

Full wwPDB X-ray Structure Validation Report (i)

Sep 6, 2023 – 11:46 PM EDT

PDB ID : 4GCW

Title : Crystal structure of RNase Z in complex with precursor tRNA(Thr) Authors Pellegrini, O.; Li de la Sierra-Gallay, I.; Piton, J.; Gilet, L.; Condon, C.

2012-07-31 Deposited on

3.00 Å(reported) Resolution

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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

> The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity 4.02b-467

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13

EDS 2.35

20191225.v01 (using entries in the PDB archive December 25th 2019) Percentile statistics

> Refmac 5.8.0158

CCP4 7.0.044 (Gargrove)

Ideal geometry (proteins) Engh & Huber (2001) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

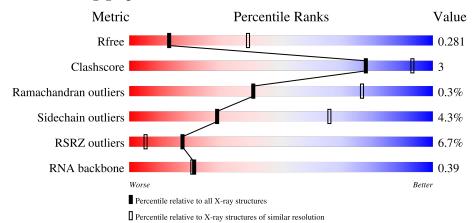
Validation Pipeline (wwPDB-VP) 2.35

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 3.00 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	320	2%	82%			13%		
2	В	76	21% 25%	32%	14%	•	28%		



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3618 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 Ribonuclease Z.

\mathbf{M}	ol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1		A	307	Total 2400	C 1527	N 410	O 456	S 7	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	MET	ILE	engineered mutation	UNP P54548
A	228	MET	LEU	engineered mutation	UNP P54548
A	308	LYS	-	expression tag	UNP P54548
A	309	LEU	-	expression tag	UNP P54548
A	310	ALA	-	expression tag	UNP P54548
A	311	ALA	-	expression tag	UNP P54548
A	312	ALA	-	expression tag	UNP P54548
A	313	LEU	-	expression tag	UNP P54548
A	314	GLU	_	expression tag	UNP P54548
A	315	HIS	-	expression tag	UNP P54548
A	316	HIS	-	expression tag	UNP P54548
A	317	HIS	-	expression tag	UNP P54548
A	318	HIS	-	expression tag	UNP P54548
A	319	HIS	-	expression tag	UNP P54548
A	320	HIS	-	expression tag	UNP P54548

• Molecule 2 is a RNA chain called TRNA(THR).

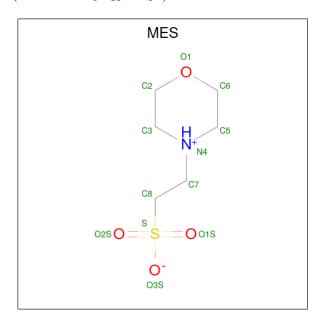
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	55	Total 1172	C 525	N 209	O 384	P 54	0	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Zn 2 2	0	0

• Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	Λ	1	Total	С	N	О	S	0	0
4	A	1	12	6	1	4	1		0

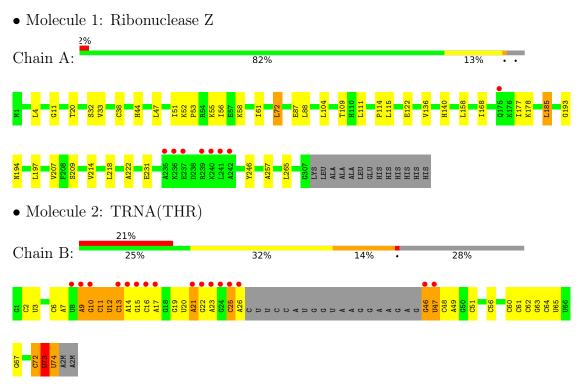
• Molecule 5 is water.

ſ	Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
	5	A	26	Total O 26 26	0	0
	5	В	6	Total O 6 6	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.





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	$174.08\text{\AA} 42.55\text{\AA} 110.89\text{Å}$	Depositor
a, b, c, α , β , γ	90.00° 127.18° 90.00°	Depositor
Resolution (Å)	43.30 - 3.00	Depositor
Resolution (A)	42.44 - 3.00	EDS
% Data completeness	99.1 (43.30-3.00)	Depositor
(in resolution range)	99.1 (42.44-3.00)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) > 1$	2.19 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
D.D.	0.227 , 0.256	Depositor
R, R_{free}	0.244 , 0.281	DCC
R_{free} test set	662 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	65.5	Xtriage
Anisotropy	0.668	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36, 56.5	EDS
L-test for twinning ²	$< L > = 0.48, < L^2> = 0.30$	Xtriage
Estimated twinning fraction	0.024 for -h-2*l,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3618	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.39% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, OMU, ZN

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.36	0/2447	0.60	0/3309	
2	В	0.90	0/1262	1.52	20/1963 (1.0%)	
All	All	0.60	0/3709	1.04	$20/5272 \ (0.4\%)$	

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
2	В	9	A	P-O3'-C3'	11.04	132.94	119.70
2	В	12	U	P-O3'-C3'	10.54	132.35	119.70
2	В	21	A	P-O3'-C3'	9.71	131.35	119.70
2	В	11	С	P-O3'-C3'	9.50	131.09	119.70
2	В	46	G	P-O3'-C3'	9.41	131.00	119.70
2	В	13	С	P-O3'-C3'	7.33	128.50	119.70
2	В	3	U	O4'-C1'-N1	6.08	113.06	108.20
2	В	15	G	P-O3'-C3'	5.85	126.72	119.70
2	В	47	U	C3'-C2'-C1'	5.63	106.00	101.50
2	В	25	С	O4'-C1'-N1	5.55	112.64	108.20
2	В	62	С	O4'-C1'-N1	5.50	112.60	108.20
2	В	51	С	O4'-C1'-N1	5.30	112.44	108.20
2	В	56	С	O4'-C1'-N1	5.30	112.44	108.20
2	В	65	U	O4'-C1'-N1	5.24	112.39	108.20
2	В	13	С	O4'-C1'-N1	5.17	112.34	108.20
2	В	10	G	N9-C1'-C2'	5.16	120.70	114.00
2	В	72	С	O4'-C1'-N1	5.09	112.27	108.20
2	В	19	G	P-O3'-C3'	5.07	125.79	119.70
2	В	64	С	O4'-C1'-N1	5.02	112.22	108.20
2	В	12	U	O4'-C1'-N1	5.02	112.22	108.20

There are no chirality outliers.



There are no planarity outliers.

5.2 Too-close contacts (i)

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	2400	0	2413	18	0
2	В	1172	0	597	1	0
3	A	2	0	0	0	0
4	A	12	0	13	1	0
5	A	26	0	0	0	0
5	В	6	0	0	0	0
All	All	3618	0	3023	19	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 3.

All (19) 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:A:38:CYS:HB3	1:A:72:LEU:HD22	1.81	0.62
1:A:122:GLU:HG3	1:A:136:VAL:HA	1.82	0.60
1:A:87:GLU:HG3	1:A:114:PRO:HB2	1.94	0.49
1:A:53:PRO:HA	1:A:56:ILE:HD12	1.94	0.49
1:A:207:VAL:HG21	1:A:222:ALA:HA	1.96	0.48
1:A:168:ILE:HG23	1:A:185:LEU:HD21	1.95	0.48
1:A:61:ILE:HD11	1:A:72:LEU:HD21	1.95	0.47
1:A:140:HIS:HA	1:A:246:TYR:HB3	1.97	0.47
2:B:72:C:H5"	2:B:73:OMU:H5	1.95	0.47
1:A:257:ALA:HB2	1:A:265:LEU:HD13	1.96	0.46
1:A:178:LYS:HA	1:A:197:LEU:HD21	1.98	0.45
1:A:33:VAL:HG21	1:A:51:ILE:HG23	1.99	0.45
1:A:209:SER:HB2	1:A:218:LEU:HD21	1.97	0.45
1:A:32:SER:HB3	4:A:403:MES:H62	1.99	0.44
1:A:104:LEU:HD23	1:A:111:LEU:HD21	2.00	0.44
1:A:177:ILE:HG23	1:A:193:GLY:HA2	2.01	0.42
1:A:52:LYS:HD2	1:A:55:LYS:HE3	2.02	0.41
1:A:194:ASN:HA	1:A:197:LEU:HD12	2.01	0.41
1:A:44:HIS:HA	1:A:47:LEU:HD12	2.03	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	305/320~(95%)	288 (94%)	16 (5%)	1 (0%)	41 76	

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	GLY

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	258/268 (96%)	247 (96%)	11 (4%)	29 66	

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

Mol	Chain	Res	Type
1	A	4	LEU
1	A	20	THR
1	A	58	LYS
1	A	72	LEU
1	A	88	LEU
1	A	109	THR
1	A	115	LEU

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Mol	Chain	Res	Type
1	A	158	LEU
1	A	185	LEU
1	A	214	VAL
1	A	231	GLU

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

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	В	54/76 (71%)	24 (44%)	9 (16%)

All (24) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	В	2	С
2	В	6	С
2	В	10	G
2	В	11 12	С
2 2 2	В	12	U
2	В	13	С
2	В	14	A
2	В	16	С
2	В	17	A
2 2 2	В	20 21	U
2	В	21	A
2	В	22	G
2	В	23	A
2	В	25	С
2 2 2 2 2	В	26	A
2	В	47	U
2	В	48	С
2	В	49	A
2	В	60	С
2	В	61	С
2	В	63	A U C A C C G
2 2	В	67 73	G
	В		OMU
2	В	74	OMU



All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	В	7	A
2	В	9	A
2	В	11	С
2	В	12	U
2	В	21	A
2	В	46	G
2	В	47	U
2	В	48	С
2	В	60	С

5.4 Non-standard residues in protein, DNA, RNA chains (i)

2 non-standard protein/DNA/RNA residues 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	Dog	Dog	Dog	Dog	Dog	Dog	Ros	Ros	Pog	Dog	Dog	Dog	Pos	Dog	Dog	Dag	Dog	Dog	Link	Bo	ond leng	ths	В	ond ang	les
MOI	туре	Chain		Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2																		
2	OMU	В	74	2	19,22,23	0.58	0	26,31,34	0.77	1 (3%)																		
2	OMU	В	73	2	19,22,23	0.69	0	26,31,34	1.53	3 (11%)																		

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	OMU	В	74	2	-	5/9/27/28	0/2/2/2
2	OMU	В	73	2	-	1/9/27/28	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	73	OMU	CM2-O2'-C2'	4.45	126.19	114.52
2	В	73	OMU	O2'-C2'-C1'	4.18	117.23	109.08
2	В	74	OMU	CM2-O2'-C2'	2.12	120.09	114.52
2	В	73	OMU	C1'-N1-C2	2.01	121.21	117.57

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	73	OMU	C1'-C2'-O2'-CM2
2	В	74	OMU	O4'-C1'-N1-C6
2	В	74	OMU	C2'-C1'-N1-C6
2	В	74	OMU	O4'-C1'-N1-C2
2	В	74	OMU	C2'-C1'-N1-C2
2	В	74	OMU	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	73	OMU	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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 Lin		Bond lengths			Bond angles				
WIOI	Type	Chain	laili ites	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MES	A	403	-	12,12,12	0.69	0	14,16,16	0.37	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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MES	A	403	-	-	2/6/14/14	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	MES	C8-C7-N4-C3
4	A	403	MES	C8-C7-N4-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	MES	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^{th} 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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	307/320 (95%)	0.23	8 (2%) 56 27	44, 63, 90, 105	0
2	В	53/76 (69%)	1.12	16 (30%) 0 0	62, 117, 154, 155	0
All	All	360/396 (90%)	0.36	24 (6%) 17 5	44, 66, 129, 155	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	46	G	4.9
2	В	16	С	4.8
2	В	15	G	4.5
2	В	47	U	3.9
2	В	9	A	3.7
1	A	240	LYS	3.2
2	В	13	С	3.2
1	A	237	GLU	3.2
1	A	242	ALA	3.1
2	В	22	G	3.1
2	В	25	С	3.1
2	В	8	U	3.0
1	A	236	LYS	3.0
2	В	26	A	2.9
2	В	23	A	2.9
1	A	239	ARG	2.7
2	В	10	G	2.6
2	В	24	G	2.6
2	В	17	A	2.4
1	A	241	LEU	2.4
2	В	21	A	2.3
1	A	175	GLN	2.3
2	В	14	A	2.1
1	A	235	ALA	2.0



6.2 Non-standard residues in protein, DNA, RNA chains (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^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	OMU	В	73	21/22	0.79	0.33	106,109,113,113	0
2	OMU	В	74	21/22	0.91	0.26	105,107,110,110	0

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^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
4	MES	A	403	12/12	0.87	0.35	110,111,116,116	0
3	ZN	A	402	1/1	0.96	0.21	68,68,68,68	0
3	ZN	A	401	1/1	0.99	0.18	70,70,70,70	0

6.5 Other polymers (i)

There are no such residues in this entry.

