

wwPDB X-ray Structure Validation Summary Report (i)

Sep 17, 2023 – 06:38 PM EDT

PDB ID : 4XES

Title : Structure of active-like neurotensin receptor

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Deposited on : 2014-12-24

Resolution : 2.60 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:

MolProbity : 4.02b-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)

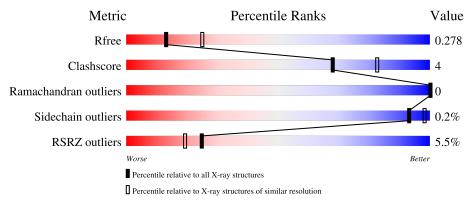
Validation Pipeline (wwPDB-VP) : 2.35.1

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 >=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	541	80%	7%	13%
2	В	6	17%		



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3923 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 Neurotensin receptor type 1, Endolysin chimera.

\mathbf{Mol}	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace	
1	Δ	471	Total	С	N	О	S	164	0	0	
1	11	711	3714	2409	634	652	19	104	U		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	ASP	-	expression tag	UNP P20789
A	34	TYR	-	expression tag	UNP P20789
A	35	LYS	-	expression tag	UNP P20789
A	36	ASP	-	expression tag	UNP P20789
A	37	ASP	-	expression tag	UNP P20789
A	38	ASP	-	expression tag	UNP P20789
A	39	ASP	-	expression tag	UNP P20789
A	40	ALA	-	expression tag	UNP P20789
A	41	THR	-	expression tag	UNP P20789
A	42	SER	-	expression tag	UNP P20789
A	86	LEU	ALA	engineered mutation	UNP P20789
A	166	ALA	GLU	engineered mutation	UNP P20789
A	215	ALA	GLY	engineered mutation	UNP P20789
A	360	ALA	VAL	engineered mutation	UNP P20789
A	989	ALA	-	linker	UNP P20789
A	990	HIS	-	linker	UNP P20789
A	991	HIS	-	linker	UNP P20789
A	992	HIS	-	linker	UNP P20789
A	993	HIS	-	linker	UNP P20789
A	994	HIS	-	linker	UNP P20789
A	995	HIS	-	linker	UNP P20789
A	996	HIS	-	linker	UNP P20789
A	997	HIS	-	linker	UNP P20789
A	998	HIS	-	linker	UNP P20789
A	999	HIS	-	linker	UNP P20789
A	1000	GLY	-	linker	UNP P20789
A	1001	GLY	-	linker	UNP P20789

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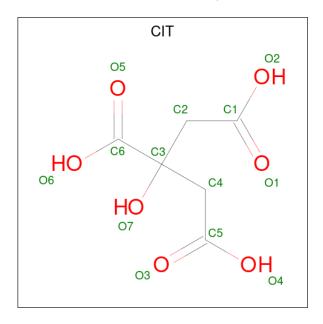
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Chain	Residue	Modelled	Actual	Comment	Reference
A	1012	GLY	ARG	conflict	UNP P00720
A	1054	THR	CYS	conflict	UNP P00720
A	1097	ALA	CYS	$\operatorname{conflict}$	UNP P00720
A	1122	ASN	GLN	conflict	UNP P00720
A	1123	ASN	GLN	$\operatorname{conflict}$	UNP P00720
A	1137	ARG	ILE	conflict	UNP P00720
A	1162	GLY	-	expression tag	UNP P00720
A	1163	SER	-	expression tag	UNP P00720
A	1164	GLY	-	expression tag	UNP P00720
A	1165	SER	-	expression tag	UNP P00720

• Molecule 2 is a protein called Neurotensin/neuromedin N.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
2	В	6	Total 58	C 38	N 12	O 8	0	0	0

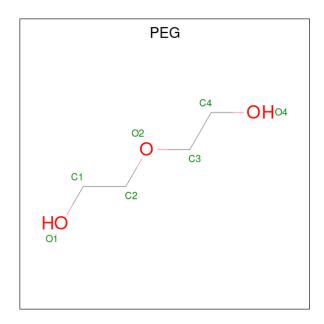
 \bullet Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: $\mathrm{C_6H_8O_7}).$



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total (C O 5 7	0	0

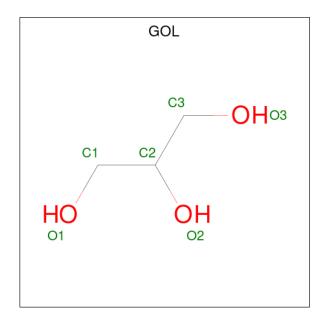
 $\bullet \ \, \text{Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$)}. \\$





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
1	Δ	1	Total C O	0	0	
-1	11	1	7 4 3	U	O O	
1	A	1	Total C O	0	0	
4	Λ	1	7 4 3	U	0	
1	A	1	Total C O	0	0	
4	Λ	1	7 4 3			
1	Λ	1	Total C O	0	0	
4	Λ	Λ 1	7 4 3	0	U	
1	Λ	A 1	Total C O	0	0	
4	A		7 4 3	U		

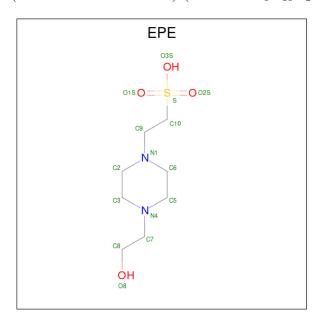
 \bullet Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $\mathrm{C_3H_8O_3}).$





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0

• Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf		
6	Λ	1	Total	С	N	О	S	0	0
0	0 A	1	15	8	2	4	1	0	
6	Λ	1	Total	С	N	О	S	0	0
	A	1	15	8	2	4	1		

• Molecule 7 is water.

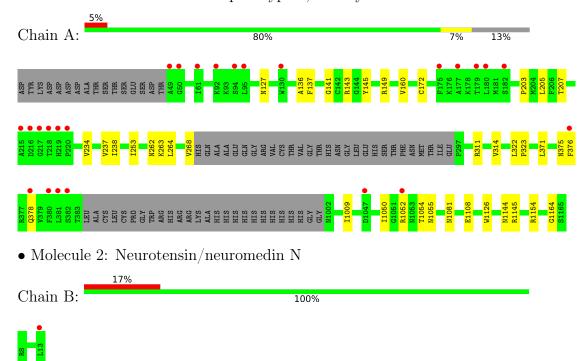
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	53	Total O 53 53	0	0
7	В	2	Total O 2 2	0	0



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: Neurotensin receptor type 1, Endolysin chimera





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants	49.84Å 88.44Å 161.33Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.00 - 2.60	Depositor
rtesolution (A)	34.16 - 2.60	EDS
% Data completeness	99.3 (34.00-2.60)	Depositor
(in resolution range)	99.4 (34.16-2.60)	EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.68 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
D D.	0.230 , 0.280	Depositor
R, R_{free}	0.235 , 0.278	DCC
R_{free} test set	1209 reflections (5.36%)	wwPDB-VP
Wilson B-factor (Å ²)	56.3	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.30 , 54.7	EDS
L-test for twinning ²	$ < L > = 0.47, < L^2> = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3923	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.67% 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: CIT, EPE, GOL, PEG

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	Cilaiii	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.49	0/3797	0.63	0/5159	
2	В	0.41	0/59	0.56	0/77	
All	All	0.48	0/3856	0.63	0/5236	

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 (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	3714	0	3787	28	0
2	В	58	0	63	0	0
3	A	13	0	5	0	0
4	A	35	0	50	1	0
5	A	18	0	24	2	0
6	A	30	0	36	0	0
7	A	53	0	0	1	0
7	В	2	0	0	0	0
All	All	3923	0	3965	28	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 28 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ (\rm \mathring{A}) \end{array}$	$egin{aligned} \operatorname{Clash} \ \operatorname{overlap}\ (ext{Å}) \end{aligned}$
1:A:234:VAL:O	1:A:238:ILE:HG13	1.83	0.78
1:A:1052:ARG:HG2	1:A:1052:ARG:HH11	1.56	0.68
1:A:371:LEU:HA	7:A:1335:HOH:O	1.94	0.66
1:A:1009:ILE:HD11	1:A:1164:GLY:HA2	1.77	0.66
1:A:1052:ARG:HG2	1:A:1052:ARG:NH1	2.08	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	A	465/541~(86%)	443 (95%)	22 (5%)	0	100	100
2	В	4/6 (67%)	4 (100%)	0	0	100	100
All	All	469/547 (86%)	447 (95%)	22 (5%)	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.

\mathbf{Mol}	Chain	Analysed	Analysed Rotameric Outliers		Percentiles	
1	A	400/459 (87%)	399 (100%)	1 (0%)	92 98	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
2	В	6/6 (100%)	6 (100%)	0	100	100	
All	All	406/465 (87%)	405 (100%)	1 (0%)	93	98	

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	376	PHE

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 (i)

11 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).

	Mol	Type	Chain	Dag	Link	Bond lengths			Bond angles		
	IVIOI	туре	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
	4	PEG	A	1204	-	6,6,6	0.29	0	5,5,5	0.35	0
Ī	4	PEG	A	1203	-	6,6,6	0.68	0	5,5,5	0.55	0



Mol	Tuno	Chain	Res	Link	Вс	ond leng	ths	В	ond ang	les
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EPE	A	1210	-	15,15,15	2.09	1 (6%)	18,20,20	1.30	2 (11%)
4	PEG	A	1202	-	6,6,6	0.57	0	5,5,5	0.17	0
5	GOL	A	1209	-	5,5,5	0.17	0	5,5,5	0.62	0
5	GOL	A	1208	-	5,5,5	0.37	0	5,5,5	0.20	0
5	GOL	A	1207	-	5,5,5	0.36	0	5,5,5	0.33	0
3	CIT	A	1201	-	12,12,12	1.08	0	17,17,17	1.58	2 (11%)
4	PEG	A	1205	-	6,6,6	0.55	0	5,5,5	0.11	0
6	EPE	A	1211	-	15,15,15	1.89	1 (6%)	18,20,20	1.29	2 (11%)
4	PEG	A	1206	-	6,6,6	0.65	0	5,5,5	0.57	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
4	PEG	A	1204	-	-	3/4/4/4	-
4	PEG	A	1203	-	-	1/4/4/4	-
6	EPE	A	1210	-	-	6/9/19/19	0/1/1/1
4	PEG	A	1202	-	-	2/4/4/4	-
5	GOL	A	1209	-	-	3/4/4/4	-
5	GOL	A	1208	-	-	4/4/4/4	-
5	GOL	A	1207	-	-	2/4/4/4	-
3	CIT	A	1201	-	-	9/16/16/16	-
4	PEG	A	1205	-	-	2/4/4/4	-
6	EPE	A	1211	-	-	5/9/19/19	0/1/1/1
4	PEG	A	1206	-	-	3/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
6	A	1210	EPE	C10-S	-7.65	1.66	1.77
6	A	1211	EPE	C10-S	-6.91	1.67	1.77

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
3	A	1201	CIT	O6-C6-C3	4.00	119.99	113.05
6	A	1211	EPE	O1S-S-C10	3.61	111.26	106.92

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
6	A	1210	EPE	O2S-S-C10	3.37	110.98	106.92
3	A	1201	CIT	O5-C6-C3	-3.17	117.76	122.25
6	A	1211	EPE	O3S-S-C10	3.13	110.83	105.77

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1201	CIT	C1-C2-C3-O7
3	A	1201	CIT	C1-C2-C3-C4
3	A	1201	CIT	C1-C2-C3-C6
5	A	1207	GOL	C1-C2-C3-O3
5	A	1208	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1203	PEG	1	0
5	A	1209	GOL	2	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	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$		$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	A	471/541 (87%)	0.18	25 (5%) 26	20	29, 63, 88, 108	53 (11%)
2	В	6/6 (100%)	0.47	1 (16%) 1	1	49, 52, 61, 69	0
All	All	477/547 (87%)	0.19	26 (5%) 25	19	29, 63, 88, 108	53 (11%)

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	381	LEU	4.8
1	A	175	PHE	4.6
1	A	95	LEU	4.4
1	A	94	SER	3.9
1	A	382	SER	3.7

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^{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	$ m B ext{-}factors(\AA^2)$	Q<0.9
4	PEG	A	1206	7/7	0.73	0.30	63,64,72,74	0
5	GOL	A	1207	6/6	0.79	0.23	69,73,74,77	0
6	EPE	A	1211	15/15	0.80	0.26	82,92,113,121	0
4	PEG	A	1202	7/7	0.81	0.17	58,60,62,63	0
4	PEG	A	1204	7/7	0.84	0.29	86,88,94,95	0
4	PEG	A	1205	7/7	0.85	0.24	73,76,78,78	0
4	PEG	A	1203	7/7	0.88	0.22	48,56,60,64	0
5	GOL	A	1208	6/6	0.90	0.32	64,70,73,74	0
5	GOL	A	1209	6/6	0.92	0.21	56,57,64,68	0
3	CIT	A	1201	13/13	0.92	0.20	51,56,62,62	0
6	EPE	A	1210	15/15	0.94	0.16	47,49,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.

