



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:26 PM UTC

PDB ID : 6FB2 / pdb\_00006fb2  
Title : Crystal Structure of a Tailored I-CreI Homing Endonuclease Protein (3115 variant) in complex with its target DNA (Haemoglobin beta subunit gene) in the presence of Manganese  
Authors : Molina, R.; Prieto, J.  
Deposited on : 2017-12-18  
Resolution : 2.95 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  
Xtriage (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

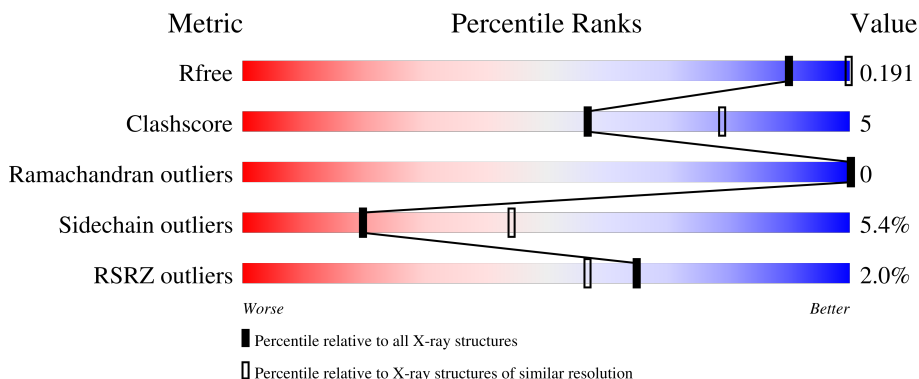
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	153	 2% 83% 14%
2	B	154	 3% 91% 6%
3	D	14	 64% 36%
4	F	14	 86% 14%
5	E	10	 60% 40%

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Mol	Chain	Length	Quality of chain
6	G	10	 80% 20%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 3480 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 DNA endonuclease I-CreI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	153	1236	794	211	230	1	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	SER	GLY	conflict	UNP P05725
A	33	VAL	TYR	conflict	UNP P05725
A	38	ARG	GLN	conflict	UNP P05725
A	40	GLN	SER	conflict	UNP P05725
A	44	ASP	GLN	conflict	UNP P05725
A	68	ALA	ARG	conflict	UNP P05725
A	70	SER	ARG	conflict	UNP P05725
A	75	LYS	ASP	conflict	UNP P05725
A	77	ARG	ILE	conflict	UNP P05725

- Molecule 2 is a protein called DNA endonuclease I-CreI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	154	1250	810	207	232	1	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	33	GLY	TYR	conflict	UNP P05725
B	38	LYS	GLN	conflict	UNP P05725
B	44	LYS	GLN	conflict	UNP P05725
B	68	TYR	ARG	conflict	UNP P05725
B	70	SER	ARG	conflict	UNP P05725
B	75	ASN	ASP	conflict	UNP P05725
B	77	TYR	ILE	conflict	UNP P05725

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Chain	Residue	Modelled	Actual	Comment	Reference
B	132	VAL	ILE	conflict	UNP P05725

- Molecule 3 is a DNA chain called DNA (5'-D(\*TP\*CP\*AP\*GP\*AP\*CP\*TP\*TP\*CP\*TP\*CP\*CP\*AP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	14	276	134	46	83	13	0	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(\*TP\*CP\*TP\*GP\*AP\*CP\*TP\*CP\*CP\*TP\*GP\*TP\*GP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	F	14	282	136	47	86	13	0	0	0

- Molecule 5 is a DNA chain called DNA (5'-D(P\*AP\*GP\*GP\*AP\*GP\*TP\*CP\*AP\*GP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	E	10	212	99	45	58	10	0	0	0

- Molecule 6 is a DNA chain called DNA (5'-D(P\*AP\*GP\*AP\*AP\*GP\*TP\*CP\*TP\*GP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	G	10	210	99	42	59	10	0	0	0

- Molecule 7 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	Mn	0	0
			3	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	6	Total	O	0	0
			6	6		

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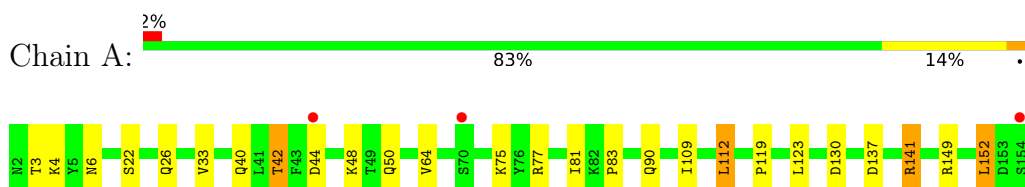
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total O 1 1	0	0
8	F	2	Total O 2 2	0	0
8	E	1	Total O 1 1	0	0
8	G	1	Total O 1 1	0	0

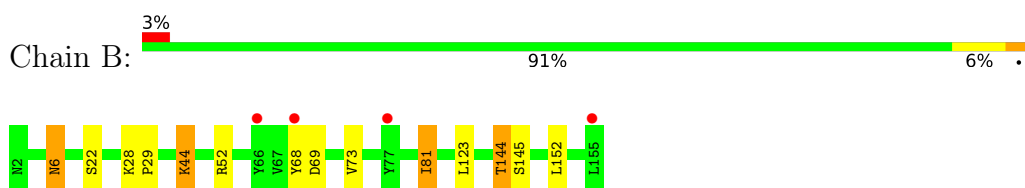
### 3 Residue-property plots [i](#)

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.

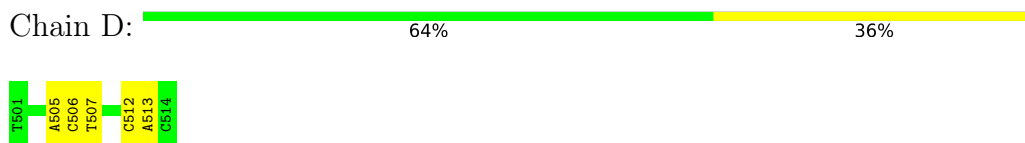
- Molecule 1: DNA endonuclease I-CreI



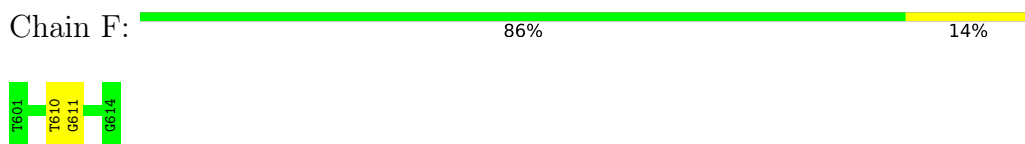
- Molecule 2: DNA endonuclease I-CreI



- Molecule 3: DNA (5'-D(\*TP\*CP\*AP\*GP\*AP\*CP\*TP\*TP\*CP\*TP\*CP\*CP\*AP\*C)-3')



- Molecule 4: DNA (5'-D(\*TP\*CP\*TP\*GP\*AP\*CP\*TP\*CP\*CP\*TP\*GP\*TP\*GP\*G)-3')

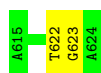


- Molecule 5: DNA (5'-D(P\*AP\*GP\*GP\*AP\*GP\*TP\*CP\*AP\*GP\*A)-3')



- Molecule 6: DNA (5'-D(P\*AP\*GP\*AP\*AP\*GP\*TP\*CP\*TP\*GP\*A)-3')

Chain G:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.89Å 67.36Å 90.87Å 90.00° 96.80° 90.00°	Depositor
Resolution (Å)	41.99 – 2.95 41.99 – 2.95	Depositor EDS
% Data completeness (in resolution range)	97.1 (41.99-2.95) 97.4 (41.99-2.95)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.95Å)	Xtrriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, $R_{free}$	0.187 , 0.235 0.193 , 0.191	Depositor DCC
$R_{free}$ test set	532 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.2	Xtrriage
Anisotropy	0.636	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.4	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	0.95	EDS
Total number of atoms	3480	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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: MN

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	0.29	0/1258	0.73	1/1698 (0.1%)
2	B	0.28	0/1278	0.71	1/1726 (0.1%)
3	D	0.15	0/307	0.73	0/470
4	F	0.11	0/314	0.63	0/483
5	E	0.10	0/239	0.61	0/366
6	G	0.12	0/236	0.53	0/361
All	All	0.25	0/3632	0.69	2/5104 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	81	ILE	N-CA-C	6.05	116.79	110.62
1	A	81	ILE	N-CA-C	5.37	115.58	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	1236	0	1276	13	0
2	B	1250	0	1285	7	0
3	D	276	0	160	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	282	0	160	1	0
5	E	212	0	112	3	0
6	G	210	0	113	1	0
7	A	3	0	0	0	0
8	A	6	0	0	1	0
8	B	1	0	0	0	0
8	E	1	0	0	1	0
8	F	2	0	0	0	0
8	G	1	0	0	0	0
All	All	3480	0	3106	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 5.

All (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)
2:B:22:SER:HB3	2:B:44:LYS:HG2	1.81	0.62
2:B:144:THR:OG1	2:B:145:SER:N	2.33	0.62
1:A:119:PRO:HB3	1:A:152:LEU:HD21	1.83	0.61
1:A:130:ASP:OD1	1:A:141:ARG:NH2	2.33	0.60
1:A:44:ASP:OD2	1:A:75:LYS:NZ	2.35	0.59
1:A:4:LYS:HA	1:A:90:GLN:HE22	1.67	0.59
2:B:6:ASN:OD1	2:B:6:ASN:N	2.31	0.58
6:G:622:DT:H2''	6:G:623:DG:C8	2.39	0.57
1:A:22:SER:HB3	1:A:44:ASP:HB3	1.89	0.55
1:A:42:THR:OG1	8:A:301:HOH:O	2.18	0.52
1:A:26:GLN:NE2	8:E:701:HOH:O	2.34	0.51
3:D:512:DC:H2''	3:D:513:DA:C8	2.46	0.50
5:E:521:DC:H2''	5:E:522:DA:C8	2.46	0.50
1:A:109:ILE:HA	1:A:112:LEU:HD22	1.95	0.49
2:B:52:ARG:NH1	2:B:69:ASP:OD1	2.47	0.48
1:A:48:LYS:HE2	1:A:50:GLN:HB3	1.95	0.47
2:B:68:TYR:OH	3:D:506:DC:O5'	2.27	0.45
1:A:64:VAL:HG11	1:A:83:PRO:HB3	1.98	0.44
1:A:123:LEU:HD13	1:A:149:ARG:HD3	1.98	0.44
1:A:137:ASP:OD1	1:A:137:ASP:N	2.51	0.44
3:D:512:DC:H4'	3:D:513:DA:OP1	2.17	0.44
5:E:517:DG:H2'	5:E:518:DA:C8	2.53	0.43
4:F:610:DT:H2''	4:F:611:DG:C8	2.53	0.43
3:D:506:DC:H2'	3:D:507:DT:H71	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:505:DA:H2''	3:D:506:DC:O5'	2.18	0.43
1:A:77:ARG:NH2	5:E:517:DG:O6	2.50	0.43
2:B:28:LYS:HA	2:B:29:PRO:HD3	1.90	0.43
2:B:68:TYR:HH	3:D:506:DC:P	2.42	0.40

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	151/153 (99%)	143 (95%)	8 (5%)	0	100	100
2	B	153/154 (99%)	143 (94%)	10 (6%)	0	100	100
All	All	304/307 (99%)	286 (94%)	18 (6%)	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	140/140 (100%)	132 (94%)	8 (6%)	18	42
2	B	141/140 (101%)	134 (95%)	7 (5%)	22	47
All	All	281/280 (100%)	266 (95%)	15 (5%)	20	45

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	6	ASN
1	A	33	VAL
1	A	40	GLN
1	A	42	THR
1	A	112	LEU
1	A	141	ARG
1	A	152	LEU
2	B	6	ASN
2	B	44	LYS
2	B	73	VAL
2	B	81	ILE
2	B	123	LEU
2	B	144	THR
2	B	152	LEU

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

Mol	Chain	Res	Type
1	A	26	GLN
1	A	92	GLN
1	A	99	GLN
1	A	103	ASN
1	A	111	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

Of 3 ligands modelled in this entry, 3 are 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

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 [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	153/153 (100%)	-0.09	3 (1%) 65 57	26, 55, 99, 123	0
2	B	154/154 (100%)	0.01	4 (2%) 57 49	16, 49, 91, 109	1 (0%)
3	D	14/14 (100%)	-0.38	0 100 100	35, 57, 71, 75	0
4	F	14/14 (100%)	-0.27	0 100 100	47, 58, 77, 88	0
5	E	10/10 (100%)	-0.63	0 100 100	29, 55, 75, 79	0
6	G	10/10 (100%)	-0.80	0 100 100	21, 45, 76, 76	0
All	All	355/355 (100%)	-0.10	7 (1%) 65 57	16, 54, 96, 123	1 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	68	TYR	5.4
2	B	155	LEU	3.0
1	A	154	SER	2.5
2	B	77	TYR	2.4
2	B	66[A]	TYR	2.2
1	A	70	SER	2.2
1	A	44	ASP	2.0

### 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

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
7	MN	A	201	1/1	0.97	0.09	52,52,52,52	0
7	MN	A	202	1/1	0.99	0.04	54,54,54,54	0
7	MN	A	203	1/1	0.99	0.06	52,52,52,52	0

## 6.5 Other polymers

There are no such residues in this entry.