

wwPDB X-ray Structure Validation Summary Report (i)

Oct 3, 2023 – 07:10 PM EDT

PDB ID : 6MTG

Title : A Single Reactive Noncanonical Amino Acid is Able to Dramatically Stabilize

Protein Structure

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Deposited on : 2018-10-19

Resolution : 1.85 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:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

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

Xtriage (Phenix) : 1.13 EDS : 2.35.1

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

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

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

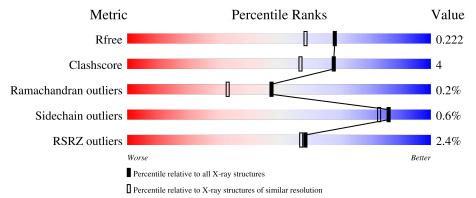
Validation Pipeline (wwPDB-VP) : 2.35.1

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 1.85 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	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	302	88%	7% • •	
1	В	302	92%		

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	PEG	A	402	_	-	X	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5388 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 Homoserine O-succinyltransferase.

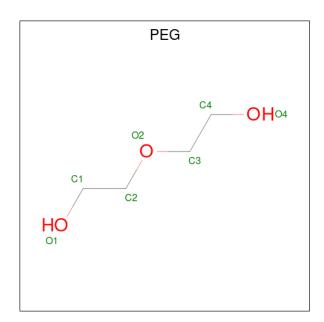
\mathbf{Mol}	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	291	Total 2382	C 1538	N 395	O 445	S 4	0	4	0
1	В	292	Total 2426		N 415	O 447	S 4	0	9	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	ILE	PRO	engineered mutation	UNP P07623
A	297	HIS	-	expression tag	UNP P07623
A	298	HIS	-	expression tag	UNP P07623
A	299	HIS	-	expression tag	UNP P07623
A	300	HIS	-	expression tag	UNP P07623
A	301	HIS	-	expression tag	UNP P07623
A	302	HIS	-	expression tag	UNP P07623
В	257	ILE	PRO	engineered mutation	UNP P07623
В	297	HIS	-	expression tag	UNP P07623
В	298	HIS	-	expression tag	UNP P07623
В	299	HIS	-	expression tag	UNP P07623
В	300	HIS	-	expression tag	UNP P07623
В	301	HIS	-	expression tag	UNP P07623
В	302	HIS	-	expression tag	UNP P07623

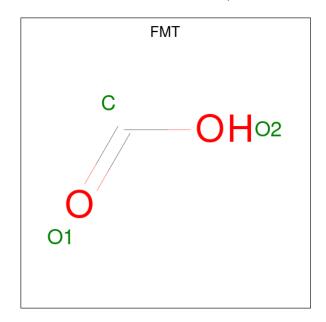
• Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).





M	lol	Chain	Residues	Atoms	ZeroOcc	AltConf
	2	A	1	Total C O 7 4 3	0	0
	2	A	1	Total C O 7 4 3	0	0

 \bullet Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: $\mathrm{CH_2O_2}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0

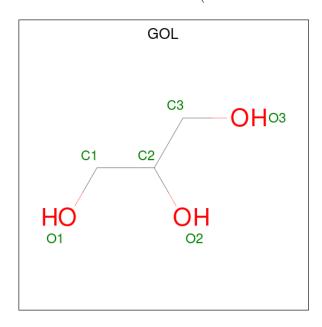
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total C O 3 1 2	0	0
3	В	1	Total C O 3 1 2	0	0
3	В	1	Total C O 3 1 2	0	0

 \bullet Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $\mathrm{C_3H_8O_3}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	Total C O 6 3 3	0	0

• Molecule 5 is water.

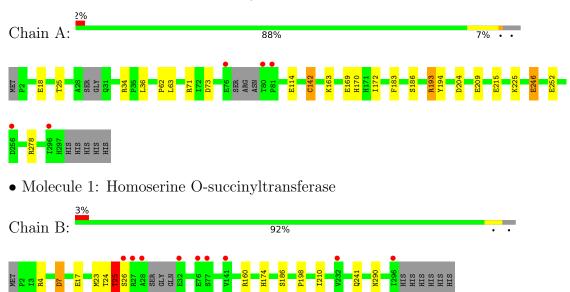
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	284	Total O 284 284	0	0
5	В	260	Total O 261 261	0	1



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: Homoserine O-succinyltransferase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	51.95Å 100.04Å 125.22Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.89 - 1.85	Depositor
Resolution (A)	29.88 - 1.85	EDS
% Data completeness	99.1 (29.89-1.85)	Depositor
(in resolution range)	99.1 (29.88-1.85)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) > 1$	1.89 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
P. P.	0.169 , 0.218	Depositor
R, R_{free}	0.179 , 0.222	DCC
R_{free} test set	2829 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31, 38.1	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5388	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.25% 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: PEG, CSD, GOL, FMT

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).

Mal	Chain		nd lengths	Bond angles		
IVIOI	Mol Chain		# Z > 5	RMSZ	# Z > 5	
1	A	0.99	$4/2446 \ (0.2\%)$	1.06	8/3338 (0.2%)	
1	В	0.93	$1/2489 \ (0.0\%)$	1.01	2/3394 (0.1%)	
All	All	0.96	5/4935 (0.1%)	1.03	10/6732 (0.1%)	

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	В	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	A	246	GLU	CD-OE2	7.30	1.33	1.25
1	A	246	GLU	CD-OE1	7.29	1.33	1.25
1	A	114	GLU	CD-OE2	-6.54	1.18	1.25
1	В	186	SER	CB-OG	-5.92	1.34	1.42
1	A	172	ILE	C-O	5.42	1.33	1.23

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	160	ARG	NE-CZ-NH1	-9.07	115.76	120.30
1	A	204	ASP	CB-CG-OD1	8.15	125.64	118.30
1	В	160	ARG	NE-CZ-NH2	7.11	123.86	120.30
1	A	71	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	193	ARG	NE-CZ-NH2	-5.78	117.41	120.30



There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Chain Res		Group	
1	В	25[A]	THR	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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	2382	0	2273	14	0
1	В	2426	0	2325	20	0
2	A	14	0	19	5	0
3	A	6	0	2	0	0
3	В	9	0	3	0	0
4	В	6	0	8	3	0
5	A	284	0	0	8	0
5	В	261	0	0	6	0
All	All	5388	0	4630	36	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 4.

The worst 5 of 36 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:B:174:HIS:NE2	4:B:401:GOL:H11	1.64	1.11
1:B:4[B]:ARG:HD3	1:B:25[B]:THR:HG22	1.60	0.84
1:B:4[B]:ARG:CD	1:B:25[B]:THR:HG22	2.14	0.77
1:B:4[B]:ARG:HD3	1:B:25[B]:THR:HA	1.75	0.68
2:A:402:PEG:H42	5:B:604:HOH:O	1.94	0.67

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	hain Analysed Favoured Allowed		Outliers	Perce	ntiles	
1	A	$288/302 \ (95\%)$	281 (98%)	7 (2%)	0	100	100
1	В	295/302~(98%)	288 (98%)	5 (2%)	2 (1%)	22	9
All	All	583/604 (96%)	569 (98%)	12 (2%)	2 (0%)	47	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	25[A]	THR
1	В	25[B]	THR

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	254/269 (94%)	252 (99%)	2 (1%)	81 76		
1	В	256/269 (95%)	253 (99%)	3 (1%)	71 62		
All	All	510/538 (95%)	505 (99%)	5 (1%)	86 69		

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252[A]	GLU
1	A	252[B]	GLU
1	В	7[A]	ASP
1	В	7[B]	ASP

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Mol	Chain	Res	Type
1	В	198	PRO

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)

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 Chai		Chain	Dec	Link	В	ond leng	gths	Bond angles		
MIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	A	142	1	3,7,8	1.06	0	1,8,10	2.66	1 (100%)
1	CSD	В	142	1	3,7,8	1.29	0	1,8,10	0.97	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.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	A	142	1	-	1/2/6/8	-
1	CSD	В	142	1	-	2/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	142	CSD	OD1-SG-CB	2.66	110.61	105.54



There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	В	142	CSD	N-CA-CB-SG
1	В	142	CSD	CA-CB-SG-OD1
1	A	142	CSD	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	142	CSD	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	Mol Type Chain F		Res	Res Link	В	Bond lengths			Bond angles		
MIOI	Type	Chain	rtes	LILIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
2	PEG	A	402	-	6,6,6	0.72	0	5,5,5	0.73	0	
3	FMT	A	404	-	2,2,2	0.30	0	1,1,1	0.22	0	
3	FMT	В	402	-	2,2,2	0.65	0	1,1,1	0.03	0	
3	FMT	В	403	-	2,2,2	0.88	0	1,1,1	0.15	0	
2	PEG	A	401	-	6,6,6	0.21	0	5,5,5	0.30	0	
3	FMT	A	403	-	2,2,2	0.23	0	1,1,1	0.04	0	
3	FMT	В	404	-	2,2,2	0.24	0	1,1,1	0.14	0	
4	GOL	В	401	-	5,5,5	0.11	0	5,5,5	0.55	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.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	A	402	-	-	3/4/4/4	_
4	GOL	В	401	-	-	0/4/4/4	-
2	PEG	A	401	-	-	3/4/4/4	_

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	PEG	C1-C2-O2-C3
2	A	401	PEG	O1-C1-C2-O2
2	A	402	PEG	O2-C3-C4-O4
2	A	402	PEG	O1-C1-C2-O2
2	A	401	PEG	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	PEG	5	0
4	В	401	GOL	3	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	290/302 (96%)	-0.25	5 (1%) 70 70	19, 26, 49, 74	0
1	В	291/302~(96%)	-0.20	9 (3%) 49 47	18, 28, 51, 77	0
All	All	581/604 (96%)	-0.22	14 (2%) 59 57	18, 27, 49, 77	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	THR	5.2
1	A	81	PRO	5.2
1	В	28[A]	ALA	4.4
1	В	27[A]	ARG	3.4
1	В	296	ILE	3.0

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
1	CSD	A	142	8/9	0.96	0.12	24,27,42,51	0
1	CSD	В	142	8/9	0.96	0.12	23,31,43,47	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	GOL	В	401	6/6	0.75	0.21	38,46,53,59	6
3	FMT	В	404	3/3	0.86	0.12	57,57,58,62	0
3	FMT	A	404	3/3	0.89	0.20	48,48,48,49	0
2	PEG	A	401	7/7	0.89	0.20	47,52,56,57	0
2	PEG	A	402	7/7	0.89	0.25	23,32,34,40	7
3	FMT	В	403	3/3	0.91	0.15	31,31,43,55	0
3	FMT	В	402	3/3	0.96	0.14	30,30,38,45	0
3	FMT	A	403	3/3	0.97	0.10	24,24,29,30	0

6.5 Other polymers (i)

There are no such residues in this entry.

