



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:18 AM GMT

PDB ID : 3E3Y
Title : Q138F HincII bound to GTTAAC and cocrystallized with 5 mM Ca²⁺
Authors : Horton, N.C.; Babic, A.C.; Little, E.J.; Manohar, V.M.
Deposited on : 2008-08-08
Resolution : 2.13 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
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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

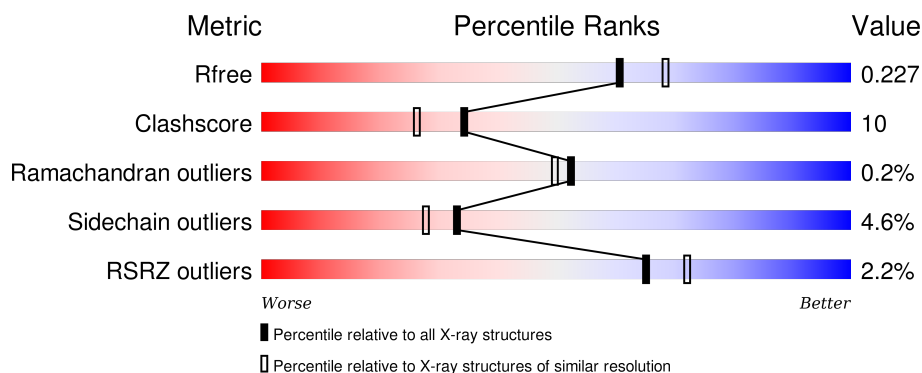
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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}	91344	1693 (2.16-2.12)
Clashscore	102246	1824 (2.16-2.12)
Ramachandran outliers	100387	1798 (2.16-2.12)
Sidechain outliers	100360	1798 (2.16-2.12)
RSRZ outliers	91569	1699 (2.16-2.12)

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	257	<div> <div></div> <div>79%</div> <div>13%</div> <div>6%</div> </div>
1	B	257	<div> <div>3%</div> <div>72%</div> <div>20%</div> <div>6%</div> </div>
2	E	14	<div> <div>57%</div> <div>43%</div> </div>
2	F	14	<div> <div>79%</div> <div>21%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NA	A	260	-	-	-	X
4	NA	B	260	-	-	-	X
4	NA	F	15	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4873 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 HindII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1929	1259	302	362	6			
1	B	241	Total	C	N	O	S	0	0	0
			1923	1253	305	359	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ASN	LYS	CONFLICT	UNP P44413
A	138	PHE	GLN	ENGINEERED	UNP P44413
B	67	ASN	LYS	CONFLICT	UNP P44413
B	138	PHE	GLN	ENGINEERED	UNP P44413

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	14	Total	C	N	O	P	0	0	0
			284	135	54	82	13			
2	F	14	Total	C	N	O	P	0	0	0
			284	135	54	82	13			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	199	Total O 199 199	0	0
5	B	161	Total O 161 161	0	0
5	E	47	Total O 47 47	0	0
5	F	41	Total O 41 41	0	0

- Molecule 1: Type-2 restriction enzyme HindII



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.48Å 91.64Å 65.78Å 90.00° 104.92° 90.00°	Depositor
Resolution (Å)	43.06 – 2.13 43.06 – 2.13	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.06-2.13) 99.9 (43.06-2.13)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.180 , 0.234 0.170 , 0.227	Depositor DCC
R_{free} test set	1605 reflections (4.96%)	DCC
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 62.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 32369 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4873	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CA

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	0.31	0/1973	0.46	0/2678
1	B	0.29	0/1967	0.46	0/2666
2	E	0.68	0/318	1.41	3/489 (0.6%)
2	F	0.69	0/318	1.37	3/489 (0.6%)
All	All	0.38	0/4576	0.69	6/6322 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	12	DG	O4'-C1'-N9	10.94	115.66	108.00
2	F	12	DG	O4'-C1'-N9	9.29	114.50	108.00
2	E	12	DG	C1'-O4'-C4'	-6.58	103.52	110.10
2	F	6	DT	C5-C4-O4	-5.63	120.96	124.90
2	E	3	DC	O4'-C1'-N1	-5.23	104.34	108.00
2	F	12	DG	C1'-O4'-C4'	-5.05	105.05	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1929	0	1813	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1923	0	1822	51	0
2	E	284	0	158	4	0
2	F	284	0	158	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	F	1	0	0	0	0
5	A	199	0	0	2	0
5	B	161	0	0	2	0
5	E	47	0	0	0	0
5	F	41	0	0	0	0
All	All	4873	0	3951	84	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 10.

All (84) 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:70:ILE:HD13	1:B:79:LEU:HD21	1.53	0.90
1:A:11:ILE:HG12	1:A:44:PHE:CE2	2.21	0.76
1:B:11:ILE:HG12	1:B:44:PHE:CE2	2.23	0.74
1:B:141:ASN:ND2	1:B:209:GLN:HE21	1.87	0.72
1:A:10:ASP:O	1:A:14:ILE:HG12	1.89	0.72
1:A:4:ILE:HD11	1:A:126:LEU:HD22	1.72	0.69
1:A:14:ILE:HG13	1:A:44:PHE:CE1	2.27	0.69
1:B:195:PRO:HA	1:B:198:LEU:HD23	1.73	0.69
1:B:170:GLU:HB2	1:B:212:VAL:HB	1.75	0.68
1:B:127:ASP:HB3	1:B:168:TYR:CD1	2.31	0.66
1:A:110:ASN:HD22	1:A:110:ASN:N	1.93	0.65
1:B:38:GLU:C	1:B:40:LEU:H	2.01	0.64
1:A:132:ASN:HD22	1:A:134:SER:H	1.44	0.63
1:A:14:ILE:HG13	1:A:44:PHE:HE1	1.63	0.63
1:A:132:ASN:HD22	1:A:132:ASN:C	2.02	0.63
1:B:73:HIS:HD2	1:B:97:GLU:OE2	1.82	0.62
1:A:132:ASN:ND2	1:A:134:SER:H	2.00	0.60
1:B:52:LEU:HD22	1:B:119:LYS:HB2	1.84	0.59
1:A:205:ALA:HA	1:B:203:ALA:O	2.02	0.59
1:B:67:ASN:HB3	1:B:70:ILE:HD12	1.85	0.59
1:A:127:ASP:HB3	1:A:168:TYR:CD1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:LYS:HB3	1:B:6:PRO:HD3	1.84	0.58
1:A:4:ILE:CD1	1:A:126:LEU:HD22	2.34	0.57
1:A:203:ALA:O	1:B:205:ALA:HA	2.04	0.57
1:A:108:LYS:HE3	1:A:110:ASN:ND2	2.19	0.57
1:B:195:PRO:HA	1:B:198:LEU:CD2	2.34	0.57
1:B:141:ASN:HD22	1:B:209:GLN:HE21	1.51	0.56
1:B:4:ILE:CD1	1:B:126:LEU:HD22	2.37	0.55
1:B:56:GLN:HE22	1:B:113:ALA:H	1.52	0.55
1:B:38:GLU:HG2	1:B:171:VAL:HG11	1.88	0.55
1:B:133:ILE:HD11	1:B:174:GLU:HB3	1.88	0.54
1:A:71:ILE:HD13	1:A:71:ILE:H	1.72	0.54
1:B:91:ARG:NE	1:B:108:LYS:HD3	2.22	0.54
1:B:91:ARG:CZ	1:B:108:LYS:HD3	2.37	0.54
1:B:109:GLN:NE2	1:B:110:ASN:N	2.56	0.53
1:B:56:GLN:NE2	1:B:113:ALA:H	2.06	0.53
1:B:140:PRO:HG3	5:B:279:HOH:O	2.08	0.52
1:A:194:GLU:HG3	5:A:299:HOH:O	2.08	0.52
1:A:85:LEU:HD22	1:A:163:LEU:HD21	1.92	0.52
1:A:110:ASN:N	5:A:440:HOH:O	2.43	0.51
1:A:123:TYR:O	1:A:164:PHE:HA	2.10	0.51
1:B:11:ILE:O	1:B:14:ILE:HG13	2.12	0.50
1:A:147:LYS:HA	1:A:150:GLN:HE21	1.76	0.50
1:B:108:LYS:HZ1	2:F:11:DC:H5''	1.77	0.50
1:A:173:TRP:CE3	1:A:180:LEU:HG	2.46	0.50
1:B:14:ILE:HD12	1:B:15:LEU:N	2.28	0.49
1:A:52:LEU:O	1:A:117:LEU:HA	2.13	0.49
1:A:4:ILE:HG13	1:A:117:LEU:HD22	1.95	0.49
1:B:108:LYS:NZ	2:F:11:DC:H5''	2.27	0.49
1:B:109:GLN:O	2:E:7:DT:H4'	2.13	0.48
1:B:38:GLU:C	1:B:40:LEU:N	2.66	0.48
1:A:4:ILE:HG23	1:A:11:ILE:HD12	1.96	0.47
1:B:41:VAL:HG21	1:B:169:LEU:CD2	2.45	0.47
1:B:109:GLN:NE2	1:B:110:ASN:H	2.13	0.47
1:B:38:GLU:O	1:B:40:LEU:HD23	2.14	0.47
1:B:169:LEU:HD12	1:B:186:SER:O	2.15	0.47
1:B:38:GLU:O	1:B:40:LEU:N	2.48	0.46
1:B:73:HIS:CD2	1:B:97:GLU:OE2	2.67	0.46
1:A:132:ASN:HD21	1:A:134:SER:HB3	1.82	0.45
1:B:127:ASP:HB3	1:B:168:TYR:CE1	2.51	0.45
1:B:72:GLY:HA2	1:B:97:GLU:HG3	1.99	0.44
1:A:5:LYS:HB3	1:A:6:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ILE:HG12	1:A:208:ILE:HD13	2.00	0.44
1:A:110:ASN:ND2	1:A:110:ASN:N	2.61	0.44
1:B:140:PRO:HD2	1:B:210:PHE:O	2.17	0.44
1:B:139:ALA:HA	1:B:140:PRO:HD3	1.87	0.43
1:A:85:LEU:HA	1:A:85:LEU:HD12	1.90	0.43
1:B:67:ASN:N	1:B:68:PRO:HD3	2.34	0.42
1:B:167:ASN:ND2	5:B:303:HOH:O	2.52	0.42
1:B:14:ILE:HD12	1:B:15:LEU:HG	2.02	0.42
1:B:108:LYS:HZ2	1:B:108:LYS:HB2	1.84	0.41
1:B:123:TYR:O	1:B:164:PHE:HA	2.20	0.41
1:B:141:ASN:ND2	2:E:9:DA:H62	2.19	0.41
1:B:109:GLN:N	1:B:109:GLN:HE21	2.19	0.41
1:B:42:TYR:CE2	1:B:55:LYS:HG2	2.55	0.41
1:B:70:ILE:CD1	1:B:79:LEU:HD21	2.38	0.41
2:E:8:DA:H2'	2:E:9:DA:O4'	2.21	0.41
1:A:59:TYR:HH	1:A:123:TYR:HH	1.65	0.41
1:A:93:LYS:HE3	2:E:14:DC:OP2	2.21	0.41
1:A:3:PHE:CZ	1:A:119:LYS:HB3	2.56	0.41
1:A:127:ASP:HB3	1:A:168:TYR:CE1	2.56	0.40
1:B:57:TYR:CE1	1:B:107:GLU:HB2	2.56	0.40
1:B:39:LYS:HE3	1:B:39:LYS:HB3	1.92	0.40
1:A:132:ASN:ND2	1:A:132:ASN:C	2.73	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	236/257 (92%)	230 (98%)	6 (2%)	0	100	100
1	B	237/257 (92%)	229 (97%)	7 (3%)	1 (0%)	39	33
All	All	473/514 (92%)	459 (97%)	13 (3%)	1 (0%)	52	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	39	LYS

5.3.2 Protein sidechains ⓘ

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	197/229 (86%)	189 (96%)	8 (4%)	37	34
1	B	196/229 (86%)	186 (95%)	10 (5%)	29	24
All	All	393/458 (86%)	375 (95%)	18 (5%)	33	28

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	ILE
1	A	85	LEU
1	A	110	ASN
1	A	118	VAL
1	A	132	ASN
1	A	138	PHE
1	A	148	LEU
1	A	231	LEU
1	B	38	GLU
1	B	55	LYS
1	B	86	LEU
1	B	108	LYS
1	B	109	GLN
1	B	138	PHE
1	B	198	LEU
1	B	215	LEU
1	B	216	ASP
1	B	231	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	48	ASN
1	A	98	ASN
1	A	103	ASN
1	A	132	ASN
1	A	150	GLN
1	A	211	HIS
1	B	56	GLN
1	B	73	HIS
1	B	109	GLN
1	B	141	ASN
1	B	167	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 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 [i](#)

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 ⓘ

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, 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	242/257 (94%)	-0.19	3 (1%) 81 85	18, 29, 43, 61	0
1	B	241/257 (93%)	0.05	8 (3%) 50 59	19, 34, 51, 66	0
2	E	14/14 (100%)	-0.47	0 100 100	20, 28, 32, 33	0
2	F	14/14 (100%)	-0.49	0 100 100	19, 28, 37, 39	0
All	All	511/542 (94%)	-0.09	11 (2%) 65 72	18, 31, 49, 66	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	177	GLY	4.3
1	B	40	LEU	3.8
1	A	20	VAL	3.2
1	B	220	ASN	3.1
1	A	175	LEU	2.9
1	B	20	VAL	2.6
1	B	181	VAL	2.6
1	B	41	VAL	2.2
1	B	18	GLN	2.1
1	B	222	THR	2.0
1	B	109	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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(Å ²)	Q<0.9
4	NA	A	260	1/1	0.97	0.18	4.36	30,30,30,30	0
4	NA	B	260	1/1	0.97	0.16	3.46	33,33,33,33	0
4	NA	F	15	1/1	0.96	0.14	2.52	39,39,39,39	0
3	CA	B	259	1/1	0.99	0.11	-0.85	30,30,30,30	0
3	CA	A	259	1/1	0.99	0.08	-1.87	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.