



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:18 PM UTC

PDB ID : 4APT / pdb\_00004apt  
Title : The structure of the AXH domain of ataxin-1.  
Authors : Rees, M.; Chen, Y.W.; de Chiara, C.; Pastore, A.  
Deposited on : 2012-04-05  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

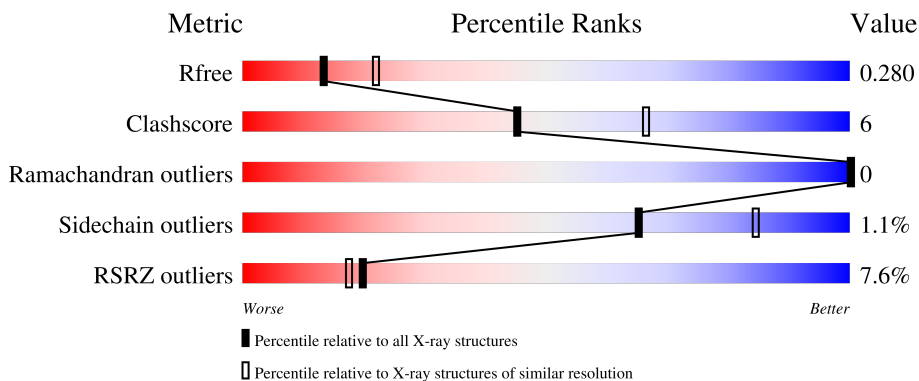
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	126	 6% 75% 24% .
1	B	126	 9% 85% 14% .
1	C	126	 8% 85% 13% ..
1	D	126	 7% 81% 17% .

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 3881 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 ATAXIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	125	961	613	154	188	6	0	0	0
1	B	125	961	613	154	188	6	0	0	0
1	C	125	961	613	154	188	6	0	0	0
1	D	124	952	607	152	187	6	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	564	GLY	-	expression tag	UNP P54253
A	565	ALA	-	expression tag	UNP P54253
A	566	MET	-	expression tag	UNP P54253
B	564	GLY	-	expression tag	UNP P54253
B	565	ALA	-	expression tag	UNP P54253
B	566	MET	-	expression tag	UNP P54253
C	564	GLY	-	expression tag	UNP P54253
C	565	ALA	-	expression tag	UNP P54253
C	566	MET	-	expression tag	UNP P54253
D	564	GLY	-	expression tag	UNP P54253
D	565	ALA	-	expression tag	UNP P54253
D	566	MET	-	expression tag	UNP P54253

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Na	0	0
			1	1		

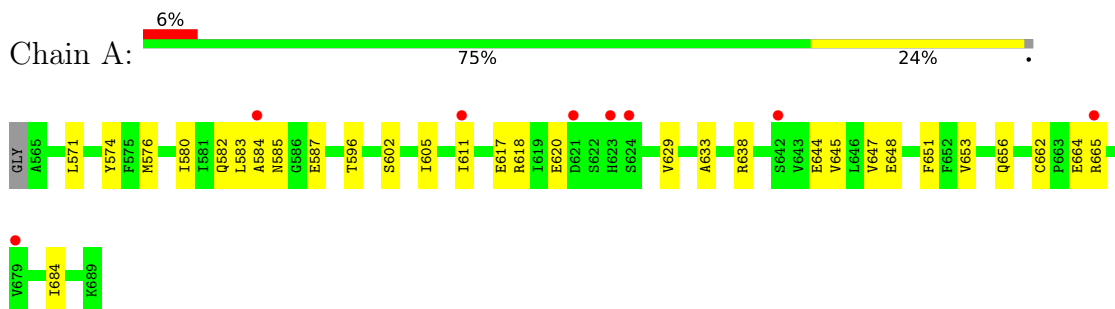
- Molecule 3 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	A	10	Total 10	O 10	0	0
3	B	9	Total 9	O 9	0	0
3	C	16	Total 16	O 16	0	0
3	D	10	Total 10	O 10	0	0

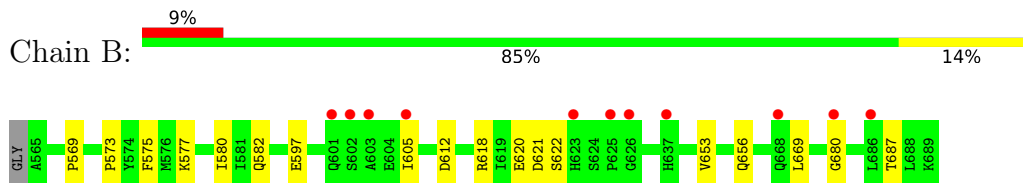
### 3 Residue-property plots [i](#)

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.

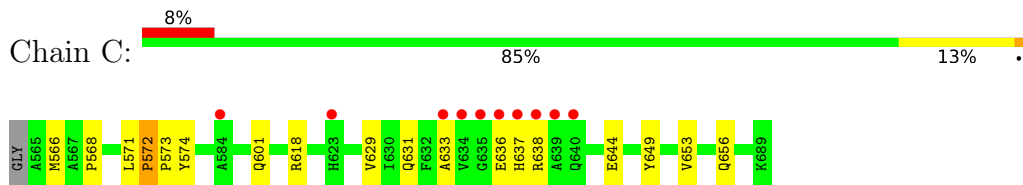
- Molecule 1: ATAXIN-1



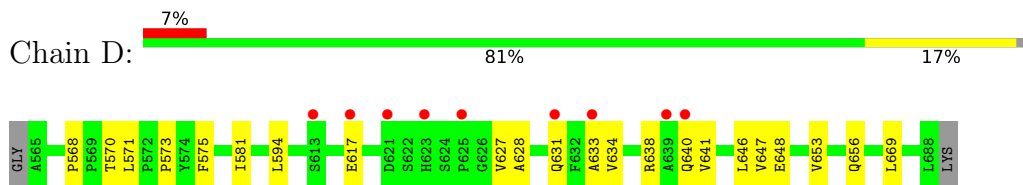
- Molecule 1: ATAXIN-1



- Molecule 1: ATAXIN-1



- Molecule 1: ATAXIN-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.47Å 80.83Å 139.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.41 – 2.50 40.41 – 2.50	Depositor EDS
% Data completeness (in resolution range)	84.4 (40.41-2.50) 84.2 (40.41-2.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.94 (at 2.51Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.236 , 0.288 0.232 , 0.280	Depositor DCC
$R_{free}$ test set	729 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.7	Xtrriage
Anisotropy	0.100	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3881	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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: NA

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	0.27	0/981	0.76	0/1331
1	B	0.28	0/981	0.79	1/1331 (0.1%)
1	C	0.30	0/981	0.77	2/1331 (0.2%)
1	D	0.28	0/972	0.78	1/1320 (0.1%)
All	All	0.28	0/3915	0.77	4/5313 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	634	VAL	N-CA-C	5.99	116.23	107.37
1	C	572	PRO	CA-C-N	5.33	124.94	119.56
1	C	572	PRO	C-N-CA	5.33	124.94	119.56
1	B	605	ILE	N-CA-C	5.15	115.36	110.42

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	961	0	954	20	0
1	B	961	0	954	11	0
1	C	961	0	954	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	952	0	941	12	0
2	D	1	0	0	0	0
3	A	10	0	0	1	0
3	B	9	0	0	0	0
3	C	16	0	0	0	0
3	D	10	0	0	0	0
All	All	3881	0	3803	45	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 6.

All (45) 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:633:ALA:HB1	1:C:638:ARG:HG3	1.72	0.70
1:A:617:GLU:OE2	1:A:638:ARG:NH2	2.25	0.68
1:C:629:VAL:HG22	1:C:644:GLU:HG2	1.77	0.64
1:D:633:ALA:HB1	1:D:638:ARG:HD2	1.81	0.62
1:D:631:GLN:HE21	1:D:640:GLN:HB3	1.64	0.61
1:A:629:VAL:HG22	1:A:644:GLU:HG2	1.81	0.61
1:A:584:ALA:HB2	1:A:602:SER:HA	1.83	0.59
1:C:571:LEU:HD22	1:C:649:TYR:HD2	1.70	0.57
1:C:568:PRO:HD3	1:D:570:THR:HG23	1.86	0.57
1:B:597:GLU:OE1	1:C:601:GLN:NE2	2.39	0.56
1:A:651:PHE:HE1	1:B:569:PRO:HD3	1.72	0.55
1:B:653:VAL:HB	1:B:656:GLN:HB3	1.88	0.54
1:D:653:VAL:HB	1:D:656:GLN:HB3	1.90	0.54
1:C:618:ARG:HB3	1:C:631:GLN:HB3	1.93	0.51
1:A:583:LEU:HB2	1:A:587:GLU:HB3	1.91	0.51
1:A:584:ALA:HB1	1:A:605:ILE:HD12	1.93	0.50
1:A:633:ALA:HB1	1:A:638:ARG:HB3	1.93	0.49
1:B:680:GLY:HA2	1:C:636:GLU:HA	1.95	0.48
1:D:568:PRO:HA	1:D:571:LEU:HD12	1.95	0.48
1:A:618:ARG:HH12	1:A:620:GLU:HB2	1.78	0.48
1:B:621:ASP:OD1	1:B:622:SER:N	2.47	0.47
1:A:582:GLN:NE2	3:A:2002:HOH:O	2.37	0.47
1:C:653:VAL:HB	1:C:656:GLN:HB3	1.97	0.47
1:D:627:VAL:HG22	1:D:646:LEU:HD23	1.96	0.47
1:C:574:TYR:HE2	1:D:573:PRO:HB2	1.80	0.46
1:A:580:ILE:HB	1:B:580:ILE:HB	1.96	0.46
1:A:664:GLU:H	1:A:664:GLU:CD	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:ILE:HD11	1:A:684:ILE:HB	1.97	0.45
1:A:647:VAL:O	1:A:662:CYS:N	2.49	0.45
1:B:618:ARG:NE	1:B:620:GLU:OE2	2.50	0.44
1:A:574:TYR:HE2	1:B:573:PRO:HB2	1.82	0.44
1:A:596:THR:HG23	1:A:684:ILE:HD13	2.00	0.44
1:A:648:GLU:HB3	1:A:665:ARG:HG2	2.01	0.43
1:B:577:LYS:HD3	1:B:669:LEU:O	2.19	0.43
1:D:581:ILE:HG13	1:D:594:LEU:HD11	2.00	0.42
1:D:648:GLU:HG3	1:D:669:LEU:HD12	2.01	0.42
1:D:617:GLU:OE2	1:D:640:GLN:NE2	2.50	0.42
1:A:576:MET:HG2	1:B:582:GLN:O	2.20	0.41
1:C:566:MET:HG2	1:D:641:VAL:HG11	2.02	0.41
1:A:585:ASN:OD1	1:A:587:GLU:HB2	2.20	0.41
1:C:572:PRO:HA	1:C:573:PRO:HD3	1.72	0.41
1:A:653:VAL:HB	1:A:656:GLN:HB3	2.02	0.41
1:A:620:GLU:O	1:A:629:VAL:N	2.46	0.40
1:B:612:ASP:HB2	1:B:687:THR:OG1	2.20	0.40
1:D:628:ALA:HB2	1:D:647:VAL:HG12	2.02	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	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
1	B	123/126 (98%)	122 (99%)	1 (1%)	0	100	100
1	C	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
1	D	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
All	All	491/504 (97%)	482 (98%)	9 (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	111/111 (100%)	109 (98%)	2 (2%)	51	77
1	B	111/111 (100%)	110 (99%)	1 (1%)	70	87
1	C	111/111 (100%)	110 (99%)	1 (1%)	70	87
1	D	110/111 (99%)	109 (99%)	1 (1%)	70	87
All	All	443/444 (100%)	438 (99%)	5 (1%)	65	84

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	571	LEU
1	A	645	VAL
1	B	575	PHE
1	C	637	HIS
1	D	575	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	656	GLN
1	A	668	GLN
1	D	631	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

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](#)

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, 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	125/126 (99%)	0.82	8 (6%) 25 22	31, 59, 107, 150	0
1	B	125/126 (99%)	0.59	11 (8%) 15 14	24, 50, 100, 128	0
1	C	125/126 (99%)	0.40	10 (8%) 18 16	18, 45, 107, 150	0
1	D	124/126 (98%)	0.61	9 (7%) 21 19	28, 59, 109, 136	0
All	All	499/504 (99%)	0.61	38 (7%) 20 17	18, 54, 108, 150	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	639	ALA	5.2
1	C	633	ALA	4.3
1	C	635	GLY	3.8
1	A	642	SER	3.4
1	C	637	HIS	3.4
1	C	636	GLU	3.4
1	D	617	GLU	3.2
1	B	637	HIS	3.1
1	D	621	ASP	3.1
1	B	601	GLN	3.0
1	C	634	VAL	2.9
1	D	625	PRO	2.9
1	A	623	HIS	2.9
1	B	680	GLY	2.9
1	B	623	HIS	2.8
1	B	602	SER	2.8
1	B	603	ALA	2.7
1	B	668	GLN	2.6
1	A	584	ALA	2.6
1	D	623	HIS	2.6
1	C	640	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	625	PRO	2.4
1	C	638	ARG	2.4
1	D	640	GLN	2.4
1	C	584	ALA	2.4
1	A	624	SER	2.3
1	A	679	VAL	2.3
1	D	639	ALA	2.3
1	B	626	GLY	2.3
1	D	631	GLN	2.3
1	D	633	ALA	2.2
1	B	686	LEU	2.2
1	A	621	ASP	2.2
1	C	623	HIS	2.2
1	A	665	ARG	2.2
1	A	611	ILE	2.1
1	D	613	SER	2.1
1	B	605	ILE	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 oligosaccharides 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( $\text{\AA}^2$ )	Q<0.9
2	NA	D	1690	1/1	0.58	0.14	60,60,60,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.