



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 16, 2017 – 10:32 PM EDT

PDB ID : 3EBC
Title : Structure of N141A HincII with Cognate DNA
Authors : Little, E.J.; Babic, A.C.; Horton, N.C.
Deposited on : unknown
Resolution : 2.55 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

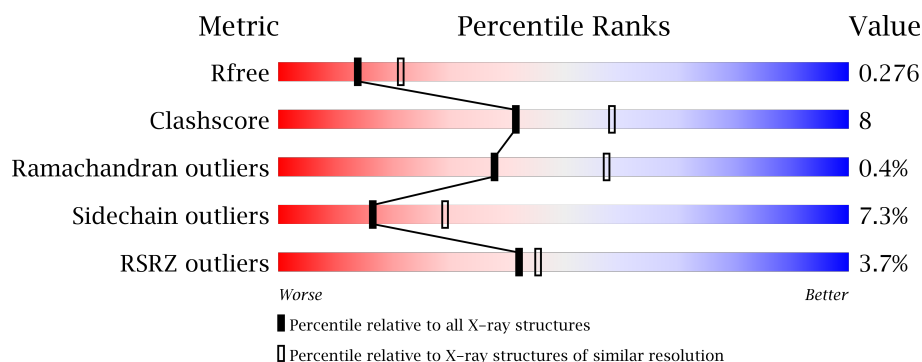
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	100719	4993 (2.58-2.50)
Clashscore	112137	5755 (2.58-2.50)
Ramachandran outliers	110173	5652 (2.58-2.50)
Sidechain outliers	110143	5654 (2.58-2.50)
RSRZ outliers	101464	5026 (2.58-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	317	<div> <div>3%</div> <div>62%</div> <div>13%</div> <div>•</div> <div>24%</div> </div>
1	B	317	<div> <div>3%</div> <div>58%</div> <div>16%</div> <div>•</div> <div>23%</div> </div>
2	E	14	<div> <div>36%</div> <div>64%</div> </div>
3	F	14	<div> <div>14%</div> <div>50%</div> <div>36%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4759 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 Type-2 restriction enzyme HincII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1934	1262	306	360	6			
1	B	244	Total	C	N	O	S	0	0	0
			1956	1278	310	362	6			

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP P17743
A	0	ALA	-	EXPRESSION TAG	UNP P17743
A	130	THR	ARG	CONFLICT	UNP P17743
A	141	ALA	ASN	ENGINEERED	UNP P17743
A	173	TRP	SER	CONFLICT	UNP P17743
A	259	ARG	-	EXPRESSION TAG	UNP P17743
A	260	SER	-	EXPRESSION TAG	UNP P17743
A	261	ARG	-	EXPRESSION TAG	UNP P17743
A	262	GLU	-	EXPRESSION TAG	UNP P17743
A	263	LEU	-	EXPRESSION TAG	UNP P17743
A	264	VAL	-	EXPRESSION TAG	UNP P17743
A	265	ASP	-	EXPRESSION TAG	UNP P17743
A	266	PRO	-	EXPRESSION TAG	UNP P17743
A	267	ASN	-	EXPRESSION TAG	UNP P17743
A	268	SER	-	EXPRESSION TAG	UNP P17743
A	269	VAL	-	EXPRESSION TAG	UNP P17743
A	270	GLN	-	EXPRESSION TAG	UNP P17743
A	271	ALA	-	EXPRESSION TAG	UNP P17743
A	272	ARG	-	EXPRESSION TAG	UNP P17743
A	273	LEU	-	EXPRESSION TAG	UNP P17743
A	274	GLN	-	EXPRESSION TAG	UNP P17743
A	275	ASP	-	EXPRESSION TAG	UNP P17743
A	276	VAL	-	EXPRESSION TAG	UNP P17743
A	277	ASP	-	EXPRESSION TAG	UNP P17743
A	278	GLY	-	EXPRESSION TAG	UNP P17743

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Chain	Residue	Modelled	Actual	Comment	Reference
A	279	THR	-	EXPRESSION TAG	UNP P17743
A	280	ILE	-	EXPRESSION TAG	UNP P17743
A	281	ASP	-	EXPRESSION TAG	UNP P17743
A	282	THR	-	EXPRESSION TAG	UNP P17743
A	283	ARG	-	EXPRESSION TAG	UNP P17743
A	284	SER	-	EXPRESSION TAG	UNP P17743
A	285	LYS	-	EXPRESSION TAG	UNP P17743
A	286	LEU	-	EXPRESSION TAG	UNP P17743
A	287	ALA	-	EXPRESSION TAG	UNP P17743
A	288	ALA	-	EXPRESSION TAG	UNP P17743
A	289	ALA	-	EXPRESSION TAG	UNP P17743
A	290	GLN	-	EXPRESSION TAG	UNP P17743
A	291	LEU	-	EXPRESSION TAG	UNP P17743
A	292	TYR	-	EXPRESSION TAG	UNP P17743
A	293	THR	-	EXPRESSION TAG	UNP P17743
A	294	ARG	-	EXPRESSION TAG	UNP P17743
A	295	ALA	-	EXPRESSION TAG	UNP P17743
A	296	SER	-	EXPRESSION TAG	UNP P17743
A	297	GLN	-	EXPRESSION TAG	UNP P17743
A	298	PRO	-	EXPRESSION TAG	UNP P17743
A	299	GLU	-	EXPRESSION TAG	UNP P17743
A	300	LEU	-	EXPRESSION TAG	UNP P17743
A	301	ALA	-	EXPRESSION TAG	UNP P17743
A	302	PRO	-	EXPRESSION TAG	UNP P17743
A	303	GLU	-	EXPRESSION TAG	UNP P17743
A	304	ASP	-	EXPRESSION TAG	UNP P17743
A	305	PRO	-	EXPRESSION TAG	UNP P17743
A	306	GLU	-	EXPRESSION TAG	UNP P17743
A	307	ASP	-	EXPRESSION TAG	UNP P17743
A	308	LEU	-	EXPRESSION TAG	UNP P17743
A	309	GLU	-	EXPRESSION TAG	UNP P17743
A	310	HIS	-	EXPRESSION TAG	UNP P17743
A	311	HIS	-	EXPRESSION TAG	UNP P17743
A	312	HIS	-	EXPRESSION TAG	UNP P17743
A	313	HIS	-	EXPRESSION TAG	UNP P17743
A	314	HIS	-	EXPRESSION TAG	UNP P17743
A	315	HIS	-	EXPRESSION TAG	UNP P17743
B	-1	MET	-	EXPRESSION TAG	UNP P17743
B	0	ALA	-	EXPRESSION TAG	UNP P17743
B	130	THR	ARG	CONFLICT	UNP P17743
B	141	ALA	ASN	ENGINEERED	UNP P17743
B	173	TRP	SER	CONFLICT	UNP P17743

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Chain	Residue	Modelled	Actual	Comment	Reference
B	259	ARG	-	EXPRESSION TAG	UNP P17743
B	260	SER	-	EXPRESSION TAG	UNP P17743
B	261	ARG	-	EXPRESSION TAG	UNP P17743
B	262	GLU	-	EXPRESSION TAG	UNP P17743
B	263	LEU	-	EXPRESSION TAG	UNP P17743
B	264	VAL	-	EXPRESSION TAG	UNP P17743
B	265	ASP	-	EXPRESSION TAG	UNP P17743
B	266	PRO	-	EXPRESSION TAG	UNP P17743
B	267	ASN	-	EXPRESSION TAG	UNP P17743
B	268	SER	-	EXPRESSION TAG	UNP P17743
B	269	VAL	-	EXPRESSION TAG	UNP P17743
B	270	GLN	-	EXPRESSION TAG	UNP P17743
B	271	ALA	-	EXPRESSION TAG	UNP P17743
B	272	ARG	-	EXPRESSION TAG	UNP P17743
B	273	LEU	-	EXPRESSION TAG	UNP P17743
B	274	GLN	-	EXPRESSION TAG	UNP P17743
B	275	ASP	-	EXPRESSION TAG	UNP P17743
B	276	VAL	-	EXPRESSION TAG	UNP P17743
B	277	ASP	-	EXPRESSION TAG	UNP P17743
B	278	GLY	-	EXPRESSION TAG	UNP P17743
B	279	THR	-	EXPRESSION TAG	UNP P17743
B	280	ILE	-	EXPRESSION TAG	UNP P17743
B	281	ASP	-	EXPRESSION TAG	UNP P17743
B	282	THR	-	EXPRESSION TAG	UNP P17743
B	283	ARG	-	EXPRESSION TAG	UNP P17743
B	284	SER	-	EXPRESSION TAG	UNP P17743
B	285	LYS	-	EXPRESSION TAG	UNP P17743
B	286	LEU	-	EXPRESSION TAG	UNP P17743
B	287	ALA	-	EXPRESSION TAG	UNP P17743
B	288	ALA	-	EXPRESSION TAG	UNP P17743
B	289	ALA	-	EXPRESSION TAG	UNP P17743
B	290	GLN	-	EXPRESSION TAG	UNP P17743
B	291	LEU	-	EXPRESSION TAG	UNP P17743
B	292	TYR	-	EXPRESSION TAG	UNP P17743
B	293	THR	-	EXPRESSION TAG	UNP P17743
B	294	ARG	-	EXPRESSION TAG	UNP P17743
B	295	ALA	-	EXPRESSION TAG	UNP P17743
B	296	SER	-	EXPRESSION TAG	UNP P17743
B	297	GLN	-	EXPRESSION TAG	UNP P17743
B	298	PRO	-	EXPRESSION TAG	UNP P17743
B	299	GLU	-	EXPRESSION TAG	UNP P17743
B	300	LEU	-	EXPRESSION TAG	UNP P17743

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Chain	Residue	Modelled	Actual	Comment	Reference
B	301	ALA	-	EXPRESSION TAG	UNP P17743
B	302	PRO	-	EXPRESSION TAG	UNP P17743
B	303	GLU	-	EXPRESSION TAG	UNP P17743
B	304	ASP	-	EXPRESSION TAG	UNP P17743
B	305	PRO	-	EXPRESSION TAG	UNP P17743
B	306	GLU	-	EXPRESSION TAG	UNP P17743
B	307	ASP	-	EXPRESSION TAG	UNP P17743
B	308	LEU	-	EXPRESSION TAG	UNP P17743
B	309	GLU	-	EXPRESSION TAG	UNP P17743
B	310	HIS	-	EXPRESSION TAG	UNP P17743
B	311	HIS	-	EXPRESSION TAG	UNP P17743
B	312	HIS	-	EXPRESSION TAG	UNP P17743
B	313	HIS	-	EXPRESSION TAG	UNP P17743
B	314	HIS	-	EXPRESSION TAG	UNP P17743
B	315	HIS	-	EXPRESSION TAG	UNP P17743

- Molecule 2 is a DNA chain called 5'-D(*DGP*DCP*DCP*DGP*DGP*DTP*DCP*DGP*DAP*DCP*DGP*DGP*DGP*DC)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	14	Total	C	N	O	P	0	0	0
			286	135	57	81	13			

- Molecule 3 is a DNA chain called 5'-D(*DGP*DCP*DCP*DCP*DGP*DTP*DCP*DGP*DAP*DCP*DCP*DGP*DGP*DC)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	14	Total	C	N	O	P	0	0	0
			281	133	53	82	13			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	123	Total	O	0	0
			123	123		

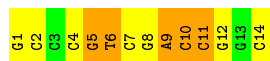
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	133	Total 133	O 133	0	0
5	E	23	Total 23	O 23	0	0
5	F	22	Total 22	O 22	0	0

- Molecule 3: 5'-D(*DGP*DCP*DCP*DCP*DGP*DTP*DCP*DGP*DAP*DCP*DCP*DGP*DGP*DC)-3'

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.55Å 91.57Å 70.59Å 90.00° 107.46° 90.00°	Depositor
Resolution (Å)	43.56 – 2.55 39.96 – 2.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.56-2.55) 95.8 (39.96-2.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.191 , 0.279 0.190 , 0.276	Depositor DCC
R_{free} test set	857 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4759	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% 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: 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	0.51	0/1978	0.62	0/2680
1	B	0.47	0/2000	0.61	0/2709
2	E	0.94	0/321	1.89	15/495 (3.0%)
3	F	0.94	0/314	1.97	11/482 (2.3%)
All	All	0.57	0/4613	0.94	26/6366 (0.4%)

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	9	DA	O4'-C1'-N9	14.80	118.36	108.00
3	F	7	DC	O4'-C1'-N1	13.34	117.34	108.00
3	F	10	DC	O4'-C1'-N1	9.99	114.99	108.00
3	F	4	DC	O4'-C1'-N1	9.10	114.37	108.00
3	F	12	DG	O4'-C1'-N9	7.56	113.29	108.00

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	1934	0	1843	23	0
1	B	1956	0	1879	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	286	0	154	1	0
3	F	281	0	157	4	0
4	A	1	0	0	0	0
5	A	123	0	0	2	0
5	B	133	0	0	5	0
5	E	23	0	0	0	0
5	F	22	0	0	0	0
All	All	4759	0	4033	65	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 65 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:B:54:PHE:O	1:B:55:LYS:HB2	1.52	1.05
1:B:133:ILE:C	1:B:136:SER:N	2.20	0.95
1:B:130:THR:HG22	1:B:171:VAL:HB	1.73	0.71
1:A:70:ILE:HG13	1:A:79:LEU:HD21	1.76	0.68
1:A:161:PHE:O	1:A:223:ARG:HD2	1.95	0.67

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	235/317 (74%)	222 (94%)	12 (5%)	1 (0%)	38	57
1	B	238/317 (75%)	223 (94%)	14 (6%)	1 (0%)	38	57
All	All	473/634 (75%)	445 (94%)	26 (6%)	2 (0%)	38	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	55	LYS
1	A	132	ASN

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	198/280 (71%)	185 (93%)	13 (7%)	19	34
1	B	201/280 (72%)	185 (92%)	16 (8%)	14	25
All	All	399/560 (71%)	370 (93%)	29 (7%)	16	29

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	60	LEU
1	B	91	ARG
1	B	216	ASP
1	B	81	ASN
1	B	118	VAL

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

Mol	Chain	Res	Type
1	A	132	ASN
1	B	237	GLN
1	B	121	GLN
1	A	81	ASN
1	A	240	GLN

5.3.3 RNA [i](#)

There are no RNA molecules 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 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 ⓘ

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, 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	241/317 (76%)	-0.04	9 (3%) 42 45	10, 24, 42, 48	0
1	B	244/317 (76%)	0.12	10 (4%) 38 41	10, 28, 47, 52	0
2	E	14/14 (100%)	-0.41	0 100 100	11, 27, 35, 38	0
3	F	14/14 (100%)	-0.39	0 100 100	11, 29, 37, 41	0
All	All	513/662 (77%)	0.02	19 (3%) 42 45	10, 26, 45, 52	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	258	LEU	5.3
1	A	177	GLY	4.3
1	B	175	LEU	4.1
1	B	33	ALA	4.0
1	B	136	SER	4.0

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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MN	A	316	1/1	0.84	0.10	-	99,99,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.