

wwPDB X-ray Structure Validation Summary Report (i)

Sep 6, 2023 – 02:56 PM EDT

PDB ID	:	4FL8
Title	:	HIV-1 protease complexed with gem-diol-amine tetrahedral intermediate
Authors	:	Tie, Y.F.; Shen, C.H.; Weber, I.T.
Deposited on		
Resolution	:	1.20 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:

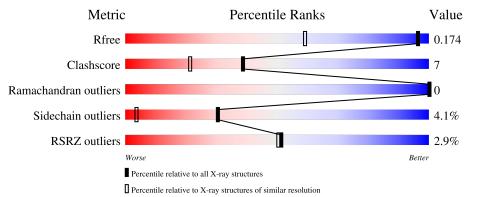
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.20 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	1223 (1.22-1.18)
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)
RSRZ outliers	127900	1200 (1.22-1.18)

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		Quali	ty of chain		
1	А	99	%	88%			9% ••
1	В	99		85%			13% •
2	С	7	29%	14%	29%	29	9%
3	D	7	43%		29%	14%	14%

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
5	GOL	А	104[A]	-	-	Х	-



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 1973 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Λ	99	Total	С	Ν	0	S	0	10	0
	A	99	805	529	136	137	3	0		
1	В	99	Total	С	Ν	0	S	0	16	0
1	D	99	845	560	138	144	3	0		

• Molecule 1 is a protein called HIV-1 protease.

Thora are 10 d	liceroponeios	hotwoon	the modelled	and	reference sequences:
There are 10 u	inscrepancies	Detween	the modelled	anu	reference sequences.

Chain	Residue	Modelled	Actual	Comment	Reference
А	7	LYS	GLN	engineered mutation	UNP P03367
А	33	ILE	LEU	engineered mutation	UNP P03367
А	63	ILE	LEU	engineered mutation	UNP P03367
А	67	ALA	CYS	engineered mutation	UNP P03367
А	95	ALA	CYS	engineered mutation	UNP P03367
В	7	LYS	GLN	engineered mutation	UNP P03367
В	33	ILE	LEU	engineered mutation	UNP P03367
В	63	ILE	LEU	engineered mutation	UNP P03367
В	67	ALA	CYS	engineered mutation	UNP P03367
В	95	ALA	CYS	engineered mutation	UNP P03367

• Molecule 2 is a protein called heptapeptide.

Mol	Chain	Residues	A	4ton	ns		ZeroOcc	AltConf	Trace
2	С	7	Total 52	$\begin{array}{c} \mathrm{C} \\ 35 \end{array}$	N 7	O 10	0	7	0

• Molecule 3 is a protein called heptapeptide.

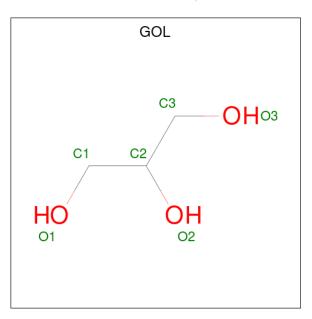
Mol	Chain	Residues	I	Aton	ns		ZeroOcc	AltConf	Trace
3	D	7	Total 56	$\begin{array}{c} \mathrm{C} \\ 35 \end{array}$		O 13	0	7	0

• Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	3	Total Cl 3 3	0	0
4	В	2	Total Cl 2 2	0	0

• Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	1
5	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

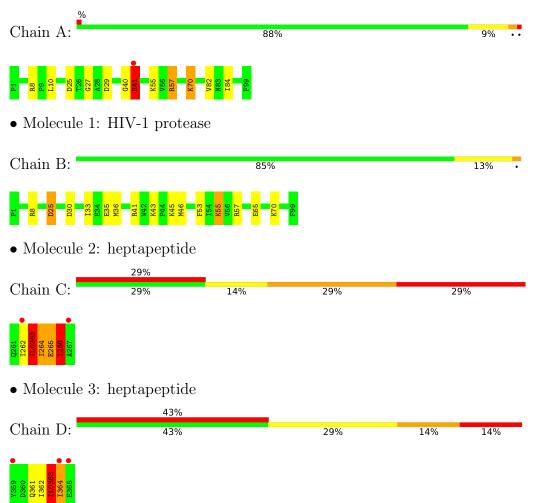
• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	91	Total O 91 91	0	0
6	В	100	Total O 100 100	0	0
6	С	2	Total O 2 2	0	0
6	D	5	Total O 5 5	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: HIV-1 protease



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	58.41Å 86.20Å 46.36Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 - 1.20	Depositor
Resolution (A)	34.68 - 1.20	EDS
% Data completeness	94.5 (10.00-1.20)	Depositor
(in resolution range)	88.9 (34.68-1.20)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$4.77 (at 1.20 \text{\AA})$	Xtriage
Refinement program	SHELXL-97	Depositor
D D.	0.142 , 0.176	Depositor
R, R_{free}	0.144 , 0.174	DCC
R_{free} test set	3506 reflections $(5.01%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	11.6	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.35, 59.1	EDS
L-test for twinning ²	$ \langle L \rangle = 0.49, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	1973	wwPDB-VP
Average B, all atoms $(Å^2)$	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.96% 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: GOL, CL, IL0 $\,$

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	Bo	ond angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.79	0/853	1.29	7/1149~(0.6%)
1	В	0.71	0/913	1.32	7/1231~(0.6%)
2	С	0.72	0/41	2.22	3/53~(5.7%)
3	D	0.48	0/45	1.64	0/58
All	All	0.75	0/1852	1.34	17/2491~(0.7%)

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	0	3
3	D	0	2
All	All	0	5

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	В	8[A]	ARG	CD-NE-CZ	10.22	137.91	123.60
1	В	8[B]	ARG	CD-NE-CZ	10.22	137.91	123.60
1	А	57[A]	ARG	CD-NE-CZ	9.43	136.79	123.60
1	А	57[B]	ARG	CD-NE-CZ	9.43	136.79	123.60
1	А	29	ASP	CB-CG-OD1	8.59	126.03	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
2	С	263[A]	IL0	Peptide,Mainchain
2	С	266[A]	ILE	Peptide
3	D	363[B]	IL0	Peptide,Mainchain

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	805	0	898	12	0
1	В	845	0	961	13	0
2	С	52	0	43	4	0
3	D	56	0	39	4	0
4	А	3	0	0	0	0
4	В	2	0	0	0	0
5	А	6	0	8	4	0
5	В	6	0	8	0	0
6	А	91	0	0	4	0
6	В	100	0	0	3	0
6	С	2	0	0	0	0
6	D	5	0	0	2	0
All	All	1973	0	1957	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 7.

The worst 5 of 28 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:35[B]:GLU:HG2	6:B:629:HOH:O	1.82	0.80
1:B:45[A]:LYS:HE3	6:B:688:HOH:O	1.83	0.78
2:C:266[A]:ILE:HG13	6:D:402:HOH:O	1.84	0.78
1:B:46[A]:MET:SD	1:B:55:LYS:HG2	2.25	0.76
1:B:46[A]:MET:SD	1:B:55:LYS:HE2	2.28	0.73

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	Percer	ntiles
1	А	107/99~(108%)	107~(100%)	0	0	100	100
1	В	114/99~(115%)	114 (100%)	0	0	100	100
2	\mathbf{C}	4/7~(57%)	3~(75%)	1 (25%)	0	100	100
3	D	4/7~(57%)	3~(75%)	1 (25%)	0	100	100
All	All	229/212~(108%)	227~(99%)	2(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 side chain 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	А	91/81~(112%)	88~(97%)	3~(3%)	38 5
1	В	98/81 (121%)	95~(97%)	3(3%)	40 6
2	С	4/5~(80%)	2~(50%)	2 (50%)	0 0
3	D	5/6~(83%)	4 (80%)	1 (20%)	1 0
All	All	198/173~(114%)	189~(96%)	9~(4%)	30 3

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	С	264[A]	ILE
3	D	364[B]	ILE
1	В	43[A]	LYS

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Mol	Chain	Res	Type
1	В	43[B]	LYS
1	В	55	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	2	GLN
1	А	18	GLN
1	А	98	ASN
1	В	2	GLN
1	В	98	ASN

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	Turne	Chain	Dec	Tinle	Bond lengths			Bond angles		
IVIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	IL0	D	363[B]	3	7,8,8	0.83	0	$5,\!10,\!10$	1.88	1 (20%)
2	ILO	С	263[A]	2	7,8,8	0.60	0	5,10,10	1.91	1 (20%)

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
3	ILO	D	363[B]	3	-	10/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IL0	С	263[A]	2	-	7/10/10/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	263[A]	IL0	OXT-C-O	-4.11	104.03	111.27
3	D	363[B]	IL0	OXT-C-O	-3.95	104.32	111.27

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	С	263[A]	IL0	O-C-CA-CB
2	С	263[A]	IL0	N-CA-CB-CG1
2	С	263[A]	IL0	N-CA-CB-CG2
2	С	263[A]	IL0	C-CA-CB-CG1
3	D	363[B]	IL0	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

	Mol	Chain	Res	Type	Clashes	Symm-Clashes
	3	D	363[B]	IL0	1	0
ſ	2	С	263[A]	IL0	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 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



	Mol	Type	Chain	Res	Res Link Bond lengths				Bond angles		
	10101	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
ſ	5	GOL	А	104[A]	-	$5,\!5,\!5$	0.84	0	$5,\!5,\!5$	1.38	1 (20%)
	5	GOL	В	503	-	$5,\!5,\!5$	0.78	0	$5,\!5,\!5$	1.13	1 (20%)

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).

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
5	GOL	А	104[A]	-	-	1/4/4/4	-
5	GOL	В	503	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	А	104[A]	GOL	C3-C2-C1	-2.56	101.75	111.70
5	В	503	GOL	C3-C2-C1	-2.07	103.67	111.70

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	А	104[A]	GOL	O1-C1-C2-C3
5	В	503	GOL	C1-C2-C3-O3
5	В	503	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	104[A]	GOL	4	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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	$Q{<}0.9$
1	А	99/99~(100%)	-0.17	1 (1%) 82 82	9, 15, 32, 56	0
1	В	99/99~(100%)	-0.27	0 100 100	9, 15, 26, 31	0
2	С	6/7~(85%)	2.24	2(33%) 0 1	18, 25, 27, 27	6 (100%)
3	D	6/7~(85%)	2.29	3 (50%) 0 0	12, 22, 30, 32	6 (100%)
All	All	210/212 (99%)	-0.08	6 (2%) 51 50	9, 15, 30, 56	12~(5%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	364[B]	ILE	7.0
2	С	262[A]	ILE	6.4
3	D	359[B]	TYR	3.8
1	А	41	ARG	3.6
2	С	267[A]	ALA	2.6

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	$B-factors(Å^2)$	Q < 0.9
2	IL0	С	263[A]	9/9	0.79	0.22	23,30,36,37	9
3	ILO	D	363[B]	9/9	0.87	0.13	16,22,31,34	9

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
5	GOL	В	503	6/6	0.63	0.24	28,30,34,35	6
5	GOL	А	104[A]	6/6	0.86	0.25	28,30,37,41	6
4	CL	А	102	1/1	0.94	0.05	43,43,43,43	0
4	CL	А	103	1/1	0.96	0.07	34,34,34,34	0
4	CL	В	502	1/1	1.00	0.05	$15,\!15,\!15,\!15$	1
4	CL	А	101	1/1	1.00	0.04	17,17,17,17	0
4	CL	В	501	1/1	1.00	0.05	18,18,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.

