

wwPDB X-ray Structure Validation Summary Report (i)

Nov 6, 2023 – 02:09 pm GMT

PDB ID	:	7Z4S
Title	:	Crystal structure of SARS-CoV-2 Mpro in complex with cyclic peptide GM4
		including unnatural amino acids.
Authors	:	Owen, C.D.; Miura, T.; Malla, T.; Lukacik, L.; Strain-Damerell, C.M.; Tum-
		ber, A.; Brewitz, L.; McDonough, M.A.; Salah, E.; Terasaka, N.; Katoh, T.;
		Kawamura, A.; Schofield, C.J.; Suga, H.; Walsh, M.A.
Deposited on	:	2022-03-04
Resolution	:	1.70 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* 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:

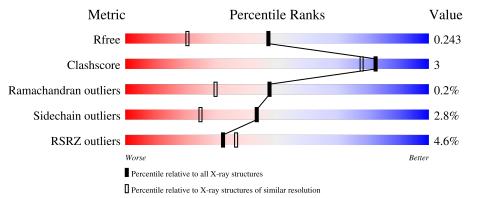
Xtriage (Phenix) EDS Percentile statistics Refmac	: : : :	 1.8.4, CSD as541be (2020) 1.13 2.36 20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158
Ideal geometry (proteins) Ideal geometry (DNA, RNA)	: :	0
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.70 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	А	306	<mark>6%</mark> 93%	7% •
1	В	306	4% 92%	7% •
2	С	15	87%	13%
2	D	15	67% 27%	7%



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 5298 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.

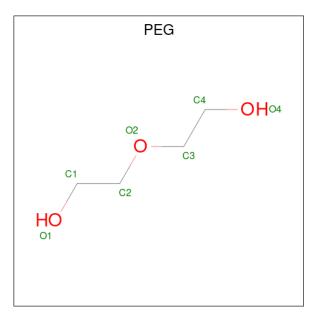
• Molecule 1 is a protein called 3C-like proteinase nsp5.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	306	Total 2390	C 1511	N 405	O 450	S 24	0	3	0
1	В	302	Total 2356	C 1489	N 401	0 443	S 23	0	3	0

• Molecule 2 is a protein called Macrocyclic peptide inhibitor.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
0	С	15	Total	С	Ν	Ο	S	0	0	1
		10	112	74	20	17	1	0		
0	Л	15	Total	С	Ν	Ο	S	0	0	1
	2 D	15	112	74	20	17	1	0		

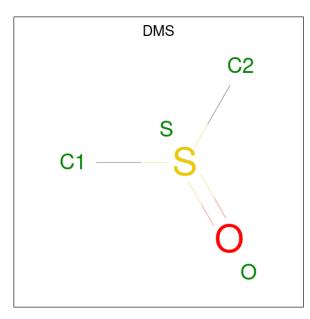
• Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).





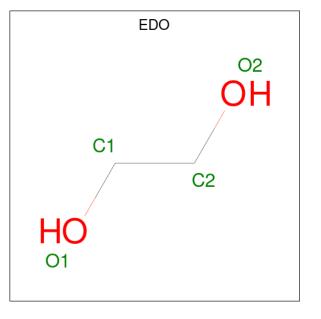
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0

• Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	А	1	Total 4	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	0 1	S 1	0	0

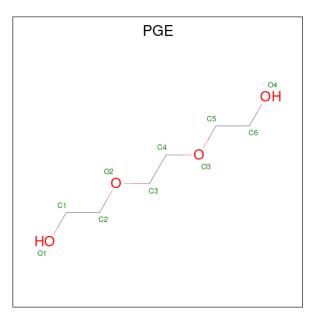
• Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	1	Total C O 10 6 4	0	0

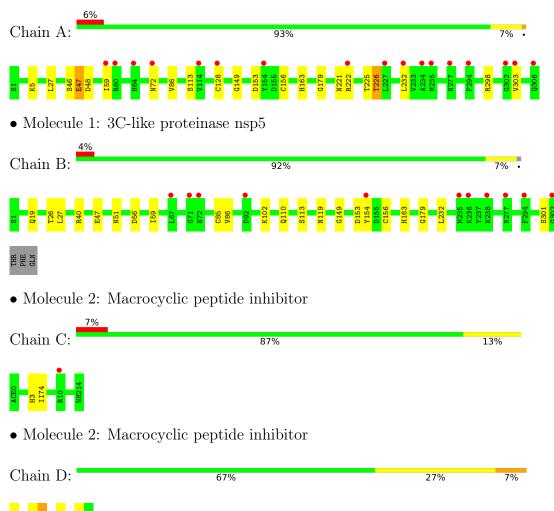
• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	132	Total O 132 132	0	0
7	В	148	Total O 148 148	0	0
7	С	4	Total O 4 4	0	0
7	D	8	Total O 8 8	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: 3C-like proteinase nsp5



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	54.52Å 56.11 Å 63.24 Å	Denesiter
a, b, c, α , β , γ	113.87° 110.53° 90.92°	Depositor
Resolution (Å)	53.23 - 1.70	Depositor
Resolution (A)	$48.82 \ - \ 1.70$	EDS
% Data completeness	99.6 (53.23-1.70)	Depositor
(in resolution range)	98.9 (48.82-1.70)	EDS
R _{merge}	0.13	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.22 (at 1.70 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D D.	0.198 , 0.234	Depositor
R, R_{free}	0.210 , 0.243	DCC
R_{free} test set	3340 reflections $(4.87%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	22.6	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34 , 36.5	EDS
L-test for twinning ²	$< L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.007 for -h,k,-k-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5298	wwPDB-VP
Average B, all atoms $(Å^2)$	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.86% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



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: EDO, ACE, NH2, PEG, PGE, CSO, DMS, DTY, II7

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		
WIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.48	0/2435	0.67	0/3307	
1	В	0.48	0/2400	0.67	0/3260	
2	С	0.41	0/91	0.68	0/120	
2	D	0.48	0/91	0.75	0/120	
All	All	0.48	0/5017	0.67	0/6807	

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
2	С	1	2
2	D	1	2
All	All	2	4

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	С	13	CYS	CA
2	D	13	CYS	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	С	4	II7	Mainchain,Peptide
2	D	4	II7	Mainchain,Peptide



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	А	2390	0	2328	9	0
1	В	2356	0	2299	15	0
2	С	112	0	94	4	0
2	D	112	0	93	2	0
3	А	7	0	10	1	0
3	В	7	0	10	0	0
4	А	4	0	6	0	0
5	В	8	0	12	0	0
6	В	10	0	14	0	0
7	А	132	0	0	0	0
7	В	148	0	0	0	0
7	С	4	0	0	0	0
7	D	8	0	0	0	0
All	All	5298	0	4866	25	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.

The worst 5 of 25 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:102:LYS:NZ	1:B:156:CSO:SG	2.43	0.92
1:B:163:HIS:HE1	2:C:3:HIS:HD2	1.19	0.90
1:B:163:HIS:HE1	2:C:3:HIS:CD2	2.02	0.77
1:B:163:HIS:CE1	2:C:3:HIS:HD2	2.06	0.74
1:B:19:GLN:HE21	1:B:26:THR:HG21	1.61	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	Perce	ntiles
1	А	306/306~(100%)	302~(99%)	4 (1%)	0	100	100
1	В	302/306~(99%)	299~(99%)	3~(1%)	0	100	100
2	\mathbf{C}	11/15~(73%)	9~(82%)	2(18%)	0	100	100
2	D	11/15~(73%)	9~(82%)	1 (9%)	1 (9%)	1	0
All	All	630/642~(98%)	619~(98%)	10~(2%)	1 (0%)	47	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	13	CYS

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	ysed Rotameric Outliers		Percentiles		
1	А	265/262~(101%)	254~(96%)	11 (4%)	30 12		
1	В	261/262~(100%)	255~(98%)	6(2%)	50 33		
2	С	9/9~(100%)	9 (100%)	0	100 100		
2	D	9/9~(100%)	9~(100%)	0	100 100		
All	All	544/542~(100%)	527~(97%)	17 (3%)	43 21		

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	110[A]	GLN
1	В	301	SER
1	А	221	ASN
1	А	222	ARG
1	А	226	THR



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	119	ASN
1	В	163	HIS
2	D	3	HIS
1	В	273	GLN
2	С	3	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 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	Mol Type Chain Res		Link	Bond lengths			Bond angles			
	Type	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
1	CSO	А	156	1	3,6,7	0.89	0	$0,\!6,\!8$	-	-
2	II7	D	4	2	7,7,8	0.63	0	4,9,11	1.52	1 (25%)
2	II7	С	4	2	7,7,8	0.57	0	4,9,11	1.41	0
1	CSO	В	156	1	3,6,7	1.04	0	0,6,8	-	-

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
1	CSO	А	156	1	-	0/1/5/7	-
2	II7	D	4	2	-	0/0/10/12	0/1/1/1
2	II7	С	4	2	-	0/0/10/12	0/1/1/1
1	CSO	В	156	1	-	0/1/5/7	-



There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	D	4	II7	C4-C3-C2	2.19	89.90	86.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	А	156	CSO	1	0
1	В	156	CSO	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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).

Mal		una Chain Bag		Tinle	B	Bond lengths			Bond angles		
		Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	gles # Z > 2 0 0 0 0 0		
5	EDO	В	402	-	$3,\!3,\!3$	0.19	0	$2,\!2,\!2$	0.22	0	
3	PEG	В	401	-	6,6,6	0.15	0	$5,\!5,\!5$	0.14	0	
6	PGE	В	403	-	9,9,9	0.26	0	8,8,8	0.16	0	
3	PEG	А	401	-	$6,\!6,\!6$	0.23	0	$5,\!5,\!5$	0.18	0	
5	EDO	В	404	-	3,3,3	0.04	0	2,2,2	0.11	0	
4	DMS	А	402	-	3,3,3	0.30	0	3,3,3	0.13	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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	В	402	-	-	0/1/1/1	-
3	PEG	В	401	-	-	2/4/4/4	-
6	PGE	В	403	-	-	5/7/7/7	-
3	PEG	А	401	-	-	0/4/4/4	-
5	EDO	В	404	-	-	1/1/1/1	-

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	В	403	PGE	O2-C3-C4-O3
6	В	403	PGE	O1-C1-C2-O2
3	В	401	PEG	O2-C3-C4-O4
6	В	403	PGE	O3-C5-C6-O4
6	В	403	PGE	C1-C2-O2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	401	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^{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 $>$	#RSRZ>2	$OWAB(Å^2)$	$\mathbf{Q}{<}0.9$
1	А	305/306~(99%)	0.43	17 (5%) 24 27	22, 33, 57, 74	0
1	В	301/306~(98%)	0.14	11 (3%) 41 46	21, 33, 56, 79	0
2	С	11/15~(73%)	0.93	1 (9%) 9 10	32, 43, 57, 66	0
2	D	11/15~(73%)	0.04	0 100 100	28, 30, 35, 51	0
All	All	628/642~(97%)	0.29	29 (4%) 32 36	21, 33, 57, 79	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	154	TYR	7.1
1	А	232	LEU	5.0
1	А	235	MET	3.7
1	В	302	GLY	3.4
1	А	72	ASN	3.2

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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q < 0.9
2	II7	D	4	7/8	0.89	0.10	25,30,32,34	0
2	II7	С	4	7/8	0.90	0.14	36,37,40,41	0
2	DTY	С	1	12/13	0.93	0.08	28,34,38,38	0
2	DTY	D	1	12/13	0.94	0.09	22,26,33,34	0
1	CSO	В	156	7/8	0.96	0.08	29,34,37,39	0
1	CSO	А	156	7/8	0.97	0.11	30,35,37,39	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	B-factors(Å ²)	Q<0.9
6	PGE	В	403	10/10	0.66	0.16	$50,\!54,\!60,\!61$	0
3	PEG	В	401	7/7	0.80	0.15	45,49,61,65	0
3	PEG	А	401	7/7	0.85	0.15	34,39,56,56	0
5	EDO	В	404	4/4	0.90	0.11	56,67,67,69	0
4	DMS	А	402	4/4	0.95	0.14	42,46,52,53	0
5	EDO	В	402	4/4	0.96	0.12	35,41,41,49	0

6.5 Other polymers (i)

There are no such residues in this entry.

