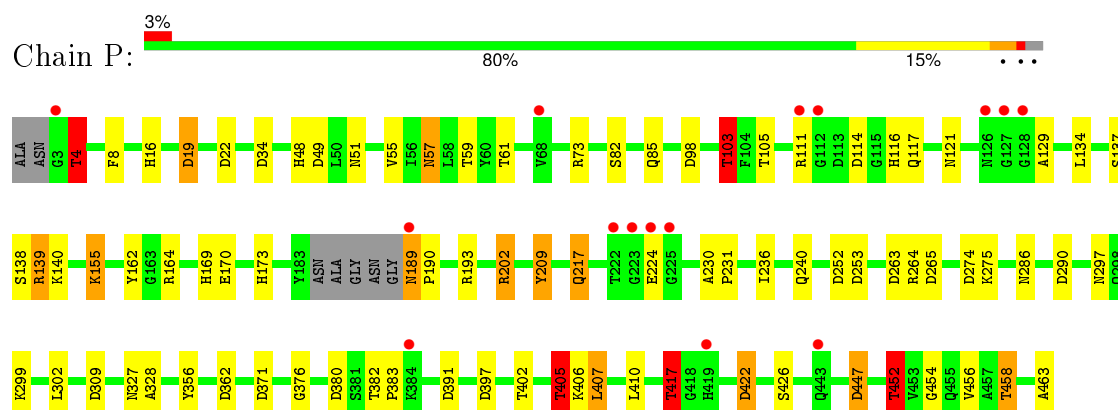
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	284	Total	O	0	0
			284	284		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: SERRALYSIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.00 Å 57.55 Å 161.81 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.10 14.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.7 (15.00-2.10) 96.7 (14.99-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.52 (at 2.10 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.164 , 0.221 0.147 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	25.5	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 29201 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3696	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, CA

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	P	0.87	1/3477 (0.0%)	1.66	52/4724 (1.1%)

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	P	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	117	GLN	CD-OE1	-5.53	1.11	1.24

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	193	ARG	NE-CZ-NH1	-15.72	112.44	120.30
1	P	265	ASP	CB-CG-OD1	11.53	128.68	118.30
1	P	202	ARG	NE-CZ-NH1	-11.40	114.60	120.30
1	P	253	ASP	CB-CG-OD1	10.90	128.11	118.30
1	P	103	THR	N-CA-CB	-10.62	90.13	110.30
1	P	452	THR	N-CA-CB	-10.40	90.54	110.30
1	P	49	ASP	CB-CG-OD1	9.32	126.69	118.30
1	P	114	ASP	CB-CG-OD2	-9.28	109.95	118.30
1	P	164	ARG	NE-CZ-NH2	-9.24	115.68	120.30
1	P	405	THR	N-CA-CB	-9.22	92.78	110.30
1	P	447	ASP	CA-CB-CG	9.13	133.48	113.40
1	P	34	ASP	CB-CG-OD1	9.10	126.49	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	263	ASP	CB-CG-OD2	8.68	126.11	118.30
1	P	253	ASP	CB-CG-OD2	-8.00	111.10	118.30
1	P	193	ARG	NH1-CZ-NH2	7.61	127.77	119.40
1	P	356	TYR	CB-CG-CD2	7.41	125.44	121.00
1	P	362	ASP	CB-CG-OD2	7.16	124.75	118.30
1	P	371	ASP	CB-CG-OD1	7.07	124.66	118.30
1	P	290	ASP	CB-CG-OD1	7.01	124.61	118.30
1	P	309	ASP	CB-CG-OD1	6.69	124.32	118.30
1	P	202	ARG	NH1-CZ-NH2	6.68	126.75	119.40
1	P	458	THR	N-CA-CB	-6.68	97.61	110.30
1	P	422	ASP	CB-CG-OD1	-6.52	112.43	118.30
1	P	447	ASP	CB-CG-OD2	6.47	124.12	118.30
1	P	380	ASP	CB-CG-OD1	6.20	123.88	118.30
1	P	274	ASP	CB-CG-OD1	6.18	123.86	118.30
1	P	22	ASP	CB-CG-OD2	6.08	123.77	118.30
1	P	356	TYR	CB-CG-CD1	-6.07	117.36	121.00
1	P	129	ALA	N-CA-CB	-6.06	101.61	110.10
1	P	162	TYR	CB-CG-CD1	-5.96	117.42	121.00
1	P	73	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	P	114	ASP	CB-CG-OD1	5.89	123.60	118.30
1	P	376	GLY	CA-C-O	-5.75	110.25	120.60
1	P	452	THR	CA-CB-OG1	5.75	121.07	109.00
1	P	309	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	P	264	ARG	NE-CZ-NH2	5.73	123.17	120.30
1	P	98	ASP	CB-CG-OD1	5.72	123.44	118.30
1	P	48	HIS	CA-CB-CG	-5.71	103.89	113.60
1	P	19	ASP	CB-CG-OD1	5.66	123.39	118.30
1	P	202	ARG	CG-CD-NE	-5.64	99.96	111.80
1	P	139	ARG	CD-NE-CZ	-5.62	115.73	123.60
1	P	170	GLU	OE1-CD-OE2	-5.59	116.59	123.30
1	P	397	ASP	CB-CG-OD2	5.50	123.25	118.30
1	P	4	THR	N-CA-CB	-5.45	99.95	110.30
1	P	391	ASP	CB-CG-OD1	5.38	123.14	118.30
1	P	155	LYS	CB-CG-CD	-5.35	97.68	111.60
1	P	169	HIS	CE1-NE2-CD2	5.25	119.71	106.60
1	P	371	ASP	OD1-CG-OD2	-5.14	113.53	123.30
1	P	252	ASP	CB-CG-OD1	5.12	122.91	118.30
1	P	202	ARG	CD-NE-CZ	5.08	130.71	123.60
1	P	173	HIS	CB-CA-C	-5.08	100.25	110.40
1	P	417	THR	N-CA-CB	-5.05	100.70	110.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	209[B]	TYR	Mainchain
1	P	297	ASN	Mainchain

## 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	P	3403	0	3163	39	0
2	P	8	0	0	0	0
3	P	1	0	0	0	0
4	P	284	0	0	6	0
All	All	3696	0	3163	39	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 6.

All (39) 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:P:85:GLN:HE22	1:P:121:ASN:HD21	1.32	0.78
1:P:103:THR:HG21	4:P:2071:HOH:O	1.86	0.75
1:P:82:SER:H	1:P:85:GLN:HE21	1.34	0.73
1:P:57:ASN:HA	1:P:103:THR:HG22	1.70	0.72
1:P:452:THR:HG21	1:P:456:VAL:HG23	1.70	0.71
1:P:61:THR:HG23	1:P:116:HIS:CE1	2.26	0.70
1:P:111:ARG:C	1:P:111:ARG:N	2.46	0.68
1:P:402:THR:HA	1:P:405:THR:HG22	1.80	0.64
1:P:417:THR:HB	1:P:422:ASP:OD1	1.98	0.64
1:P:202:ARG:NH2	1:P:209[B]:TYR:HB3	2.15	0.62
1:P:16:HIS:HD2	1:P:19:ASP:OD2	1.85	0.59
1:P:406:LYS:O	1:P:407:LEU:HB2	2.05	0.55
1:P:230:ALA:HB1	1:P:231:PRO:HD2	1.88	0.54
1:P:217:GLN:NE2	1:P:217:GLN:H	2.05	0.54
1:P:405:THR:HG21	1:P:463:ALA:OXT	2.08	0.53
1:P:452:THR:HG23	1:P:454:GLY:O	2.08	0.53

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:217:GLN:HE21	1:P:217:GLN:H	1.60	0.50
1:P:286:ASN:HD21	1:P:327:ASN:HD21	1.60	0.48
1:P:236:ILE:O	1:P:240:GLN:HG3	2.14	0.48
1:P:155:LYS:CE	4:P:2108:HOH:O	2.63	0.47
1:P:286:ASN:ND2	1:P:327:ASN:HD21	2.13	0.46
1:P:302:LEU:N	1:P:302:LEU:HD22	2.30	0.46
1:P:61:THR:HG23	1:P:116:HIS:HE1	1.77	0.46
1:P:103:THR:HG23	4:P:2040:HOH:O	2.15	0.46
1:P:405:THR:CG2	1:P:407:LEU:H	2.29	0.46
1:P:382:THR:HB	1:P:383:PRO:CD	2.46	0.45
1:P:405:THR:CG2	1:P:463:ALA:OXT	2.65	0.45
1:P:4:THR:HG21	1:P:8:PHE:HD1	1.81	0.45
1:P:382:THR:HB	1:P:383:PRO:HD2	1.98	0.45
1:P:452:THR:HG21	1:P:456:VAL:CG2	2.42	0.44
1:P:224:GLU:O	1:P:275:LYS:HE2	2.18	0.43
1:P:103:THR:CG2	4:P:2040:HOH:O	2.67	0.42
1:P:302:LEU:HD21	1:P:328:ALA:HB2	2.01	0.42
1:P:452:THR:CG2	1:P:454:GLY:O	2.68	0.42
1:P:155:LYS:HE3	4:P:2108:HOH:O	2.19	0.41
1:P:4:THR:HG23	1:P:8:PHE:HB3	2.02	0.41
1:P:299:LYS:HE3	4:P:2205:HOH:O	2.21	0.41
1:P:59:THR:HA	1:P:105:THR:O	2.21	0.41
1:P:189:ASN:N	1:P:190:PRO:CD	2.84	0.41

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	P	452/463 (98%)	445 (98%)	7 (2%)	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	P	350/354 (99%)	330 (94%)	20 (6%)	25	22

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	4	THR
1	P	51	ASN
1	P	55	VAL
1	P	57	ASN
1	P	103	THR
1	P	134	LEU
1	P	137	SER
1	P	138	SER
1	P	139	ARG
1	P	140	LYS
1	P	189	ASN
1	P	217	GLN
1	P	405	THR
1	P	407	LEU
1	P	410	LEU
1	P	417	THR
1	P	426	SER
1	P	447	ASP
1	P	452	THR
1	P	458	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	16	HIS
1	P	85	GLN
1	P	117	GLN
1	P	189	ASN
1	P	217	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	P	286	ASN
1	P	321	GLN
1	P	411	ASN
1	P	419	HIS
1	P	443	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

### 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	P	456/463 (98%)	-0.38	15 (3%)	50 59	20, 28, 47, 68	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	222	THR	7.9
1	P	127	GLY	6.6
1	P	443	GLN	4.4
1	P	68	VAL	3.9
1	P	224	GLU	3.8
1	P	111	ARG	3.3
1	P	189	ASN	3.2
1	P	3	GLY	3.2
1	P	128	GLY	2.9
1	P	126	ASN	2.8
1	P	419	HIS	2.4
1	P	223	GLY	2.2
1	P	384	LYS	2.2
1	P	225	GLY	2.2
1	P	112	GLY	2.0

### 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	CA	P	502	1/1	1.00	0.15	6.85	23,23,23,23	0
2	CA	P	503	1/1	1.00	0.11	1.88	24,24,24,24	0
2	CA	P	504	1/1	1.00	0.11	1.40	25,25,25,25	0
2	CA	P	501	1/1	1.00	0.09	0.34	24,24,24,24	0
2	CA	P	505	1/1	1.00	0.08	-0.13	25,25,25,25	0
2	CA	P	506	1/1	0.99	0.08	-0.21	24,24,24,24	0
2	CA	P	507	1/1	0.99	0.08	-0.43	26,26,26,26	0
3	ZN	P	600	1/1	1.00	0.06	-0.74	28,28,28,28	0
2	CA	P	500	1/1	0.98	0.10	-0.79	39,39,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.