



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 01:14 am BST

PDB ID : 5W1C  
Title : Crystal structure of MBP fused activation-induced cytidine deaminase (AID)  
in complex with cytidine  
Authors : Qiao, Q.; Wang, L.; Wu, H.  
Deposited on : 2017-06-02  
Resolution : 3.18 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

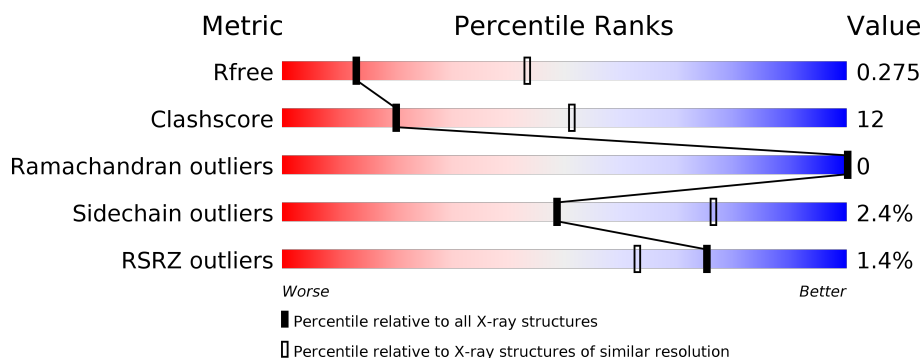
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.18 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	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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  $\geq 3$ , 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	549	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>21%</div> <div>..</div> </div> </div>
1	B	549	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>..</div> </div> </div>
2	D	12	<div> <div>25%</div> <div>75%</div> </div>
3	G	12	<div> <div>50%</div> <div>50%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CTN	A	2002	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9129 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 MBP fused activation-induced cytidine deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	543	Total	C	N	O	S	0	0	0
			4303	2765	727	796	15			
1	A	543	Total	C	N	O	S	0	0	0
			4302	2765	727	795	15			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P0AEY0
B	368	ASN	-	linker	UNP P0AEY0
B	369	ALA	-	linker	UNP P0AEY0
B	370	ALA	-	linker	UNP P0AEY0
B	371	ALA	-	linker	UNP P0AEY0
B	372	GLU	-	linker	UNP P0AEY0
B	373	PHE	LEU	engineered mutation	UNP Q9GZX7
B	1007	ASP	ASN	engineered mutation	UNP Q9GZX7
B	1008	PRO	ARG	engineered mutation	UNP Q9GZX7
B	1009	ALA	ARG	engineered mutation	UNP Q9GZX7
B	1010	THR	LYS	engineered mutation	UNP Q9GZX7
B	1012	THR	LEU	engineered mutation	UNP Q9GZX7
B	1042	GLU	PHE	engineered mutation	UNP Q9GZX7
B	1058	ALA	GLU	engineered mutation	UNP Q9GZX7
B	1130	ALA	HIS	engineered mutation	UNP Q9GZX7
B	1131	GLU	ARG	engineered mutation	UNP Q9GZX7
B	1141	TYR	PHE	engineered mutation	UNP Q9GZX7
B	1145	GLU	PHE	engineered mutation	UNP Q9GZX7
B	1181	GLN	LEU	engineered mutation	UNP Q9GZX7
A	1	MET	-	initiating methionine	UNP P0AEY0
A	368	ASN	-	linker	UNP P0AEY0
A	369	ALA	-	linker	UNP P0AEY0
A	370	ALA	-	linker	UNP P0AEY0
A	371	ALA	-	linker	UNP P0AEY0
A	372	GLU	-	linker	UNP P0AEY0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	373	PHE	LEU	engineered mutation	UNP Q9GZX7
A	1007	ASP	ASN	engineered mutation	UNP Q9GZX7
A	1008	PRO	ARG	engineered mutation	UNP Q9GZX7
A	1009	ALA	ARG	engineered mutation	UNP Q9GZX7
A	1010	THR	LYS	engineered mutation	UNP Q9GZX7
A	1012	THR	LEU	engineered mutation	UNP Q9GZX7
A	1042	GLU	PHE	engineered mutation	UNP Q9GZX7
A	1058	ALA	GLU	engineered mutation	UNP Q9GZX7
A	1130	ALA	HIS	engineered mutation	UNP Q9GZX7
A	1131	GLU	ARG	engineered mutation	UNP Q9GZX7
A	1141	TYR	PHE	engineered mutation	UNP Q9GZX7
A	1145	GLU	PHE	engineered mutation	UNP Q9GZX7
A	1181	GLN	LEU	engineered mutation	UNP Q9GZX7

- Molecule 2 is a DNA chain called DNA (5'-D(\*GP\*TP\*TP\*CP\*AP\*AP\*GP\*GP\*CP\*CP\*AP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	12	Total	C	N	O	P	0	0	0
			243	116	48	68	11			

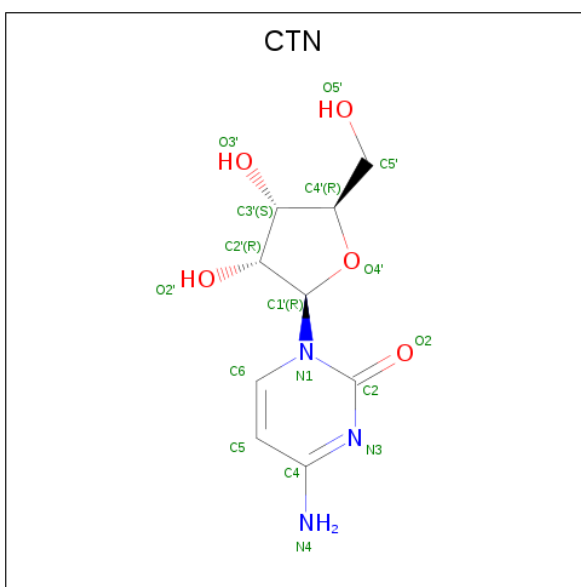
- Molecule 3 is a DNA chain called DNA (5'-D(\*CP\*TP\*GP\*GP\*CP\*CP\*TP\*TP\*GP\*AP\*AP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	12	Total	C	N	O	P	0	0	0
			241	116	43	71	11			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is 4-AMINO-1-BETA-D-RIBOFURANOSYL-2(1H)-PYRIMIDINONE (three-letter code: CTN) (formula: C<sub>9</sub>H<sub>13</sub>N<sub>3</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			17	9	3	5		
5	A	1	Total	C	N	O	0	0
			17	9	3	5		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	A	1	Total	Ca	0	0
			1	1		

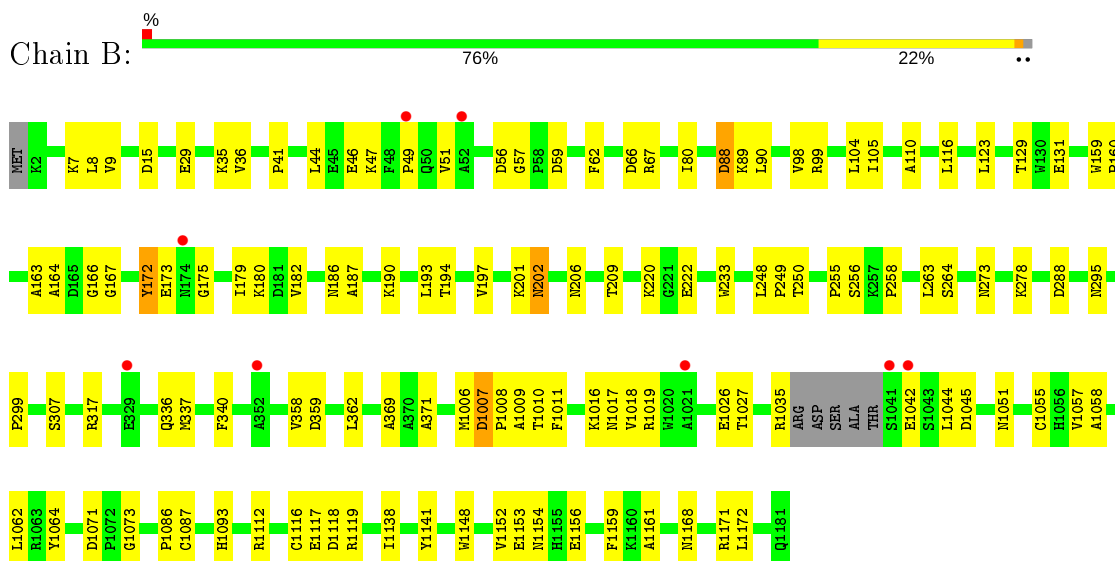
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	O	0	0
			1	1		
7	A	1	Total	O	0	0
			1	1		

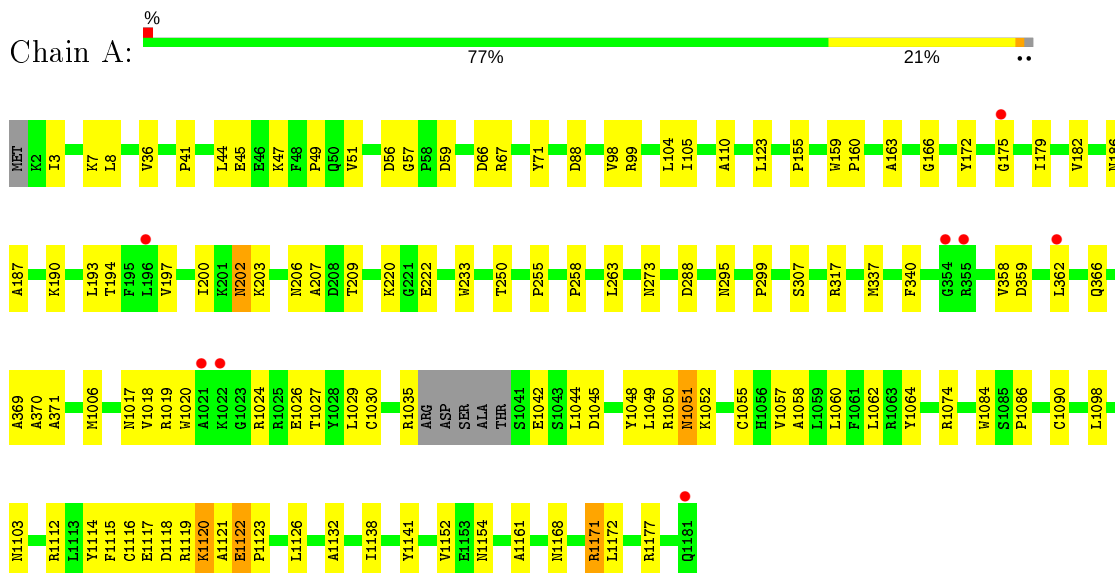
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: MBP fused activation-induced cytidine deaminase



- Molecule 1: MBP fused activation-induced cytidine deaminase



- Molecule 2: DNA (5'-D(\*GP\*TP\*TP\*CP\*AP\*AP\*GP\*GP\*CP\*CP\*AP\*G)-3')

Chain D:  25% 75%



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

Chain G:  50% 50%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.46 Å   39.82 Å   155.30 Å 90.00°   90.27°   90.00°	Depositor
Resolution (Å)	125.45 – 3.18 125.45 – 3.18	Depositor EDS
% Data completeness (in resolution range)	98.5 (125.45-3.18) 98.5 (125.45-3.18)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 3.19 Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.232   ,   0.270 0.238   ,   0.275	Depositor DCC
$R_{free}$ test set	1423 reflections (5.39%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	97.4	Xtriage
Anisotropy	0.722	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 65.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9129	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 69.72 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5265e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: ZN, CA, CTN

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	0.44	0/4413	0.60	1/5989 (0.0%)
1	B	0.41	1/4414 (0.0%)	0.58	1/5990 (0.0%)
2	D	0.71	0/273	0.89	1/420 (0.2%)
3	G	0.76	0/269	0.93	0/413
All	All	0.45	1/9369 (0.0%)	0.62	3/12812 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1087	CYS	CB-SG	6.05	1.92	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1118	ASP	CB-CA-C	-7.38	95.63	110.40
1	A	370	ALA	N-CA-CB	-5.66	102.17	110.10
2	D	2	DT	N3-C4-O4	5.46	123.17	119.90

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	4302	0	4186	116	1
1	B	4303	0	4188	86	0
2	D	243	0	132	8	1
3	G	241	0	137	9	1
4	A	1	0	0	1	0
4	B	1	0	0	0	0
5	A	17	0	13	17	0
5	B	17	0	13	6	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	1	0	0	3	0
7	B	1	0	0	2	0
All	All	9129	0	8669	222	2

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 12.

All (222) 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)
5:A:2002:CTN:C4	7:A:3001:HOH:O	1.81	1.28
1:B:1027:THR:OG1	5:B:2002:CTN:O2	1.62	1.18
5:B:2002:CTN:C4	7:B:3001:HOH:O	1.91	1.17
1:A:179:ILE:HG22	1:A:371:ALA:HB2	1.28	1.13
5:B:2002:CTN:N4	7:B:3001:HOH:O	1.84	1.08
1:A:1119:ARG:O	1:A:1123:PRO:HD2	1.67	0.94
5:A:2002:CTN:N4	7:A:3001:HOH:O	1.86	0.94
1:B:1018:VAL:HG23	1:B:1019:ARG:O	1.67	0.93
3:G:8:DT:H2"	3:G:9:DG:C8	2.05	0.92
1:B:1007:ASP:OD2	1:B:1009:ALA:N	2.03	0.92
1:A:1090:CYS:HG	4:A:2001:ZN:ZN	0.69	0.91
1:A:1114:TYR:OH	5:A:2002:CTN:C5'	2.18	0.90
1:B:1006:MET:HG2	1:B:1007:ASP:H	1.35	0.90
1:A:1115:PHE:HA	1:A:1122:GLU:HG2	1.52	0.89
1:B:1168:ASN:HD22	1:B:1171:ARG:HE	1.21	0.87
1:A:1119:ARG:O	1:A:1123:PRO:CD	2.24	0.85
1:A:1118:ASP:O	1:A:1121:ALA:N	2.10	0.84
1:A:1019:ARG:O	1:A:1020:TRP:CD2	2.34	0.81
1:A:172:TYR:CZ	1:A:175:GLY:HA2	2.17	0.80
3:G:7:DT:H2"	3:G:8:DT:H5'	1.64	0.79
1:A:179:ILE:CG2	1:A:371:ALA:HB2	2.12	0.79
1:B:41:PRO:HG2	1:B:44:LEU:HB3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1045:ASP:OD2	1:B:1064:TYR:OH	2.01	0.77
1:A:1122:GLU:N	1:A:1123:PRO:CD	2.48	0.76
1:A:1027:THR:OG1	5:A:2002:CTN:O2	2.04	0.75
1:B:179:ILE:HG22	1:B:371:ALA:HB2	1.68	0.74
1:A:1114:TYR:OH	5:A:2002:CTN:H5'1	1.88	0.74
1:B:1168:ASN:HD22	1:B:1171:ARG:NE	1.86	0.72
1:A:172:TYR:OH	1:A:175:GLY:HA2	1.88	0.72
1:A:179:ILE:HG22	1:A:371:ALA:CB	2.14	0.72
1:A:1018:VAL:HG23	1:A:1019:ARG:O	1.90	0.71
1:B:1086:PRO:HA	5:B:2002:CTN:HN41	1.56	0.70
1:A:41:PRO:HG2	1:A:44:LEU:HB3	1.71	0.70
1:B:1006:MET:HG2	1:B:1007:ASP:N	2.05	0.69
1:A:1051:ASN:O	1:A:1052:LYS:HD3	1.93	0.68
1:A:1138:ILE:HD13	1:A:1172:LEU:HB3	1.74	0.68
1:B:1027:THR:OG1	5:B:2002:CTN:C2	2.39	0.68
1:A:1115:PHE:HD1	1:A:1122:GLU:HB2	1.59	0.67
1:A:1119:ARG:O	1:A:1123:PRO:HG2	1.94	0.67
1:A:1050:ARG:O	1:A:1057:VAL:HG12	1.95	0.66
1:A:1115:PHE:CD1	1:A:1122:GLU:HB2	2.30	0.66
1:A:1115:PHE:CD1	1:A:1122:GLU:CB	2.78	0.66
1:A:1114:TYR:OH	5:A:2002:CTN:H5'2	1.97	0.65
1:A:1035:ARG:NH1	1:A:1042:GLU:OE2	2.29	0.65
1:B:1017:ASN:OD1	1:B:1017:ASN:O	2.14	0.65
1:A:1019:ARG:O	1:A:1020:TRP:CE3	2.50	0.65
1:A:1027:THR:OG1	5:A:2002:CTN:C2	2.45	0.65
1:A:66:ASP:OD1	1:A:67:ARG:N	2.29	0.65
1:B:1168:ASN:ND2	1:B:1171:ARG:HE	1.94	0.65
1:A:1114:TYR:O	1:A:1115:PHE:CD1	2.50	0.64
1:B:1086:PRO:HA	5:B:2002:CTN:N4	2.11	0.64
1:A:1029:LEU:O	1:A:1049:LEU:N	2.30	0.64
1:A:1119:ARG:O	1:A:1123:PRO:CG	2.46	0.64
1:B:99:ARG:HH21	1:B:104:LEU:HD21	1.62	0.64
2:D:10:DC:H2''	2:D:11:DA:C8	2.34	0.63
1:A:1122:GLU:N	1:A:1123:PRO:HD2	2.13	0.63
1:B:1035:ARG:NH1	1:B:1042:GLU:OE2	2.31	0.63
1:A:1017:ASN:OD1	1:A:1017:ASN:O	2.16	0.63
1:A:1086:PRO:HA	5:A:2002:CTN:N4	2.13	0.63
1:B:160:PRO:HG3	1:B:258:PRO:HA	1.82	0.62
1:B:172:TYR:HD1	1:B:173:GLU:H	1.46	0.61
1:B:206:ASN:OD1	1:B:209:THR:OG1	2.18	0.61
3:G:7:DT:C2'	3:G:8:DT:H5'	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1024:ARG:HD2	1:A:1112:ARG:HH12	1.66	0.61
1:B:1138:ILE:HD13	1:B:1172:LEU:HB3	1.82	0.61
1:B:194:THR:HG22	1:B:358:VAL:HG21	1.82	0.61
1:A:1168:ASN:HD22	1:A:1171:ARG:HH11	1.48	0.61
1:A:99:ARG:HH21	1:A:104:LEU:HD21	1.63	0.61
1:B:180:LYS:HA	1:B:371:ALA:HB3	1.82	0.61
1:A:1030:CYS:HA	1:A:1048:TYR:HA	1.82	0.61
1:A:1115:PHE:CE1	1:A:1122:GLU:HB3	2.36	0.61
1:B:110:ALA:HB3	1:B:263:LEU:HB3	1.81	0.61
1:B:172:TYR:CD1	1:B:173:GLU:N	2.68	0.61
1:B:250:THR:HG22	1:B:255:PRO:HA	1.83	0.60
1:A:206:ASN:OD1	1:A:209:THR:OG1	2.19	0.60
1:B:172:TYR:HD1	1:B:173:GLU:N	1.99	0.60
1:A:1027:THR:CB	5:A:2002:CTN:O2	2.50	0.60
1:A:172:TYR:CZ	1:A:175:GLY:CA	2.85	0.60
1:A:1045:ASP:OD2	1:A:1064:TYR:OH	2.19	0.58
1:B:1168:ASN:ND2	1:B:1171:ARG:HH11	2.01	0.58
1:A:1019:ARG:O	1:A:1020:TRP:CG	2.57	0.58
1:B:166:GLY:O	1:B:186:ASN:ND2	2.36	0.58
1:B:7:LYS:O	1:B:273:ASN:ND2	2.37	0.57
1:B:1154:ASN:OD1	1:B:1156:GLU:N	2.37	0.57
1:A:1115:PHE:HD1	1:A:1122:GLU:CB	2.18	0.56
1:B:186:ASN:OD1	1:B:187:ALA:N	2.39	0.56
1:A:1019:ARG:HG2	1:A:1020:TRP:H	1.69	0.56
1:A:186:ASN:OD1	1:A:187:ALA:N	2.38	0.56
1:A:190:LYS:HG2	1:A:362:LEU:HD12	1.86	0.56
2:D:5:DA:C2	3:G:9:DG:N2	2.74	0.55
1:A:1114:TYR:CE1	5:A:2002:CTN:H5'2	2.42	0.55
1:A:194:THR:HG22	1:A:358:VAL:HG21	1.88	0.55
1:A:1114:TYR:CZ	5:A:2002:CTN:C5'	2.89	0.55
1:A:1114:TYR:CZ	5:A:2002:CTN:H5'2	2.43	0.54
1:A:172:TYR:CZ	1:A:175:GLY:N	2.74	0.54
1:B:1116:CYS:O	1:B:1117:GLU:HB3	2.06	0.54
1:B:1016:LYS:O	1:B:1112:ARG:HD3	2.08	0.54
3:G:10:DA:H2''	3:G:11:DA:H8	1.72	0.53
1:A:1027:THR:HG1	5:A:2002:CTN:C2	2.22	0.53
1:B:9:VAL:N	1:B:59:ASP:OD2	2.39	0.53
1:A:1116:CYS:O	1:A:1117:GLU:HB2	2.09	0.53
1:A:220:LYS:NZ	1:A:222:GLU:OE2	2.42	0.53
1:A:1006:MET:O	1:A:1152:VAL:HG13	2.08	0.52
1:B:66:ASP:OD1	1:B:67:ARG:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:LYS:HG2	1:B:362:LEU:HD12	1.90	0.52
1:A:172:TYR:OH	1:A:175:GLY:CA	2.56	0.52
3:G:10:DA:H2"	3:G:11:DA:C8	2.44	0.52
1:A:56:ASP:OD1	1:A:57:GLY:N	2.37	0.52
1:B:56:ASP:OD1	1:B:57:GLY:N	2.34	0.51
1:A:1168:ASN:ND2	1:A:1171:ARG:HH11	2.08	0.51
1:A:288:ASP:OD1	1:A:307:SER:OG	2.27	0.50
1:A:1115:PHE:CE1	1:A:1122:GLU:CB	2.94	0.50
1:A:166:GLY:O	1:A:186:ASN:ND2	2.44	0.50
1:B:62:PHE:HA	1:B:264:SER:O	2.11	0.50
1:A:1027:THR:HG23	1:A:1084:TRP:H	1.76	0.50
1:A:110:ALA:HB3	1:A:263:LEU:HB3	1.93	0.50
1:B:80:ILE:HG22	1:B:278:LYS:HE2	1.93	0.50
1:B:8:LEU:HB2	1:B:36:VAL:HG22	1.93	0.49
1:B:1168:ASN:HD22	1:B:1171:ARG:HH11	1.60	0.49
1:A:1118:ASP:C	1:A:1120:LYS:N	2.64	0.49
1:B:129:THR:HB	1:B:131:GLU:OE1	2.13	0.49
1:B:1168:ASN:HD22	1:B:1171:ARG:CZ	2.26	0.48
1:A:1050:ARG:C	1:A:1057:VAL:HG12	2.33	0.48
1:B:1007:ASP:OD2	1:B:1008:PRO:N	2.46	0.48
1:B:1168:ASN:HD22	1:B:1171:ARG:NH1	2.12	0.48
1:B:159:TRP:CE2	1:B:163:ALA:HB2	2.48	0.48
2:D:10:DC:H2"	2:D:11:DA:H8	1.76	0.48
1:A:337:MET:O	1:A:340:PHE:HB3	2.13	0.48
1:B:1027:THR:O	1:B:1057:VAL:HG11	2.14	0.48
1:B:295:ASN:OD1	1:B:299:PRO:HA	2.13	0.48
1:A:1052:LYS:HB2	1:A:1060:LEU:HD11	1.95	0.48
1:B:47:LYS:O	1:B:51:VAL:HG23	2.14	0.48
1:A:3:ILE:HD11	1:A:59:ASP:OD1	2.14	0.48
1:B:1141:TYR:HE1	1:B:1161:ALA:HB2	1.79	0.48
1:A:1114:TYR:O	1:A:1115:PHE:CG	2.66	0.48
2:D:7:DG:H2"	2:D:8:DG:C8	2.49	0.47
1:B:337:MET:O	1:B:340:PHE:HB3	2.14	0.47
5:A:2002:CTN:C5	7:A:3001:HOH:O	2.37	0.47
1:B:116:LEU:HD22	1:B:249:PRO:HD3	1.96	0.47
1:B:1008:PRO:HG3	1:B:1153:GLU:O	2.14	0.47
1:B:15:ASP:N	1:B:15:ASP:OD1	2.47	0.47
1:B:88:ASP:O	1:B:89:LYS:C	2.51	0.47
1:A:1114:TYR:CZ	5:A:2002:CTN:H5'1	2.49	0.47
1:B:172:TYR:HE1	1:B:175:GLY:CA	2.28	0.47
2:D:8:DG:H2"	2:D:9:DC:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1071:ASP:O	1:B:1073:GLY:N	2.45	0.47
1:A:47:LYS:O	1:A:51:VAL:HG23	2.15	0.47
1:B:220:LYS:NZ	1:B:222:GLU:OE2	2.47	0.47
1:A:160:PRO:HG3	1:A:258:PRO:HA	1.95	0.46
1:A:1114:TYR:CG	1:A:1115:PHE:N	2.83	0.46
1:A:1168:ASN:HD22	1:A:1171:ARG:NH1	2.12	0.46
1:B:1168:ASN:ND2	1:B:1171:ARG:NH1	2.63	0.46
3:G:7:DT:H1'	3:G:8:DT:H5'	1.98	0.46
1:A:1052:LYS:HD2	1:A:1052:LYS:HA	1.89	0.46
1:B:182:VAL:HG21	1:B:369:ALA:O	2.16	0.46
1:A:98:VAL:O	1:A:105:ILE:HG13	2.15	0.46
2:D:7:DG:H2''	2:D:8:DG:H8	1.81	0.46
1:A:182:VAL:HG21	1:A:369:ALA:O	2.16	0.46
1:A:1122:GLU:O	1:A:1126:LEU:HG	2.16	0.45
1:A:1027:THR:HB	5:A:2002:CTN:O2	2.16	0.45
1:B:1168:ASN:ND2	1:B:1171:ARG:NE	2.59	0.45
1:A:1086:PRO:HA	5:A:2002:CTN:HN42	1.82	0.45
1:A:295:ASN:OD1	1:A:299:PRO:HA	2.17	0.45
1:A:1115:PHE:HE1	1:A:1122:GLU:HB3	1.82	0.45
1:A:200:ILE:HB	1:A:207:ALA:HB2	1.99	0.45
1:A:182:VAL:O	1:A:366:GLN:NE2	2.38	0.45
1:A:202:ASN:OD1	1:A:202:ASN:N	2.49	0.45
1:B:1006:MET:CG	1:B:1007:ASP:H	2.18	0.45
1:A:172:TYR:CE2	1:A:175:GLY:HA2	2.52	0.45
1:A:49:PRO:HG3	1:A:71:TYR:CE1	2.52	0.45
1:B:202:ASN:N	1:B:202:ASN:OD1	2.50	0.44
1:B:193:LEU:HD23	1:B:358:VAL:HG13	2.00	0.44
1:B:29:GLU:OE1	1:B:35:LYS:HG3	2.18	0.44
1:A:8:LEU:HB2	1:A:36:VAL:HG22	2.00	0.44
1:B:98:VAL:O	1:B:105:ILE:HG13	2.17	0.44
2:D:11:DA:C2	3:G:3:DG:N2	2.86	0.44
2:D:11:DA:H2''	2:D:12:DG:O5'	2.18	0.44
1:A:1098:LEU:HD23	1:A:1132:ALA:HB1	2.00	0.44
1:B:1007:ASP:HB3	1:B:1010:THR:HB	1.99	0.44
1:B:88:ASP:O	1:B:90:LEU:N	2.51	0.43
1:A:1122:GLU:H	1:A:1123:PRO:HD2	1.83	0.43
1:B:123:LEU:HA	1:B:123:LEU:HD23	1.86	0.43
1:B:1148:TRP:CD1	1:B:1159:PHE:HB2	2.53	0.43
1:A:1141:TYR:HE1	1:A:1161:ALA:HB2	1.84	0.43
1:A:1118:ASP:O	1:A:1119:ARG:C	2.57	0.43
1:A:203:LYS:HD3	1:A:203:LYS:HA	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:TYR:CE1	1:B:175:GLY:HA2	2.54	0.43
1:B:288:ASP:OD1	1:B:307:SER:OG	2.33	0.43
1:A:1168:ASN:ND2	1:A:1171:ARG:NH1	2.67	0.43
1:B:46:GLU:O	1:B:49:PRO:HD2	2.18	0.43
1:A:197:VAL:O	1:A:200:ILE:HG12	2.19	0.42
1:A:7:LYS:O	1:A:273:ASN:ND2	2.52	0.42
1:B:233:TRP:CH2	1:B:317:ARG:HB3	2.54	0.42
1:B:8:LEU:HA	1:B:59:ASP:OD2	2.20	0.42
1:A:1103:ASN:OD1	1:A:1103:ASN:N	2.52	0.42
1:B:1006:MET:SD	1:B:1011:PHE:HB2	2.59	0.42
1:A:1044:LEU:HB3	1:A:1045:ASP:H	1.75	0.42
1:A:1116:CYS:O	1:A:1118:ASP:N	2.43	0.42
1:A:123:LEU:HA	1:A:123:LEU:HD23	1.90	0.42
1:A:159:TRP:CE2	1:A:163:ALA:HB2	2.55	0.42
1:A:1029:LEU:O	1:A:1048:TYR:HA	2.20	0.41
1:B:197:VAL:HG12	1:B:201:LYS:HE2	2.01	0.41
1:A:1027:THR:O	1:A:1057:VAL:HG11	2.20	0.41
1:A:1058:ALA:O	1:A:1062:LEU:HG	2.20	0.41
1:A:1177:ARG:HD2	1:A:1177:ARG:HH11	1.68	0.41
1:A:233:TRP:CH2	1:A:317:ARG:HB3	2.55	0.41
1:A:45:GLU:HG3	1:A:67:ARG:HH22	1.84	0.41
1:B:179:ILE:HG23	1:B:336:GLN:HG2	2.02	0.41
1:A:1122:GLU:CB	1:A:1123:PRO:HD3	2.50	0.41
1:B:163:ALA:HA	1:B:167:GLY:HA3	2.02	0.41
1:A:193:LEU:O	1:A:197:VAL:HG23	2.20	0.41
1:B:116:LEU:HB2	1:B:248:LEU:HD23	2.02	0.41
1:B:164:ALA:HB2	1:B:256:SER:HA	2.02	0.41
1:B:1152:VAL:HG12	1:B:1153:GLU:N	2.36	0.41
1:A:1117:GLU:C	1:A:1119:ARG:H	2.24	0.41
1:A:172:TYR:CE1	1:A:175:GLY:N	2.73	0.41
1:A:250:THR:HG22	1:A:255:PRO:HA	2.02	0.40
1:B:1044:LEU:HB3	1:B:1045:ASP:H	1.69	0.40
1:B:1058:ALA:O	1:B:1062:LEU:HG	2.21	0.40
3:G:8:DT:H2"	3:G:9:DG:H8	1.73	0.40
1:A:1035:ARG:HH22	1:A:1074:ARG:NH1	2.19	0.40
1:B:51:VAL:HG12	1:B:56:ASP:HB3	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:DG:O4'	2:D:12:DG:C2'[1_545]	1.99	0.21
3:G:9:DG:OP1	1:A:1119:ARG:NH2[1_455]	2.16	0.04

## 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	539/549 (98%)	518 (96%)	21 (4%)	0	100	100
1	B	539/549 (98%)	519 (96%)	20 (4%)	0	100	100
All	All	1078/1098 (98%)	1037 (96%)	41 (4%)	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	438/453 (97%)	427 (98%)	11 (2%)	47	76
1	B	439/453 (97%)	429 (98%)	10 (2%)	50	77
All	All	877/906 (97%)	856 (98%)	21 (2%)	49	76

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	88	ASP
1	B	172	TYR

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Mol	Chain	Res	Type
1	B	202	ASN
1	B	359	ASP
1	B	1007	ASP
1	B	1026	GLU
1	B	1051	ASN
1	B	1055	CYS
1	B	1093	HIS
1	B	1119	ARG
1	A	88	ASP
1	A	155	PRO
1	A	202	ASN
1	A	359	ASP
1	A	1026	GLU
1	A	1051	ASN
1	A	1055	CYS
1	A	1120	LYS
1	A	1122	GLU
1	A	1154	ASN
1	A	1171	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1017	ASN
1	B	1051	ASN
1	B	1168	ASN
1	B	1175	GLN
1	A	1017	ASN
1	A	1168	ASN
1	A	1175	GLN

### 5.3.3 RNA ⓘ

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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z  > 2$
5	CTN	A	2002	-	15,18,18	0.80	0	17,26,26	1.64	3 (17%)
5	CTN	B	2002	-	15,18,18	0.79	0	17,26,26	1.67	3 (17%)

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
5	CTN	A	2002	-	-	0/4/22/22	0/2/2/2
5	CTN	B	2002	-	-	3/4/22/22	0/2/2/2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2002	CTN	C2-N3-C4	3.99	120.38	116.34
5	A	2002	CTN	C2-N3-C4	3.93	120.32	116.34
5	B	2002	CTN	C3'-C2'-C1'	3.64	106.46	100.98
5	A	2002	CTN	C3'-C2'-C1'	3.54	106.31	100.98
5	B	2002	CTN	N4-C4-N3	2.21	119.98	116.49
5	A	2002	CTN	N4-C4-N3	2.20	119.96	116.49

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	2002	CTN	C2'-C1'-N1-C6
5	B	2002	CTN	O4'-C4'-C5'-O5'
5	B	2002	CTN	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2002	CTN	17	0
5	B	2002	CTN	6	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	543/549 (98%)	0.08	8 (1%) 73 61	66, 103, 138, 169	0
1	B	543/549 (98%)	0.06	8 (1%) 73 61	69, 106, 136, 175	0
2	D	12/12 (100%)	0.43	0 100 100	146, 168, 175, 179	0
3	G	12/12 (100%)	0.53	0 100 100	154, 168, 181, 198	0
All	All	1110/1122 (98%)	0.08	16 (1%) 75 63	66, 105, 144, 198	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1022	LYS	3.6
1	B	352	ALA	3.6
1	A	1181	GLN	3.5
1	B	1042	GLU	3.0
1	A	175	GLY	2.5
1	A	355	ARG	2.4
1	B	1041	SER	2.4
1	B	52	ALA	2.4
1	A	354	GLY	2.3
1	B	49	PRO	2.3
1	B	174	ASN	2.3
1	B	329	GLU	2.3
1	A	1021	ALA	2.3
1	A	196	LEU	2.1
1	B	1021	ALA	2.1
1	A	362	LEU	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 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. 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
6	CA	B	2003	1/1	0.21	0.18	120,120,120,120	0
6	CA	A	2003	1/1	0.77	0.21	118,118,118,118	0
5	CTN	B	2002	17/17	0.82	0.22	94,134,154,169	0
5	CTN	A	2002	17/17	0.83	0.20	92,129,156,158	0
4	ZN	B	2001	1/1	0.94	0.23	122,122,122,122	0
4	ZN	A	2001	1/1	0.97	0.19	136,136,136,136	0

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

There are no such residues in this entry.