



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 14, 2021 – 03:16 pm BST

PDB ID : 7O74  
Title : Structure of cyanase from *Pseudomonas lactis*  
Authors : Brag, S.; Driller, J.H.; Pedersen, B.P.  
Deposited on : 2021-04-12  
Resolution : 1.61 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

<https://www.wwpdb.org/validation/2017/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  
Xtriage (Phenix) : 1.13  
EDS : 2.18  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.18

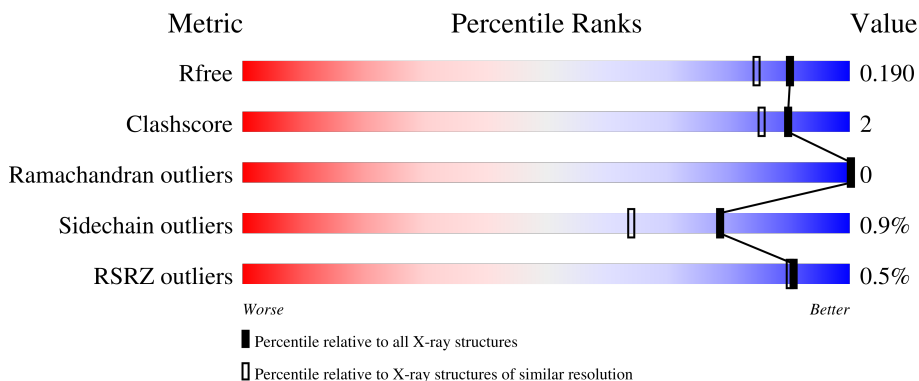
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.61 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))
$R_{free}$	130704	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (1.64-1.60)

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  $\geq 3$ , 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	156	94% 6%
1	B	156	97% .
1	C	156	91% 9%
1	D	156	95% 5%
1	E	156	96% .

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Mol	Chain	Length	Quality of chain
1	F	156	 96% .
1	G	156	 94% 6% .
1	H	156	 98% .
1	I	156	 % 91% 8% .
1	J	156	 96% .

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13985 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 Cyanate hydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	156	1219	780	203	232	4	0	4	0
1	B	156	1204	770	201	229	4	0	2	0
1	C	156	1204	770	201	229	4	0	2	0
1	D	156	1198	767	200	227	4	0	1	0
1	E	156	1225	784	204	233	4	0	5	0
1	F	156	1219	780	203	232	4	0	4	0
1	G	156	1211	774	202	231	4	0	3	0
1	H	156	1211	775	202	230	4	0	3	0
1	I	156	1206	773	201	228	4	0	2	0
1	J	156	1212	776	202	230	4	0	3	0

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total Cl 1 1	0	0
2	G	1	Total Cl 1 1	0	0
2	H	1	Total Cl 1 1	0	0
2	I	1	Total Cl 1 1	0	0
2	J	1	Total Cl 1 1	0	0

- Molecule 3 is water.

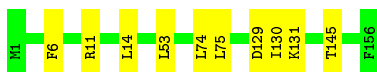
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	212	Total O 212 212	0	0
3	B	197	Total O 197 197	0	0
3	C	152	Total O 152 152	0	0
3	D	192	Total O 192 192	0	0
3	E	193	Total O 193 193	0	0
3	F	195	Total O 195 195	0	0
3	G	172	Total O 172 172	0	0
3	H	177	Total O 177 177	0	0
3	I	200	Total O 200 200	0	0
3	J	177	Total O 177 177	0	0

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

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.

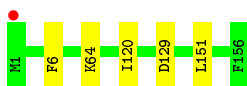
- Molecule 1: Cyanate hydratase

Chain A:  94% 6%

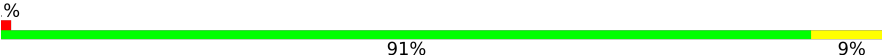


- Molecule 1: Cyanate hydratase

Chain B:  % 97% .



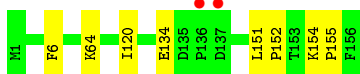
- Molecule 1: Cyanate hydratase

Chain C:  % 91% 9%



- Molecule 1: Cyanate hydratase

Chain D:  % 95% 5%



- Molecule 1: Cyanate hydratase

Chain E:  % 96% .



- Molecule 1: Cyanate hydratase

Chain F:  96%



● Molecule 1: Cyanate hydratase

Chain G:  94%

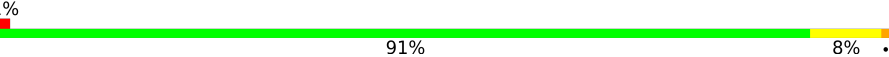


● Molecule 1: Cyanate hydratase

Chain H:  98%



● Molecule 1: Cyanate hydratase

Chain I:  91%



● Molecule 1: Cyanate hydratase

Chain J:  96%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.15Å 117.59Å 106.99Å 90.00° 94.26° 90.00°	Depositor
Resolution (Å)	43.57 – 1.61 46.54 – 1.61	Depositor EDS
% Data completeness (in resolution range)	97.2 (43.57-1.61) 89.9 (46.54-1.61)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.47 (at 1.61Å)	Xtrriage
Refinement program	PHENIX 1.19	Depositor
R, $R_{free}$	0.164 , 0.190 0.164 , 0.190	Depositor DCC
$R_{free}$ test set	2027 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.0	Xtrriage
Anisotropy	0.083	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 38.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13985	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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:  
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	0.40	0/1243	0.63	0/1685
1	B	0.39	0/1228	0.64	0/1664
1	C	0.36	0/1228	0.60	0/1664
1	D	0.38	0/1222	0.63	0/1656
1	E	0.36	0/1249	0.60	0/1693
1	F	0.39	0/1243	0.61	0/1685
1	G	0.37	0/1235	0.59	0/1674
1	H	0.37	0/1235	0.60	0/1674
1	I	0.38	0/1230	0.60	0/1667
1	J	0.37	0/1236	0.60	0/1676
All	All	0.38	0/12349	0.61	0/16738

There are no bond length outliers.

There are no bond angle outliers.

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	1219	0	1242	6	0
1	B	1204	0	1226	2	0
1	C	1204	0	1226	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1198	0	1222	4	0
1	E	1225	0	1248	3	0
1	F	1219	0	1242	5	0
1	G	1211	0	1232	5	0
1	H	1211	0	1234	2	0
1	I	1206	0	1232	8	0
1	J	1212	0	1236	4	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	212	0	0	0	0
3	B	197	0	0	2	0
3	C	152	0	0	0	0
3	D	192	0	0	1	0
3	E	193	0	0	1	0
3	F	195	0	0	1	0
3	G	172	0	0	1	0
3	H	177	0	0	1	0
3	I	200	0	0	1	0
3	J	177	0	0	1	0
All	All	13985	0	12340	43	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.

All (43) 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:I:34:ASP:O	1:I:64:LYS:NZ	2.25	0.69
1:C:47:LEU:HD21	1:C:61:VAL:HG11	1.79	0.65
1:A:14:LEU:HD21	1:A:75[A]:LEU:HG	1.79	0.64
1:G:120:ILE:HD11	1:G:151:LEU:HD12	1.81	0.62
1:J:25:LYS:NZ	3:J:301:HOH:O	2.32	0.62
1:C:120:ILE:HD11	1:C:151:LEU:HD12	1.83	0.60
1:D:120:ILE:HD11	1:D:151:LEU:HD12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ASP:OD2	1:A:131:LYS:HE3	2.03	0.59
1:C:34:ASP:O	1:C:64:LYS:NZ	2.36	0.58
1:A:130:ILE:O	1:A:131:LYS:HD3	2.04	0.57
1:F:154:LYS:NZ	3:F:1003:HOH:O	2.36	0.54
1:A:129:ASP:OD1	1:A:145:THR:HB	2.08	0.53
1:G:131:LYS:HE3	1:G:133:VAL:CG1	2.39	0.52
1:I:135:ASP:HB3	1:I:141:ARG:HG3	1.91	0.52
1:F:129:ASP:OD1	1:F:131:LYS:NZ	2.32	0.51
1:A:53:LEU:HD12	1:A:75[B]:LEU:HD21	1.92	0.50
1:E:130[B]:ILE:HD11	1:G:108:LEU:HD23	1.93	0.50
3:E:362:HOH:O	1:F:154:LYS:HG2	2.11	0.50
1:I:131:LYS:NZ	3:I:303:HOH:O	2.44	0.50
1:F:34:ASP:O	1:F:64:LYS:NZ	2.43	0.50
1:E:47:LEU:HD21	1:E:61[B]:VAL:HG11	1.94	0.49
1:E:129:ASP:OD1	1:E:131:LYS:HE2	2.13	0.49
1:H:56:GLU:HG3	3:H:406:HOH:O	2.13	0.49
1:D:64:LYS:NZ	3:D:302:HOH:O	2.41	0.48
1:B:64:LYS:NZ	3:B:305:HOH:O	2.47	0.47
1:I:130[B]:ILE:HD11	1:J:108:LEU:HD23	1.98	0.46
1:D:152:PRO:HB2	1:D:154:LYS:HE3	1.97	0.46
1:B:120:ILE:HD11	1:B:151:LEU:HD12	1.97	0.45
1:I:120:ILE:HD11	1:I:151:LEU:HD12	1.98	0.45
1:I:9:THR:HB	1:I:10:PRO:HD3	1.99	0.45
1:C:132:LYS:HG3	1:H:116:PHE:CE2	2.52	0.45
1:A:11:ARG:HD2	1:A:74:LEU:HG	1.99	0.45
1:I:11:ARG:HD2	1:I:74:LEU:HG	1.98	0.45
1:J:97:PHE:HE1	1:J:144:ILE:HD13	1.81	0.44
1:F:129:ASP:OD2	1:F:131:LYS:HE2	2.18	0.44
1:C:68:ASP:OD2	1:C:70:ASP:HB2	2.19	0.42
1:G:11:ARG:HD2	1:G:74:LEU:HG	2.01	0.42
1:J:120:ILE:HD11	1:J:151:LEU:HD12	2.01	0.42
1:I:97:PHE:HE1	1:I:144:ILE:HD13	1.85	0.42
1:C:11:ARG:HD2	1:C:74:LEU:HG	2.02	0.41
1:C:96:ARG:O	1:C:100:MET:HG3	2.21	0.41
1:G:134:GLU:HG2	3:G:411:HOH:O	2.21	0.41
3:B:405:HOH:O	1:D:155:PRO:HG3	2.20	0.40

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	158/156 (101%)	157 (99%)	1 (1%)	0	100	100
1	B	156/156 (100%)	155 (99%)	1 (1%)	0	100	100
1	C	156/156 (100%)	155 (99%)	1 (1%)	0	100	100
1	D	155/156 (99%)	154 (99%)	1 (1%)	0	100	100
1	E	159/156 (102%)	157 (99%)	2 (1%)	0	100	100
1	F	158/156 (101%)	157 (99%)	1 (1%)	0	100	100
1	G	157/156 (101%)	156 (99%)	1 (1%)	0	100	100
1	H	157/156 (101%)	154 (98%)	3 (2%)	0	100	100
1	I	156/156 (100%)	155 (99%)	1 (1%)	0	100	100
1	J	157/156 (101%)	156 (99%)	1 (1%)	0	100	100
All	All	1569/1560 (101%)	1556 (99%)	13 (1%)	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	133/129 (103%)	132 (99%)	1 (1%)	81	69
1	B	131/129 (102%)	129 (98%)	2 (2%)	65	43
1	C	131/129 (102%)	130 (99%)	1 (1%)	81	69
1	D	130/129 (101%)	128 (98%)	2 (2%)	65	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	134/129 (104%)	133 (99%)	1 (1%)	84	72
1	F	133/129 (103%)	132 (99%)	1 (1%)	81	69
1	G	132/129 (102%)	131 (99%)	1 (1%)	81	69
1	H	132/129 (102%)	131 (99%)	1 (1%)	81	69
1	I	131/129 (102%)	130 (99%)	1 (1%)	81	69
1	J	132/129 (102%)	132 (100%)	0	100	100
All	All	1319/1290 (102%)	1308 (99%)	11 (1%)	78	69

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	PHE
1	B	6	PHE
1	B	129	ASP
1	C	6	PHE
1	D	6	PHE
1	D	134	GLU
1	E	6	PHE
1	F	6	PHE
1	G	6	PHE
1	H	137	ASP
1	I	135	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

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

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	156/156 (100%)	-0.68	0 <b>100</b>   <b>100</b>	13, 19, 31, 41	0
1	B	156/156 (100%)	-0.56	1 (0%) <b>89</b>   <b>89</b>	14, 20, 36, 48	0
1	C	156/156 (100%)	-0.39	1 (0%) <b>89</b>   <b>89</b>	16, 24, 44, 64	0
1	D	156/156 (100%)	-0.55	2 (1%) <b>77</b>   <b>76</b>	13, 21, 38, 76	0
1	E	156/156 (100%)	-0.48	2 (1%) <b>77</b>   <b>76</b>	15, 21, 35, 63	0
1	F	156/156 (100%)	-0.60	0 <b>100</b>   <b>100</b>	14, 22, 34, 46	0
1	G	156/156 (100%)	-0.52	0 <b>100</b>   <b>100</b>	16, 24, 39, 46	0
1	H	156/156 (100%)	-0.55	0 <b>100</b>   <b>100</b>	15, 22, 36, 62	0
1	I	156/156 (100%)	-0.53	2 (1%) <b>77</b>   <b>76</b>	15, 21, 37, 62	0
1	J	156/156 (100%)	-0.50	0 <b>100</b>   <b>100</b>	15, 22, 38, 58	0
All	All	1560/1560 (100%)	-0.54	8 (0%) <b>91</b>   <b>90</b>	13, 22, 38, 76	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	137	ASP	4.8
1	I	136	PRO	3.8
1	B	1	MET	2.7
1	D	136	PRO	2.5
1	C	137	ASP	2.4
1	E	136	PRO	2.4
1	I	137	ASP	2.3
1	E	137	ASP	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 monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	CL	E	201	1/1	0.98	0.04	28,28,28,28	0
2	CL	H	201	1/1	0.98	0.04	23,23,23,23	0
2	CL	G	201	1/1	0.99	0.04	23,23,23,23	0
2	CL	B	201	1/1	0.99	0.03	20,20,20,20	0
2	CL	J	201	1/1	0.99	0.03	21,21,21,21	0
2	CL	C	201	1/1	1.00	0.02	24,24,24,24	0
2	CL	D	201	1/1	1.00	0.03	19,19,19,19	0
2	CL	I	201	1/1	1.00	0.04	24,24,24,24	0
2	CL	A	201	1/1	1.00	0.02	23,23,23,23	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.