



# wwPDB X-ray Structure Validation Summary Report

Apr 25, 2023 – 07:21 pm BST

PDB ID : 8BNT  
Title : The DH domain of ARHGEF2 bound to RhoA  
Authors : Bradshaw, W.J.; Katis, V.L.; Grosjean, H.; Bountra, C.; von Delft, F.; Brennan, P.E.  
Deposited on : 2022-11-25  
Resolution : 1.40 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.32.2  
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) : 2.32.2

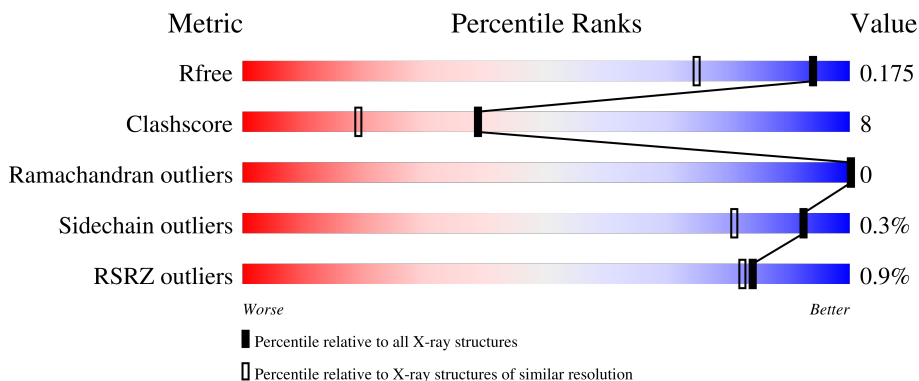
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

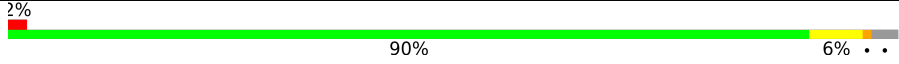

The reported resolution of this entry is 1.40 Å.

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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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  $\geq 3$ , 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	185	 2% 90% 6% . .
2	B	245	 87% 12%

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
4	FMT	B	505	-	-	X	-
4	FMT	B	510	-	-	X	-
4	FMT	B	512	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4183 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 Transforming protein RhoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	179	1462	931	243	275	13	0	9	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P61586

- Molecule 2 is a protein called Rho guanine nucleotide exchange factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	245	2201	1403	383	402	13	0	34	0

There are 2 discrepancies between the modelled and reference sequences:

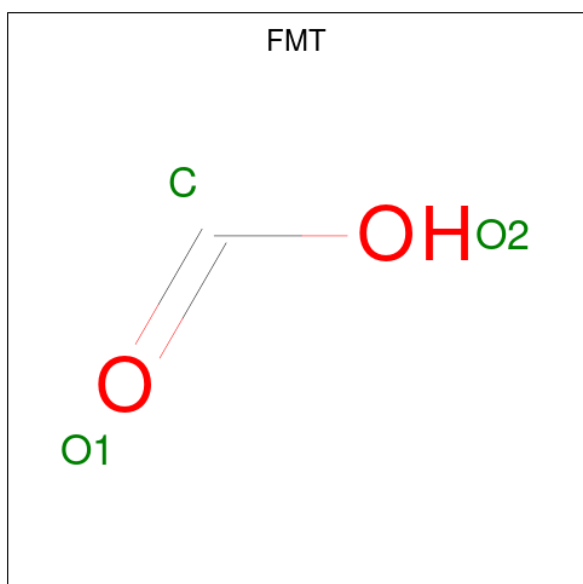
Chain	Residue	Modelled	Actual	Comment	Reference
B	204	SER	-	expression tag	UNP Q92974
B	205	MET	-	expression tag	UNP Q92974

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



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

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula:  $\text{CH}_2\text{O}_2$ ).



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


- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	156	Total O 156 156	0	3
5	B	295	Total O 299 299	0	11

### 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.

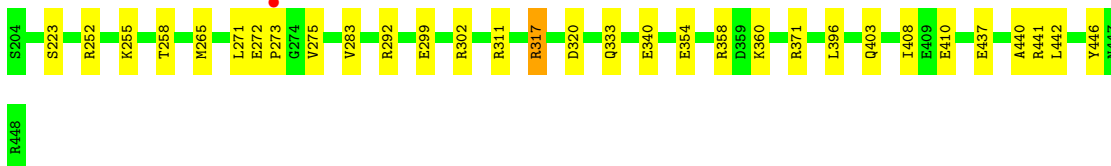
- Molecule 1: Transforming protein RhoA

Chain A:  2% 90% 6% . . .



- Molecule 2: Rho guanine nucleotide exchange factor 2

Chain B:  87% 12%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.43Å 71.43Å 196.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.84 – 1.40 57.78 – 1.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (57.84-1.40) 100.0 (57.78-1.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.21 (at 1.40Å)	Xtrriage
Refinement program	REFMAC 5.8.0352	Depositor
R, $R_{free}$	0.130 , 0.175 0.131 , 0.175	Depositor DCC
$R_{free}$ test set	2000 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.6	Xtrriage
Anisotropy	0.430	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	4183	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: DMS, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.54	0/1517	0.82	3/2050 (0.1%)
2	B	0.61	2/2323 (0.1%)	0.86	6/3118 (0.2%)
All	All	0.58	2/3840 (0.1%)	0.85	9/5168 (0.2%)

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
2	B	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	340[A]	GLU	CD-OE1	6.91	1.33	1.25
2	B	340[B]	GLU	CD-OE1	6.91	1.33	1.25

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	311	ARG	NE-CZ-NH1	-9.39	115.60	120.30
1	A	168	ARG	NE-CZ-NH1	-7.89	116.36	120.30
2	B	311	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	A	70	ARG	NE-CZ-NH1	6.47	123.53	120.30
2	B	317[A]	ARG	NE-CZ-NH2	-6.25	117.17	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ARG	Sidechain
2	B	292	ARG	Sidechain
2	B	441	ARG	Sidechain

## 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	1462	0	1484	10	0
2	B	2201	0	2288	43	0
3	A	4	0	6	0	0
3	B	16	0	24	2	0
4	A	18	0	7	0	0
4	B	27	0	12	12	0
5	A	156	0	0	4	0
5	B	299	0	0	15	0
All	All	4183	0	3821	57	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 8.

The worst 5 of 57 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)
2:B:354[A]:GLU:CG	2:B:358[A]:ARG:NH1	1.78	1.46
2:B:354[A]:GLU:HG2	2:B:358[A]:ARG:NH1	1.32	1.36
2:B:354[A]:GLU:CG	2:B:358[A]:ARG:HH11	1.41	1.18
2:B:354[A]:GLU:HG3	2:B:358[A]:ARG:NH1	1.72	0.98
2:B:408[B]:ILE:CD1	4:B:505:FMT:O2	2.15	0.95

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	186/185 (100%)	182 (98%)	4 (2%)	0	100	100
2	B	277/245 (113%)	276 (100%)	1 (0%)	0	100	100
All	All	463/430 (108%)	458 (99%)	5 (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 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	165/160 (103%)	165 (100%)	0	100	100
2	B	258/224 (115%)	257 (100%)	1 (0%)	91	78
All	All	423/384 (110%)	422 (100%)	1 (0%)	92	82

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

Mol	Chain	Res	Type
2	B	410	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	381	GLN

### 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](#)

20 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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	DMS	B	504[A]	-	3,3,3	0.44	0	3,3,3	0.07	0
3	DMS	B	502	-	3,3,3	0.42	0	3,3,3	0.69	0
4	FMT	B	511	-	2,2,2	1.14	0	1,1,1	0.31	0
3	DMS	B	501	-	3,3,3	0.72	0	3,3,3	0.32	0
4	FMT	B	508	-	2,2,2	1.07	0	1,1,1	0.20	0
4	FMT	B	505	-	2,2,2	3.32	1 (50%)	1,1,1	1.02	0
4	FMT	B	506	-	2,2,2	0.53	0	1,1,1	0.23	0
3	DMS	B	503	-	3,3,3	0.63	0	3,3,3	0.20	0
4	FMT	B	512	-	2,2,2	1.11	0	1,1,1	0.17	0
4	FMT	A	206	-	2,2,2	1.34	0	1,1,1	0.24	0
4	FMT	B	510	-	2,2,2	0.41	0	1,1,1	0.08	0
3	DMS	A	201	-	3,3,3	0.29	0	3,3,3	0.14	0
4	FMT	A	207	-	2,2,2	0.63	0	1,1,1	0.35	0
4	FMT	A	204	-	2,2,2	1.06	0	1,1,1	0.23	0
4	FMT	B	513	-	2,2,2	1.21	0	1,1,1	0.26	0
4	FMT	A	205	-	2,2,2	0.75	0	1,1,1	0.40	0
4	FMT	A	202	-	2,2,2	0.39	0	1,1,1	0.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FMT	A	203	-	2,2,2	1.06	0	1,1,1	0.30	0
4	FMT	B	507	-	2,2,2	1.05	0	1,1,1	0.29	0
4	FMT	B	509	-	2,2,2	1.17	0	1,1,1	0.28	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	505	FMT	O2-C	4.66	1.52	1.28

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	505	FMT	5	0
3	B	503	DMS	2	0
4	B	512	FMT	3	0
4	B	510	FMT	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	179/185 (96%)	-0.40	3 (1%) 70 69	11, 18, 55, 77	0
2	B	245/245 (100%)	-0.52	1 (0%) 92 91	10, 16, 37, 50	0
All	All	424/430 (98%)	-0.47	4 (0%) 84 82	10, 17, 42, 77	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	30	PHE	4.7
2	B	273[A]	PRO	2.2
1	A	181	ALA	2.1
1	A	134	MET	2.1

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	FMT	A	206	3/3	0.78	0.12	48,48,60,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FMT	B	508	3/3	0.84	0.24	55,55,57,58	0
4	FMT	A	204	3/3	0.85	0.12	53,53,54,59	0
4	FMT	B	513	3/3	0.88	0.20	54,54,55,71	0
4	FMT	B	511	3/3	0.93	0.09	32,32,43,53	0
4	FMT	B	509	3/3	0.94	0.11	34,34,42,48	0
3	DMS	B	503	4/4	0.94	0.16	36,39,49,56	4
4	FMT	B	512	3/3	0.94	0.36	39,39,57,67	0
4	FMT	A	205	3/3	0.94	0.15	46,46,55,63	0
4	FMT	A	207	3/3	0.95	0.25	31,31,35,35	3
4	FMT	A	203	3/3	0.95	0.13	37,37,53,65	0
3	DMS	B	504[A]	4/4	0.96	0.09	54,55,55,72	4
3	DMS	A	201	4/4	0.98	0.05	15,17,18,20	0
3	DMS	B	501	4/4	0.98	0.07	17,18,18,20	4
4	FMT	B	510	3/3	0.98	0.22	18,18,38,42	3
4	FMT	A	202	3/3	0.98	0.06	16,16,16,17	0
3	DMS	B	502	4/4	0.98	0.07	14,15,16,16	4
4	FMT	B	507	3/3	0.98	0.07	20,20,22,31	0
4	FMT	B	506	3/3	0.99	0.12	27,27,29,30	0
4	FMT	B	505	3/3	0.99	0.11	18,18,18,19	3

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.