Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2CKU
Title	:	Solution structure of 2F13F1 from human fibronectin
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Deposited on	:	2006-04-21

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

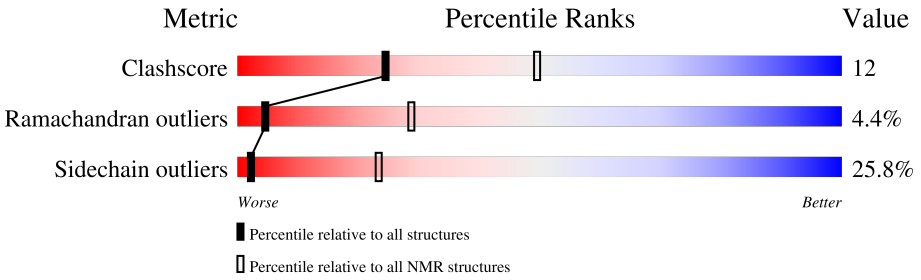
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.20
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.20

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	90	61% 30% 7% ••

2 Ensemble composition and analysis (i)

This entry contains 15 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:64-A:121 (58)	0.52	14
2	A:122-A:151 (30)	0.39	12

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 3 single-model clusters were found.

Cluster number	Models
1	3, 4, 5, 6, 7, 9, 10, 11, 13, 15
2	1, 2
Single-model clusters	8; 12; 14

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1348 atoms, of which 650 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called FIBRONECTIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	89	1348	427	650	126	135	10	0

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: FIBRONECTIN

Chain A: 61% 30% 7% ••

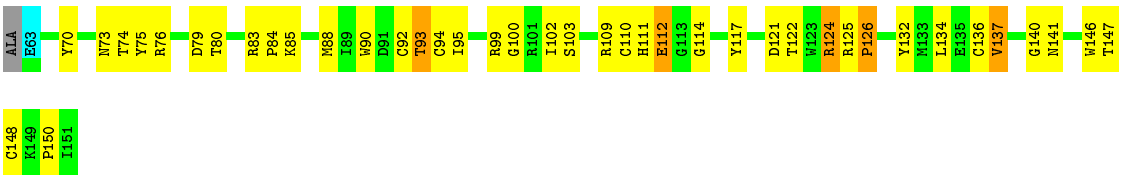
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: FIBRONECTIN

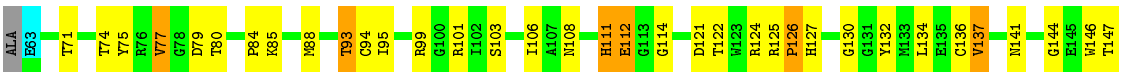
Chain A: 52% 40% 6% ••



4.2.2 Score per residue for model 2

• Molecule 1: FIBRONECTIN

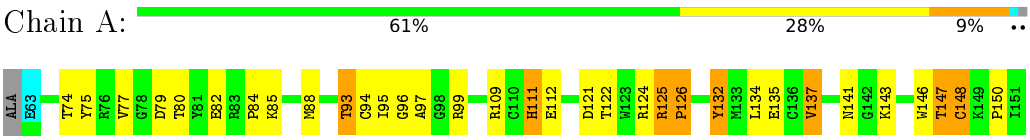
Chain A: 57% 34% 7% ••



4.2.3 Score per residue for model 3

- Molecule 1: FIBRONECTIN

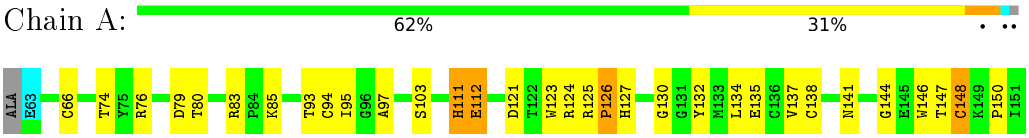
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: FIBRONECTIN

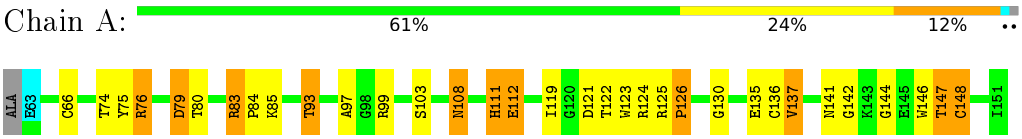
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: FIBRONECTIN

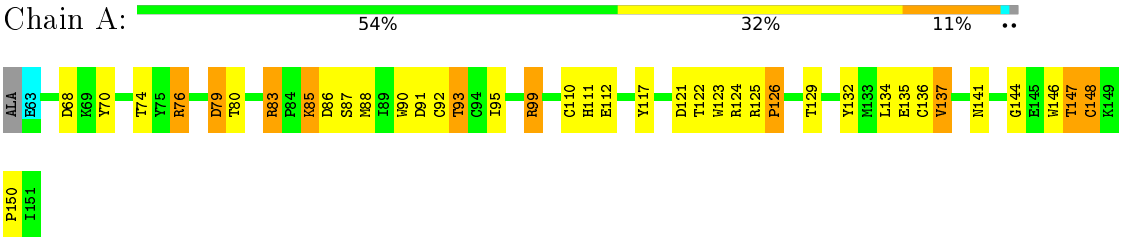
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: FIBRONECTIN

Chain A:



4.2.7 Score per residue for model 7

- Molecule 1: FIBRONECTIN

Chain A: 56% 33% 9% ••

ALA E63 C66 Y70 T71 T74 Y75 R76 D79 T80 Y81 E82 R83 P84 K85 M88 C92 T93 R99 I102 I106 A107 N108 H111 E112 D121 T122 W123 R124 H127 G130 G131 Y132 M133 L134 E135 C136 V137 N141 G142 K143 W146 T147 C148 K149 P150 I151

4.2.8 Score per residue for model 8

- Molecule 1: FIBRONECTIN

Chain A: 57% 37% • ••

ALA E63 C66 T74 Y75 R76 D79 T80 Y81 E82 R83 P84 K85 M88 I89 W90 D91 C92 T93 C94 I95 R99 I102 C110 H111 E112 Y117 T122 W123 R124 R125 P126 H127 E128 T129 G130 G131 Y132 M133 L134 V137 N141 G142 K143 W146 T147 P150 I151

4.2.9 Score per residue for model 9

- Molecule 1: FIBRONECTIN

Chain A: 59% 29% 10% ••

ALA E63 Y70 T74 T80 Y81 E82 R83 P84 K85 D86 S87 M88 C92 T93 R99 I106 A107 N108 H111 E112 D121 T122 W123 R124 R125 P126 H127 Y132 M133 L134 E135 C136 V137 C138 N141 G142 K143 W146 T147 C148 I151

4.2.10 Score per residue for model 10

- Molecule 1: FIBRONECTIN

Chain A: 57% 30% 10% •••

ALA E63 Y70 T71 T74 Y75 R76 V77 T80 R83 P84 K85 M88 I89 W90 T93 C94 I95 R99 I106 A107 N108 R109 C110 H111 E112 D121 T122 W123 R124 R125 P126 H127 G130 G131 Y132 M133 L134 E135 C136 V137 G144 E145 W146 T147 C148 K149 P150 I151

4.2.11 Score per residue for model 11

- Molecule 1: FIBRONECTIN

Chain A: 56% 34% 8% ••

ALA E63 T74 Y75 R76 V77 G78 D79 T80 Y81 E82 R83 P84 K85 M88 I89 W90 T93 C94 R99 I106 A107 N108 H111 E112 D121 T122 W123 R124 R125 P126 H127 G130 G131 Y132 M133 L134 E135 C136 V137 C138 N141 G142 W146 T147 C148 K149 P150 I151

4.2.12 Score per residue for model 12

- Molecule 1: FIBRONECTIN

Chain A: 53% 39% • •••

ALA E63 C66 Y70 N73 T74 Y75 D79 T80 Y81 E82 R83 P84 K85 M88 I89 W90 D91 C92 T93 C94 I95 R99 S103 I106 C110 H111 E112 G113 G114 Q115 S116 Y117 T122 W123 R124 R125 P126 H127 Y132 M133 L134 E135 C136 V137 N141 G142 K143

W146 T147 C148 K149 P150 I151

4.2.13 Score per residue for model 13

- Molecule 1: FIBRONECTIN

Chain A: 60% 29% 9% ••

ALA E63 C66 T74 Y75 R76 D79 T80 R83 P84 K85 M88 T93 G98 I102 N108 H111 E112 D121 T122 W123 R124 R125 P126 H127 E128 T129 Y132 M133 L134 E135 C136 V137 N141 G144 E145 W146 T147 C148 I151

4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: FIBRONECTIN

Chain A: 59% 30% 9% ••

ALA E63 T71 T74 Y75 R76 D79 T80 Y81 E82 R83 P84 K85 M88 T93 G98 R99 I106 C110 H111 E112 G113 G114 Y117 T122 H127 Y132 M133 L134 E135 C136 V137 C138 L139 G140 N141 W146 T147 C148 K149 P150 I151

4.2.15 Score per residue for model 15

- Molecule 1: FIBRONECTIN

Chain A: 58% 30% 10% ••

ALA E63 C66 Y70 T74 Y75 T80 Y81 E82 R83 P84 K85 M88 I89 W90 T93 C94 I95 G96 A97 G98 R99 S103 I106 A107 N108 R109 C110 H111 E112 I119 G120 D121 T122 W123 P126 G130 E135 C136 V137 C138 N141 G142 W146 T147 C148

I151

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *CNS*.

Of the 50 calculated structures, 15 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CNS	refinement	
NMRView	structure solution	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	689	642	640	16±3
All	All	10335	9630	9600	235

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 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:137:VAL:HG23	1:A:147:THR:HG23	0.90	1.40	14	1
1:A:137:VAL:HG23	1:A:147:THR:CG2	0.88	1.98	14	1
1:A:80:THR:HG22	1:A:93:THR:HG23	0.87	1.44	12	15
1:A:137:VAL:HG23	1:A:147:THR:HG22	0.84	1.48	3	3
1:A:137:VAL:CG2	1:A:147:THR:HG22	0.79	2.08	3	3
1:A:137:VAL:HG23	1:A:147:THR:O	0.67	1.90	15	3
1:A:122:THR:HG22	1:A:137:VAL:HG23	0.64	1.67	1	10
1:A:84:PRO:HA	1:A:88:MET:O	0.63	1.94	14	11
1:A:80:THR:HG22	1:A:93:THR:CG2	0.60	2.24	12	11
1:A:127:HIS:HB2	1:A:132:TYR:O	0.57	2.00	13	2
1:A:125:ARG:O	1:A:126:PRO:O	0.56	2.24	13	11
1:A:111:HIS:O	1:A:112:GLU:HB2	0.55	2.01	9	7
1:A:127:HIS:ND1	1:A:134:LEU:HD22	0.55	2.16	14	3
1:A:75:TYR:HB2	1:A:94:CYS:SG	0.55	2.42	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:THR:CG2	1:A:93:THR:HG23	0.54	2.31	9	15
1:A:66:CYS:HB3	1:A:102:ILE:HD13	0.54	1.80	8	2
1:A:82:GLU:HA	1:A:90:TRP:O	0.54	2.02	11	2
1:A:111:HIS:O	1:A:112:GLU:HB3	0.53	2.04	14	6
1:A:137:VAL:CG2	1:A:147:THR:OG1	0.52	2.57	14	1
1:A:71:THR:OG1	1:A:75:TYR:OH	0.52	2.27	7	3
1:A:95:ILE:HG22	1:A:95:ILE:O	0.52	2.04	6	1
1:A:124:ARG:CB	1:A:135:GLU:HA	0.51	2.36	9	2
1:A:81:TYR:CZ	1:A:92:CYS:HB3	0.51	2.41	7	1
1:A:83:ARG:HD2	1:A:84:PRO:N	0.50	2.21	14	2
1:A:70:TYR:HB3	1:A:83:ARG:HD3	0.50	1.82	12	1
1:A:135:GLU:O	1:A:148:CYS:HA	0.50	2.07	14	10
1:A:83:ARG:HD3	1:A:83:ARG:C	0.49	2.27	6	3
1:A:111:HIS:O	1:A:112:GLU:CB	0.49	2.60	1	3
1:A:110:CYS:O	1:A:117:TYR:O	0.49	2.30	1	5
1:A:95:ILE:HD12	1:A:95:ILE:N	0.48	2.24	6	2
1:A:66:CYS:N	1:A:75:TYR:O	0.47	2.45	12	3
1:A:100:GLY:O	1:A:102:ILE:HD12	0.47	2.10	1	1
1:A:122:THR:HG22	1:A:137:VAL:CG2	0.47	2.40	8	1
1:A:90:TRP:CH2	1:A:106:ILE:HG12	0.47	2.45	15	2
1:A:137:VAL:HG23	1:A:147:THR:OG1	0.46	2.10	14	1
1:A:73:ASN:O	1:A:75:TYR:CZ	0.46	2.68	1	2
1:A:85:LYS:HB3	1:A:90:TRP:CD1	0.46	2.46	8	2
1:A:77:VAL:HG13	1:A:95:ILE:O	0.46	2.10	3	1
1:A:137:VAL:N	1:A:147:THR:O	0.46	2.48	10	2
1:A:70:TYR:HB3	1:A:83:ARG:NE	0.46	2.24	7	2
1:A:70:TYR:CD2	1:A:83:ARG:HD3	0.46	2.45	1	3
1:A:127:HIS:CD2	1:A:130:GLY:HA3	0.46	2.45	8	6
1:A:85:LYS:O	1:A:87:SER:N	0.45	2.49	6	2
1:A:76:ARG:O	1:A:79:ASP:HB2	0.45	2.12	13	4
1:A:122:THR:HG22	1:A:137:VAL:HG12	0.45	1.87	10	3
1:A:137:VAL:HG23	1:A:147:THR:CB	0.45	2.41	14	1
1:A:83:ARG:HD3	1:A:84:PRO:N	0.45	2.26	7	1
1:A:81:TYR:CZ	1:A:92:CYS:HB2	0.45	2.47	8	2
1:A:134:LEU:HD12	1:A:150:PRO:HB3	0.45	1.88	6	9
1:A:127:HIS:CE1	1:A:129:THR:OG1	0.45	2.70	8	1
1:A:96:GLY:O	1:A:97:ALA:C	0.45	2.56	15	1
1:A:123:TRP:O	1:A:123:TRP:CG	0.44	2.71	6	4
1:A:123:TRP:O	1:A:123:TRP:CD1	0.44	2.70	15	1
1:A:66:CYS:O	1:A:75:TYR:N	0.44	2.50	13	3
1:A:71:THR:HG22	1:A:83:ARG:HG2	0.44	1.88	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:134:LEU:CD1	1:A:150:PRO:HB3	0.44	2.42	14	2
1:A:85:LYS:HB3	1:A:90:TRP:NE1	0.44	2.28	1	1
1:A:85:LYS:HB2	1:A:90:TRP:CD1	0.44	2.48	10	2
1:A:113:GLY:O	1:A:115:GLN:N	0.44	2.50	12	1
1:A:133:MET:O	1:A:151:ILE:N	0.43	2.51	9	1
1:A:108:ASN:O	1:A:119:ILE:HD13	0.43	2.13	5	1
1:A:137:VAL:HG12	1:A:147:THR:HG22	0.43	1.88	5	2
1:A:77:VAL:HA	1:A:94:CYS:SG	0.43	2.53	2	2
1:A:80:THR:HA	1:A:92:CYS:O	0.43	2.14	12	4
1:A:75:TYR:CE1	1:A:81:TYR:CG	0.42	3.06	14	1
1:A:109:ARG:HA	1:A:119:ILE:HD12	0.42	1.89	15	1
1:A:127:HIS:CE1	1:A:129:THR:HB	0.42	2.48	13	1
1:A:110:CYS:O	1:A:117:TYR:N	0.42	2.53	8	1
1:A:95:ILE:HD13	1:A:103:SER:HB3	0.41	1.92	1	2
1:A:70:TYR:HB3	1:A:83:ARG:CZ	0.41	2.45	9	1
1:A:127:HIS:CD2	1:A:132:TYR:CZ	0.41	3.07	9	1
1:A:70:TYR:CB	1:A:83:ARG:HD3	0.41	2.44	12	1
1:A:125:ARG:O	1:A:134:LEU:O	0.41	2.39	13	1
1:A:132:TYR:CZ	1:A:150:PRO:HB2	0.41	2.51	3	2
1:A:68:ASP:OD1	1:A:70:TYR:HB2	0.40	2.16	6	1
1:A:135:GLU:O	1:A:148:CYS:HB3	0.40	2.16	4	1
1:A:136:CYS:HA	1:A:147:THR:O	0.40	2.16	14	1
1:A:95:ILE:N	1:A:95:ILE:HD12	0.40	2.32	4	1
1:A:85:LYS:CB	1:A:90:TRP:CD1	0.40	3.04	6	1
1:A:75:TYR:CE2	1:A:81:TYR:CZ	0.40	3.09	7	1
1:A:75:TYR:CE1	1:A:81:TYR:CD1	0.40	3.09	15	1

6.3 Torsion angles (i)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	87/90 (97%)	72±2 (83±2%)	11±1 (13±2%)	4±1 (4±1%)	4	29
All	All	1305/1350 (97%)	1081 (83%)	166 (13%)	58 (4%)	4	29

All 16 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	126	PRO	13
1	A	112	GLU	10
1	A	144	GLY	6
1	A	114	GLY	4
1	A	97	ALA	4
1	A	143	LYS	4
1	A	142	GLY	3
1	A	99	ARG	2
1	A	130	GLY	2
1	A	86	ASP	2
1	A	106	ILE	2
1	A	98	GLY	2
1	A	124	ARG	1
1	A	140	GLY	1
1	A	96	GLY	1
1	A	131	GLY	1

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	73/74 (99%)	54±2 (74±3%)	19±2 (26±3%)	2 23
All	All	1095/1110 (99%)	813 (74%)	282 (26%)	2 23

All 42 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	74	THR	15
1	A	137	VAL	15
1	A	146	TRP	15
1	A	147	THR	15
1	A	141	ASN	14
1	A	85	LYS	14
1	A	93	THR	13
1	A	124	ARG	13

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Mol	Chain	Res	Type	Models (Total)
1	A	148	CYS	13
1	A	79	ASP	12
1	A	99	ARG	12
1	A	121	ASP	12
1	A	111	HIS	12
1	A	132	TYR	11
1	A	83	ARG	11
1	A	76	ARG	10
1	A	106	ILE	8
1	A	108	ASN	8
1	A	94	CYS	6
1	A	136	CYS	6
1	A	82	GLU	5
1	A	138	CYS	5
1	A	88	MET	5
1	A	103	SER	4
1	A	109	ARG	3
1	A	77	VAL	3
1	A	75	TYR	3
1	A	66	CYS	2
1	A	129	THR	2
1	A	89	ILE	2
1	A	95	ILE	2
1	A	101	ARG	1
1	A	125	ARG	1
1	A	143	LYS	1
1	A	91	ASP	1
1	A	92	CYS	1
1	A	149	LYS	1
1	A	71	THR	1
1	A	112	GLU	1
1	A	102	ILE	1
1	A	151	ILE	1
1	A	139	LEU	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided