



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:58 AM GMT

PDB ID : 4FBK
Title : Crystal structure of a covalently fused Nbs1-Mre11 complex with one manganese ion per active site
Authors : Schiller, C.B.; Lammens, K.; Hopfner, K.P.
Deposited on : 2012-05-23
Resolution : 2.38 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

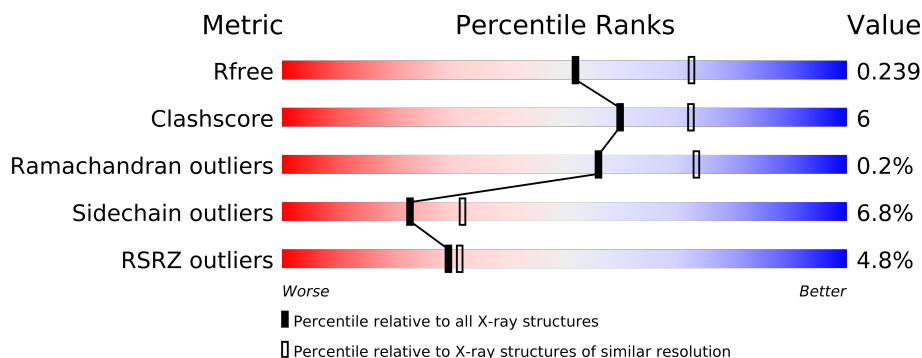
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.38 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}	66092	2963 (2.40-2.36)
Clashscore	79885	3668 (2.40-2.36)
Ramachandran outliers	78287	3600 (2.40-2.36)
Sidechain outliers	78261	3602 (2.40-2.36)
RSRZ outliers	66119	2966 (2.40-2.36)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	472	
1	B	472	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MN	A	1504	-	X
3	MN	B	1502	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6934 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DNA repair and telomere maintenance protein nbs1, DNA repair protein rad32 CHIMERIC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	98	0	0
			3428	2181	597	642	8			
1	B	406	Total	C	N	O	S	123	0	0
			3274	2085	569	612	8			

There are 30 discrepancies between the modelled and reference sequences:

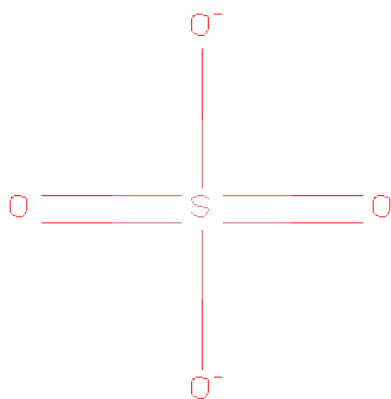
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP O43070
A	-3	PRO	-	EXPRESSION TAG	UNP O43070
A	-2	LEU	-	EXPRESSION TAG	UNP O43070
A	-1	GLY	-	EXPRESSION TAG	UNP O43070
A	0	SER	-	EXPRESSION TAG	UNP O43070
A	532	VAL	-	LINKER	UNP Q09683
A	533	ASP	-	LINKER	UNP Q09683
A	534	GLY	-	LINKER	UNP Q09683
A	535	SER	-	LINKER	UNP Q09683
A	536	ALA	-	LINKER	UNP Q09683
A	537	GLY	-	LINKER	UNP Q09683
A	538	SER	-	LINKER	UNP Q09683
A	539	ALA	-	LINKER	UNP Q09683
A	540	GLY	-	LINKER	UNP Q09683
A	541	SER	-	LINKER	UNP Q09683
B	-4	GLY	-	EXPRESSION TAG	UNP O43070
B	-3	PRO	-	EXPRESSION TAG	UNP O43070
B	-2	LEU	-	EXPRESSION TAG	UNP O43070
B	-1	GLY	-	EXPRESSION TAG	UNP O43070
B	0	SER	-	EXPRESSION TAG	UNP O43070
B	532	VAL	-	LINKER	UNP Q09683
B	533	ASP	-	LINKER	UNP Q09683
B	534	GLY	-	LINKER	UNP Q09683
B	535	SER	-	LINKER	UNP Q09683

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Chain	Residue	Modelled	Actual	Comment	Reference
B	536	ALA	-	LINKER	UNP Q09683
B	537	GLY	-	LINKER	UNP Q09683
B	538	SER	-	LINKER	UNP Q09683
B	539	ALA	-	LINKER	UNP Q09683
B	540	GLY	-	LINKER	UNP Q09683
B	541	SER	-	LINKER	UNP Q09683

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	121	Total 121	O 121	0	0
4	B	89	Total 89	O 89	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.26Å 78.87Å 222.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.88 – 2.38 47.88 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.88-2.38) 99.5 (47.88-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.37Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.222 , 0.242 0.218 , 0.239	Depositor DCC
R_{free} test set	1999 reflections (4.61%)	DCC
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 43369 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6934	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, SO4

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	0.48	0/3503	0.70	6/4746 (0.1%)
1	B	0.44	0/3348	0.71	6/4543 (0.1%)
All	All	0.46	0/6851	0.70	12/9289 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1162	PRO	CA-N-CD	-9.29	98.49	111.50
1	B	1299	PHE	N-CA-CB	-8.60	95.11	110.60
1	A	1108	ASP	CB-CA-C	-7.15	96.11	110.40
1	A	1216	PHE	N-CA-C	-6.74	92.80	111.00
1	A	1109	THR	N-CA-CB	-6.72	97.53	110.30
1	A	1114	ILE	CB-CA-C	6.58	124.77	111.60
1	B	1298	ASP	CB-CA-C	-6.01	98.38	110.40
1	B	1387	GLU	CB-CA-C	5.84	122.09	110.40
1	B	1214	GLU	CB-CA-C	5.83	122.05	110.40
1	B	1214	GLU	N-CA-CB	-5.46	100.77	110.60
1	A	1109	THR	N-CA-C	5.42	125.64	111.00
1	A	478	ASP	CB-CG-OD2	5.15	122.94	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3428	0	0	12	0
1	B	3274	0	0	28	0
2	A	15	0	0	0	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	121	0	0	0	0
4	B	89	0	0	0	0
All	All	6934	0	0	39	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (39) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1108:ASP:CB	1:A:1109:THR:CA	2.30	1.07
1:B:1383:GLY:O	1:B:1384:TYR:CD2	2.28	0.87
1:B:1211:TYR:O	1:B:1215:TRP:CD1	2.30	0.84
1:B:1266:PHE:CD2	1:B:1266:PHE:O	2.34	0.81
1:A:525:GLN:O	1:B:1122:ASN:ND2	2.20	0.75
1:B:1016:ASN:O	1:B:1179:THR:CG2	2.37	0.73
1:B:1383:GLY:C	1:B:1384:TYR:CD2	2.63	0.72
1:B:1162:PRO:CD	1:B:1163:GLU:N	2.57	0.67
1:B:1019:ARG:NH1	1:B:1055:ARG:O	2.29	0.65
1:B:1114:ILE:CG2	1:B:1116:TYR:CD1	2.80	0.64
1:B:1115:ASN:OD1	1:B:1116:TYR:N	2.30	0.64
1:A:1108:ASP:OD1	1:A:1110:ALA:N	2.33	0.62
1:A:1209:ASP:OD1	1:A:1210:LEU:N	2.32	0.62
1:B:1266:PHE:CD2	1:B:1266:PHE:C	2.73	0.61
1:B:1332:LYS:O	1:B:1336:LEU:CD1	2.49	0.61
1:B:1016:ASN:ND2	1:B:1177:GLY:CA	2.63	0.61
1:B:1209:ASP:O	1:B:1212:ARG:NH1	2.34	0.61
1:B:1383:GLY:O	1:B:1384:TYR:CG	2.53	0.60
1:A:1111:VAL:CG1	1:A:1112:CYS:N	2.68	0.57
1:B:1114:ILE:CG2	1:B:1116:TYR:CE1	2.88	0.56
1:B:1292:LEU:C	1:B:1292:LEU:CD2	2.74	0.55
1:A:1067:PHE:O	1:A:1134:HIS:CE1	2.60	0.55
1:B:1099:LEU:CD1	1:B:1099:LEU:N	2.71	0.52
1:B:1116:TYR:O	1:B:1116:TYR:CD2	2.62	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1150:GLN:OE1	1:A:1160:ARG:NH2	2.46	0.48
1:A:1211:TYR:O	1:A:1214:GLU:N	2.48	0.47
1:B:1150:GLN:OE1	1:B:1160:ARG:NH2	2.47	0.47
1:A:522:LYS:CE	1:A:1122:ASN:ND2	2.79	0.46
1:B:1292:LEU:CD2	1:B:1294:ILE:CG1	2.94	0.45
1:B:1264:GLN:CB	1:B:1266:PHE:CE1	3.01	0.44
1:B:1331:ASN:ND2	1:B:1331:ASN:N	2.66	0.43
1:A:1032:GLU:OE2	1:A:1073:SER:OG	2.37	0.43
1:A:1063:GLY:O	1:A:1222:HIS:CD2	2.72	0.42
1:B:1116:TYR:C	1:B:1116:TYR:CD2	2.93	0.41
1:B:1032:GLU:OE2	1:B:1073:SER:OG	2.38	0.41
1:A:522:LYS:NZ	1:A:1090:GLY:O	2.54	0.41
1:B:1331:ASN:O	1:B:1334:GLU:N	2.54	0.41
1:B:1334:GLU:OE1	1:B:1334:GLU:N	2.54	0.41
1:B:1331:ASN:O	1:B:1335:VAL:CG2	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	414/472 (88%)	402 (97%)	12 (3%)	0	100	100
1	B	398/472 (84%)	384 (96%)	12 (3%)	2 (0%)	38	51
All	All	812/944 (86%)	786 (97%)	24 (3%)	2 (0%)	56	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1327	PRO
1	B	1397	VAL

5.3.2 Protein sidechains ⓘ

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	384/420 (91%)	361 (94%)	23 (6%)	27	38
1	B	367/420 (87%)	339 (92%)	28 (8%)	19	26
All	All	751/840 (89%)	700 (93%)	51 (7%)	22	32

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	488	ARG
1	A	490	LEU
1	A	496	ILE
1	A	497	ARG
1	A	526	LYS
1	A	1112	CYS
1	A	1113	ASN
1	A	1115	ASN
1	A	1151	VAL
1	A	1157	TYR
1	A	1163	GLU
1	A	1164	ASN
1	A	1166	ASN
1	A	1201	ASN
1	A	1212	ARG
1	A	1213	ASP
1	A	1251	GLU
1	A	1266	PHE
1	A	1267	THR
1	A	1277	THR
1	A	1323	SER
1	A	1332	LYS
1	A	1394	ASN
1	B	483	GLU
1	B	486	ARG
1	B	488	ARG
1	B	497	ARG
1	B	1015	GLU
1	B	1100	SER

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Mol	Chain	Res	Type
1	B	1111	VAL
1	B	1142	ARG
1	B	1151	VAL
1	B	1157	TYR
1	B	1179	THR
1	B	1192	GLU
1	B	1193	ARG
1	B	1201	ASN
1	B	1210	LEU
1	B	1211	TYR
1	B	1213	ASP
1	B	1229	THR
1	B	1266	PHE
1	B	1297	LYS
1	B	1300	HIS
1	B	1305	ARG
1	B	1324	SER
1	B	1330	GLU
1	B	1331	ASN
1	B	1344	GLU
1	B	1368	LYS
1	B	1375	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
2	SO4	A	1501	-	4,4,4	0.54	0	6,6,6	0.16	0
2	SO4	A	1502	-	4,4,4	0.13	0	6,6,6	0.16	0
2	SO4	A	1503	-	4,4,4	0.45	0	6,6,6	0.33	0
2	SO4	B	1501	-	4,4,4	0.67	0	6,6,6	0.18	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	SO4	A	1501	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1502	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1503	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1501	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	424/472 (89%)	0.15	22 (5%) 26 28	20, 41, 87, 124	36 (8%)
1	B	406/472 (86%)	0.27	17 (4%) 35 37	24, 54, 94, 119	38 (9%)
All	All	830/944 (87%)	0.21	39 (4%) 29 32	20, 47, 93, 124	74 (8%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1413	LYS	4.4
1	A	481	PHE	4.1
1	B	1382	GLY	3.7
1	B	1397	VAL	3.7
1	A	520	ASN	3.6
1	A	521	PHE	3.6
1	B	1111	VAL	3.3
1	A	1326	PRO	3.0
1	A	477	ASP	3.0
1	A	1280	SER	3.0
1	A	479	LYS	2.7
1	A	478	ASP	2.7
1	A	480	ALA	2.7
1	B	1093	PRO	2.7
1	B	541	SER	2.7
1	B	1329	VAL	2.6
1	A	526	LYS	2.6
1	B	480	ALA	2.5
1	B	1211	TYR	2.5
1	B	1327	PRO	2.5
1	A	1110	ALA	2.5
1	B	1016	ASN	2.5
1	B	481	PHE	2.4
1	A	1108	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1165	ASP	2.3
1	B	1299	PHE	2.3
1	A	525	GLN	2.3
1	A	1211	TYR	2.2
1	A	1410	TYR	2.2
1	A	519	LYS	2.2
1	B	1114	ILE	2.2
1	A	486	ARG	2.1
1	A	1164	ASN	2.1
1	A	524	PHE	2.1
1	B	1098	LEU	2.1
1	A	518	ARG	2.1
1	B	1215	TRP	2.1
1	B	1371	LEU	2.0
1	A	1112	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MN	B	1502	1/1	0.27	11.99	120,120,120,120	0
3	MN	A	1504	1/1	0.18	5.87	97,97,97,97	0
2	SO4	A	1501	5/5	0.11	-0.41	35,37,38,38	0
2	SO4	B	1501	5/5	0.12	-0.66	35,37,39,39	0
2	SO4	A	1502	5/5	0.13	-0.97	49,51,51,52	0
2	SO4	A	1503	5/5	0.11	-1.04	44,45,48,48	0

6.5 Other polymers ⓘ

There are no such residues in this entry.