



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 22, 2024 – 08:47 PM EDT

PDB ID : 6QPT
Title : Crystal structure of nitrite bound synthetic core domain of nitrite reductase from *Ralstonia pickettii* (residues 1-331)
Authors : Antonyuk, S.V.; Hedison, T.M.; Eady, R.R.; Hasnain, S.S.; Scrutton, N.S.
Deposited on : 2019-02-15
Resolution : 1.90 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
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) : 2.37.1

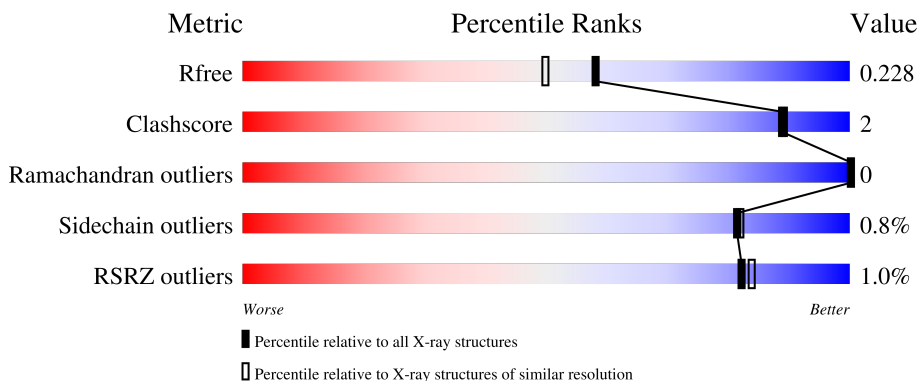
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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.



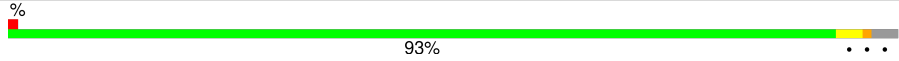
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 $\leq 5\%$. 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	331	92% 5% .
1	B	331	2% 90% 6% .
1	C	331	% 91% 6% .
1	D	331	% 91% 5% .
1	E	331	% 89% 8% .

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Mol	Chain	Length	Quality of chain
1	F	331	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16574 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 Copper-containing nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	320	2441	1569	412	451	9	0	1	0
1	B	319	2444	1571	411	454	8	0	2	0
1	C	320	2461	1581	416	456	8	0	5	0
1	D	319	2440	1568	411	453	8	0	2	0
1	E	320	2441	1568	414	451	8	0	1	0
1	F	320	2445	1571	414	452	8	0	2	0

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

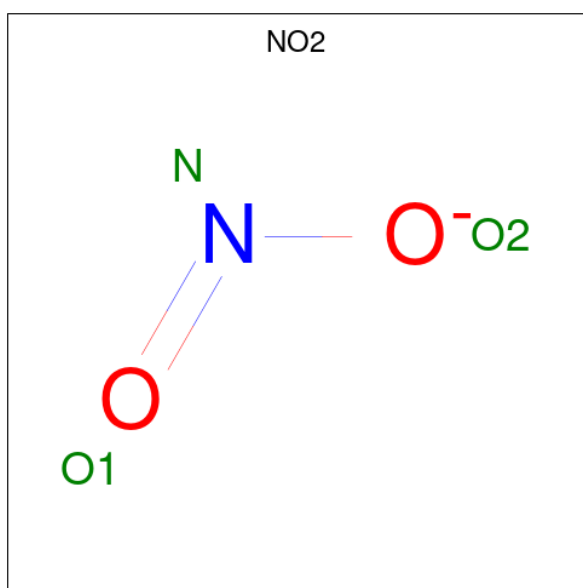
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Cu 2	0	0
2	B	2	Total 2	Cu 2	0	0
2	C	2	Total 2	Cu 2	0	0
2	D	2	Total 2	Cu 2	0	0
2	E	2	Total 2	Cu 2	0	0
2	F	2	Total 2	Cu 2	0	0

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 9 6 3	0	0
3	E	1	Total C O 10 6 4	0	0

- Molecule 4 is NITRITE ION (three-letter code: NO2) (formula: NO₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total N O 3 1 2	0	0
4	C	1	Total N O 3 1 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	N	O	0	0
			3	1	2		
4	E	1	Total	N	O	0	0
			3	1	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	319	Total	O	0	3
			320	320		
5	B	295	Total	O	0	9
			299	299		
5	C	331	Total	O	0	7
			332	332		
5	D	279	Total	O	0	8
			280	280		
5	E	353	Total	O	0	11
			356	356		
5	F	272	Total	O	0	1
			272	272		

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: Copper-containing nitrite reductase

Chain A: 

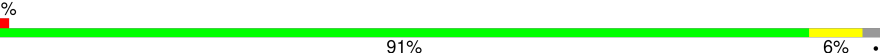


- Molecule 1: Copper-containing nitrite reductase

Chain B: 



- Molecule 1: Copper-containing nitrite reductase

Chain C: 




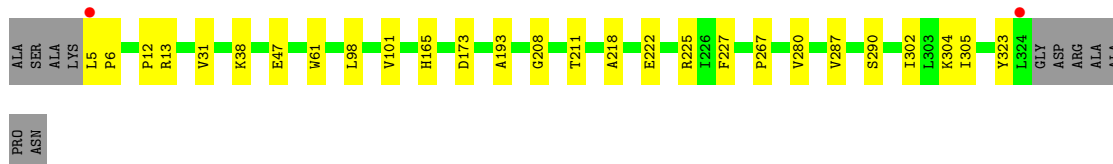
- Molecule 1: Copper-containing nitrite reductase

Chain D: 

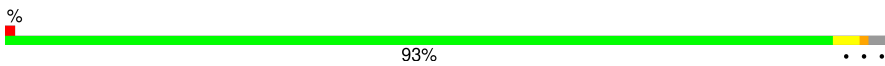


- Molecule 1: Copper-containing nitrite reductase

Chain E: 



● Molecule 1: Copper-containing nitrite reductase

Chain F:  93%

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	165.91Å 167.55Å 143.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 1.90 117.89 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.01-1.90) 99.8 (117.89-1.80)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 1.81Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.178 , 0.224 0.186 , 0.228	Depositor DCC
R_{free} test set	8903 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtrriage
Anisotropy	0.103	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.125 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16574	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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: CU, PG4, NO2

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	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.63	0/2512	0.80	0/3413
1	B	0.63	0/2518	0.78	0/3422
1	C	0.62	0/2540	0.78	0/3452
1	D	0.64	0/2514	0.78	0/3417
1	E	0.62	0/2512	0.79	0/3416
1	F	0.62	0/2519	0.78	0/3423
All	All	0.63	0/15115	0.79	0/20543

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	A	0	1
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	1
All	All	0	10

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	290	SER	Peptide

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Mol	Chain	Res	Type	Group
1	B	289	HIS	Peptide
1	B	290	SER	Peptide
1	C	289	HIS	Peptide
1	C	290	SER	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	A	2441	0	2401	8	0
1	B	2444	0	2401	13	0
1	C	2461	0	2412	15	0
1	D	2440	0	2398	10	0
1	E	2441	0	2392	13	0
1	F	2445	0	2403	8	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	9	0	11	0	0
3	E	10	0	13	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
4	E	3	0	0	0	0
5	A	320	0	0	1	0
5	B	299	0	0	0	0
5	C	332	0	0	0	0
5	D	280	0	0	1	0
5	E	356	0	0	0	0
5	F	272	0	0	0	0
All	All	16574	0	14431	56	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 2.

The worst 5 of 56 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:C:322:VAL:C	1:C:323:TYR:N	2.42	0.73
1:C:322:VAL:O	1:C:323:TYR:N	2.31	0.62
1:D:45:VAL:HG11	1:D:94:HIS:CD2	2.39	0.57
1:D:98:LEU:HB2	1:D:101:VAL:HG23	1.88	0.55
1:B:57:SER:OG	1:B:185:LEU:HA	2.08	0.53

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	319/331 (96%)	315 (99%)	4 (1%)	0	100	100
1	B	319/331 (96%)	315 (99%)	4 (1%)	0	100	100
1	C	320/331 (97%)	313 (98%)	7 (2%)	0	100	100
1	D	319/331 (96%)	314 (98%)	5 (2%)	0	100	100
1	E	319/331 (96%)	315 (99%)	4 (1%)	0	100	100
1	F	320/331 (97%)	316 (99%)	4 (1%)	0	100	100
All	All	1916/1986 (96%)	1888 (98%)	28 (2%)	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/264 (98%)	255 (99%)	3 (1%)	71	70
1	B	259/264 (98%)	258 (100%)	1 (0%)	91	91
1	C	261/264 (99%)	259 (99%)	2 (1%)	81	82
1	D	259/264 (98%)	257 (99%)	2 (1%)	81	82
1	E	257/264 (97%)	254 (99%)	3 (1%)	71	70
1	F	258/264 (98%)	256 (99%)	2 (1%)	81	82
All	All	1552/1584 (98%)	1539 (99%)	13 (1%)	81	82

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	191	GLU
1	E	13	ARG
1	F	286	LEU
1	E	173	ASP
1	F	173	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	260	ASN
1	F	127	ASN
1	C	260	ASN
1	D	51	GLN
1	D	127	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](#)

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

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PG4	E	504	-	9,9,12	0.24	0	8,8,11	0.14	0
4	NO2	E	503	2	1,2,2	0.76	0	0,1,1	-	-
4	NO2	C	503	2	1,2,2	0.88	0	0,1,1	-	-
4	NO2	D	503	2	1,2,2	0.90	0	0,1,1	-	-
3	PG4	A	503	-	8,8,12	0.29	0	7,7,11	0.21	0
4	NO2	B	503	2	1,2,2	0.85	0	0,1,1	-	-

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	PG4	A	503	-	-	3/6/6/10	-
3	PG4	E	504	-	-	2/7/7/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	504	PG4	O3-C5-C6-O4
3	E	504	PG4	O2-C3-C4-O3
3	A	503	PG4	C6-C5-O3-C4
3	A	503	PG4	C4-C3-O2-C2
3	A	503	PG4	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	322:VAL	C	323:TYR	N	2.42

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, 95th 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)	Q<0.9
1	A	320/331 (96%)	-0.33	1 (0%) 94 94	15, 25, 38, 65	3 (0%)
1	B	319/331 (96%)	-0.18	6 (1%) 66 69	16, 29, 48, 72	0
1	C	320/331 (96%)	-0.29	3 (0%) 84 85	14, 23, 42, 69	2 (0%)
1	D	319/331 (96%)	-0.13	3 (0%) 84 85	17, 31, 49, 68	0
1	E	320/331 (96%)	-0.33	2 (0%) 89 90	15, 24, 37, 57	0
1	F	320/331 (96%)	-0.20	4 (1%) 77 79	14, 28, 46, 56	0
All	All	1918/1986 (96%)	-0.24	19 (0%) 82 84	14, 27, 45, 72	5 (0%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	323	TYR	4.9
1	B	324	LEU	4.9
1	D	324	LEU	4.2
1	C	323	TYR	3.5
1	E	324	LEU	3.5

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, 95th 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
3	PG4	E	504	10/13	0.79	0.16	35,41,44,44	0
3	PG4	A	503	9/13	0.81	0.16	36,36,41,41	0
4	NO2	C	503	3/3	0.95	0.15	21,21,22,22	3
4	NO2	D	503	3/3	0.95	0.12	24,24,25,25	3
4	NO2	B	503	3/3	0.96	0.11	40,40,40,41	0
4	NO2	E	503	3/3	0.98	0.09	20,20,20,21	3
2	CU	F	501	1/1	0.99	0.07	32,32,32,32	0
2	CU	D	502	1/1	1.00	0.07	21,21,21,21	0
2	CU	E	501	1/1	1.00	0.07	22,22,22,22	0
2	CU	E	502	1/1	1.00	0.07	19,19,19,19	0
2	CU	A	501	1/1	1.00	0.07	23,23,23,23	0
2	CU	F	502	1/1	1.00	0.07	23,23,23,23	0
2	CU	A	502	1/1	1.00	0.08	19,19,19,19	0
2	CU	B	501	1/1	1.00	0.06	26,26,26,26	0
2	CU	B	502	1/1	1.00	0.06	22,22,22,22	0
2	CU	C	501	1/1	1.00	0.07	19,19,19,19	0
2	CU	C	502	1/1	1.00	0.07	17,17,17,17	0
2	CU	D	501	1/1	1.00	0.06	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.