Protein Data Bank Contents Guide:

Atomic Coordinate Entry Format Description

Version 3.30

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This format complies with the PDB Exchange Dictionary (PDBx) http://mmcif.pdb.org/dictionaries/mmcif_pdbx.dic/Index/index.html.

5. Secondary Structure Section

The secondary structure section of a PDB formatted file describes helices and sheets found in protein and polypeptide structures.

HELIX

Overview

HELIX records are used to identify the position of helices in the molecule. Helices are named, numbered, and classified by type. The residues where the helix begins and ends are noted, as well as the total length.

Record Format

COLUMNS	DATA TYPE	FIELD	DEFINITION
1 - 6	Record name	"HELIX "	
8 - 10	Integer	serNum	Serial number of the helix. This starts at 1 and increases incrementally.
12 - 14	LString(3)	helixID	Helix identifier. In addition to a serial number, each helix is given an alphanumeric character helix identifier.
16 - 18	Residue name	initResName	Name of the initial residue.
20	Character	initChainID	Chain identifier for the chain containing this helix.
22 - 25	Integer	initSeqNum	Sequence number of the initial residue.
26	AChar	initICode	Insertion code of the initial residue.
28 - 30	Residue name	endResName	Name of the terminal residue of the helix.
32	Character	endChainID	Chain identifier for the chain containing this helix.
34 - 37	Integer	endSeqNum	Sequence number of the terminal residue.
38	AChar	endICode	Insertion code of the terminal residue.
39 - 40	Integer	helixClass	Helix class (see below).
41 - 70	String	comment	Comment about this helix.
72 - 76	Integer	length	Length of this helix.

Details

^{*} Additional HELIX records with different serial numbers and identifiers occur if more than one helix is present.

- * The initial residue of the helix is the N-terminal residue.
- * Helices are classified as follows:

TYPE OF HELIX	CLASS NUMBER (COLUMNS 39 - 40)
Right-handed alpha (default) Right-handed omega Right-handed pi Right-handed gamma Right-handed 310 Left-handed alpha Left-handed omega Left-handed gamma 27 ribbon/helix Polyproline	1 2 3 4 5 6 7 8 9
LOTABLOTTHE	10

Relationships to Other Record Types

There may be related information in the REMARKs.

Example

	1			2		3			4	5	6	7	8
1234567	8901	2345	56789	901	23456	78901	123	45678	901	234567890123	45678901234	567890123	4567890
HELIX	1	HA	GLY	Α	86	GLY	Α	94	1				9
HELIX	2	HB	GLY	В	86	GLY	В	94	1				9
HELIX	21	21	PRO	J	385	LEU	J	388	5				4
HELIX	22	22	PHE	J	397	PHE	J	402	5				6

SHEET

Overview

SHEET records are used to identify the position of sheets in the molecule. Sheets are both named and numbered. The residues where the sheet begins and ends are noted.

Record Format

COLUMNS	DATA TYPE	FIELD	DEFINITION
1 - 6	Record name	"SHEET "	
8 - 10	Integer	strand	Strand number which starts at 1 for each strand within a sheet and increases by one.
12 - 14	LString(3)	sheetID	Sheet identifier.
15 - 16	Integer	numStrands	Number of strands in sheet.
18 - 20	Residue name	initResName	Residue name of initial residue.
22	Character	initChainID	Chain identifier of initial residue in strand.
23 – 26	Integer	initSeqNum	Sequence number of initial residue in strand.
27	AChar	initICode	Insertion code of initial residue in strand.
29 - 31	Residue name	endResName	Residue name of terminal residue.
33	Character	endChainID	Chain identifier of terminal residue.
34 - 37	Integer	endSeqNum	Sequence number of terminal residue.
38	AChar	endICode	Insertion code of terminal residue.
39 - 40	Integer	sense	Sense of strand with respect to previous strand in the sheet. 0 if first strand, 1 if parallel, and -1 if anti-parallel.
42 - 45	Atom	curAtom	Registration. Atom name in current strand.
46 - 48	Residue name	curResName	Registration. Residue name in current strand
50	Character	curChainId	Registration. Chain identifier in current strand.
51 - 54	Integer	curResSeq	Registration. Residue sequence number in current strand.
55	AChar	curICode	Registration. Insertion code in current strand.
57 - 60	Atom	prevAtom	Registration. Atom name in previous strand.

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61 - 63	Residue name	prevResName	Registration. Residue name in previous strand.
65	Character	prevChainId	Registration. Chain identifier in previous strand.
66 - 69	Integer	prevResSeq	Registration. Residue sequence number in previous strand.
70	AChar	prevICode	Registration. Insertion code in previous strand.

Details

- * The initial residue for a strand is its N-terminus. Strand registration information is provided in columns 39 70. Strands are listed starting with one edge of the sheet and continuing to the spatially adjacent strand.
- * The sense in columns 39 40 indicates whether strand n is parallel (sense = 1) or anti-parallel (sense = -1) to strand n-1. Sense is equal to zero (0) for the first strand of a sheet.
- * The registration (columns 42 70) of strand n to strand n-1 may be specified by one hydrogen bond between each such pair of strands. This is done by providing the hydrogen bonding between the current and previous strands. No register information should be provided for the first strand.
- * Split strands, or strands with two or more runs of residues from discontinuous parts of the amino acid sequence, are explicitly listed. Detail description can be included in the REMARK 700.

Relationships to Other Record Types

If the entry contains bifurcated sheets or beta-barrels, the relevant REMARK 700 records must be provided. See the REMARK section for details.

Examples

	1			2			3			4			5			6		7		8
123456	789012	2345	56	7890	123	34567	789012	234	45678	3901	L234	56789	901	2345	6789	01234	456	578901	12345	67890
SHEET	1	Α	5	THR	Α	107	ARG	Α	110	0										
SHEET	2	Α	5	ILE	Α	96	THR	Α	99	-1	N	LYS	Α	98	0	THR	Α	107		
SHEET	3	Α	5	ARG	Α	87	SER	Α	91	-1	N	LEU	Α	89	0	TYR	Α	97		
SHEET	4	Α	5	TRP	Α	71	ASP	Α	75	-1	N	ALA	Α	74	0	ILE	Α	88		
SHEET	5	Α	5	GLY	Α	52	PHE	Α	56	-1	N	PHE	Α	56	0	TRP	Α	71		
SHEET	1	В	5	THR	В	107	ARG	В	110	0										
SHEET	2	В	5	ILE	В	96	THR	В	99	-1	N	LYS	В	98	0	THR	В	107		
SHEET	3	В	5	ARG	В	87	SER	В	91	-1	N	LEU	В	89	0	TYR	В	97		
SHEET	4	В	5	TRP	В	71	ASP	В	75	-1	N	ALA	В	74	0	ILE	В	88		
SHEET	5	В	5	GLY	В	52	ILE	В	55	-1	N	ASP	В	54	0	GLU	В	73		

The sheet presented as BS1 below is an eight-stranded beta-barrel. This is represented by a nine-stranded sheet in which the first and last strands are identical.

SHEET	1	BS1	9	VAL	13	$_{ m ILE}$	17	0						
SHEET	2	BS1	9	ALA	70	ILE	73	1	0	TRP	72	N	ILE	17
SHEET	3	BS1	9	LYS	127	PHE	132	1	0	ILE	129	N	ILE	73
SHEET	4	BS1	9	GLY	221	ASP	225	1	0	GLY	221	N	ILE	130
SHEET	5	BS1	9	VAL	248	GLU	253	1	О	PHE	249	N	ILE	222

SHEET	6	BS1	9	LEU	276	ASP	278	1	N	LEU	277	0	GLY	252
SHEET	7	BS1	9	TYR	310	THR	318	1	0	VAL	317	N	ASP	278
SHEET	8	BS1	9	VAL	351	TYR	356	1	0	VAL	351	N	THR	318
SHEET	9	BS1	9	VAL	13	ILE	17	1	N	VAL	14	0	PRO	352

The sheet structure of this example is bifurcated. In order to represent this feature, two sheets are defined. Strands 2 and 3 of BS7 and BS8 are identical.

SHEET	1 BS7	3 HIS	662	THR	665 0						
SHEET	2 BS7	3 LYS	639	LYS	648 -1	N	PHE	643	0	HIS	662
SHEET	3 BS7	3 ASN	596	VAL	600 -1	N	TYR	598	0	ILE	646
SHEET	1 BS8	3 ASN	653	TRP	656 0						
SHEET	2 BS8	3 LYS	639	LYS	648 -1	N	LYS	647	0	THR	655
SHEET	3 BS8	3 ASN	596	VAT	600 -1	N	TYR	598	0	TLE	646

ATOM

Overview

The ATOM records present the atomic coordinates for standard amino acids and nucleotides. They also present the occupancy and temperature factor for each atom. Non-polymer chemical coordinates use the HETATM record type. The element symbol is always present on each ATOM record; charge is optional.

Changes in ATOM/HETATM records result from the standardization atom and residue nomenclature. This nomenclature is described in the Chemical Component Dictionary (ftp://ftp.wwpdb.org/pub/pdb/data/monomers).

Record Format

COLUMNS	DATA TYPE	FIELD	DEFINITION
1 - 6	Record name	"ATOM "	
7 - 11	Integer	serial	Atom serial number.
13 - 16	Atom	name	Atom name.
17	Character	altLoc	Alternate location indicator.
18 - 20	Residue name	resName	Residue name.
22	Character	chainID	Chain identifier.
23 - 26	Integer	resSeq	Residue sequence number.
27	AChar	iCode	Code for insertion of residues.
31 - 38	Real(8.3)	х	Orthogonal coordinates for X in Angstroms.
39 - 46	Real(8.3)	У	Orthogonal coordinates for Y in Angstroms.
47 - 54	Real(8.3)	Z	Orthogonal coordinates for Z in Angstroms.
55 - 60	Real(6.2)	occupancy	Occupancy.
61 - 66	Real(6.2)	tempFactor	Temperature factor.
77 - 78	LString(2)	element	Element symbol, right-justified.
79 - 80	LString(2)	charge	Charge on the atom.

Details

- * ATOM records for proteins are listed from amino to carboxyl terminus.
- * Nucleic acid residues are listed from the 5' → 3' terminus.
- * Alignment of one-letter atom name such as C starts at column 14, while two-letter atom name such as FE starts at column 13.

- * Atom nomenclature begins with atom type.
- * No ordering is specified for polysaccharides.
- * Non-blank alphanumerical character is used for chain identifier.
- * The list of ATOM records in a chain is terminated by a TER record.
- * If more than one model is present in the entry, each model is delimited by MODEL and ENDMDL records.
- * AltLoc is the place holder to indicate alternate conformation. The alternate conformation can be in the entire polymer chain, or several residues or partial residue (several atoms within one residue). If an atom is provided in more than one position, then a non-blank alternate location indicator must be used for each of the atomic positions. Within a residue, all atoms that are associated with each other in a given conformation are assigned the same alternate position indicator. There are two ways of representing alternate conformation- either at atom level or at residue level (see examples).
- * For atoms that are in alternate sites indicated by the alternate site indicator, sorting of atoms in the ATOM/HETATM list uses the following general rules:
 - In the simple case that involves a few atoms or a few residues with alternate sites, the coordinates occur one after the other in the entry.
 - In the case of a large heterogen groups which are disordered, the atoms for each conformer are listed together.
- * Alphabet letters are commonly used for insertion code. The insertion code is used when two residues have the same numbering. The combination of residue numbering and insertion code defines the unique residue.
- * If the depositor provides the data, then the isotropic B value is given for the temperature factor.
- * If there are neither isotropic B values from the depositor, nor anisotropic temperature factors in ANISOU, then the default value of 0.0 is used for the temperature factor.
- * Columns 79 80 indicate any charge on the atom, e.g., 2+, 1-. In most cases, these are blank.

Verification/Validation/Value Authority Control

The ATOM/HETATM records are checked for PDB file format, sequence information, and packing.

Relationships to Other Record Types

The ATOM records are compared to the corresponding sequence database. Sequence discrepancies appear in the SEQADV record. Missing atoms are annotated in the remarks. HETATM records are formatted in the same way as ATOM records. The sequence implied by ATOM records must be identical to that given in SEQRES, with the exception that residues that have no coordinates, e.g., due to disorder, must appear in SEQRES.

Examples

ATOM	32	N AARG	A -3	11.281	86.699	94.383	0.50	35.88	N	
ATOM	33	N BARG	A -3	11.296	86.721	94.521	0.50	35.60	N	
ATOM	34	CA AARG	A -3	12.353	85.696	94.456	0.50	36.67	С	
ATOM	35	CA BARG	A -3	12.333	85.862	95.041	0.50	36.42	С	
ATOM	36	C AARG	A -3	13.559	86.257	95.222	0.50	37.37	С	
ATOM	37	C BARG	A -3	12.759	86.530	96.365	0.50	36.39	С	
ATOM	38	O AARG	A -3	13.753	87.471	95.270	0.50	37.74	0	
ATOM	39	O BARG	A -3	12.924	87.757	96.420	0.50	37.26	0	
ATOM	40	CB AARG	A -3	12.774	85.306	93.039	0.50	37.25	С	
ATOM	41	CB BARG	A -3	13.428	85.746	93.980	0.50	36.60	С	
MOTA	42	CG AARG	A -3	11.754	84.432	92.321	0.50	38.44	С	
ATOM	43	CG BARG		12.866	85.172	92.651	0.50	37.31	С	
ATOM	44	CD AARG	A -3	11.698	84.678	90.815	0.50	38.51	С	
ATOM	45	CD BARG		3 13.374	85.886	91.406	0.50	37.66	C	
MOTA	46	NE AARG	A -3	12.984	84.447	90.163	0.50	39.94	N	
ATOM	47	NE BARG	A -3	12.644	85.487	90.195	0.50	38.24	N	
MOTA	48	CZ AARG	A -3	13.202	84.534	88.850	0.50	40.03	C	
ATOM	49	CZ BARG	A -3	3 13.114	85.582	88.947	0.50	39.55	C	
MOTA	50	NH1AARG	A -3	12.218	84.840	88.007	0.50	40.76	N	
MOTA	51	NH1BARG	A -3	14.338	86.056	88.706		40.23	N	
ATOM	52	NH2AARG	A -3	14.421	84.308	88.373	0.50	40.45	N	
	1	2		3	4	5	6		7 8	3
					4	5	U		,	
12345678	9012		23456					1234567		
12345678 ATOM	9012 32			7890123456789			67890	1234567 35 . 88	, 8901234567890 N	
		345678901	A -3	57890123456789 11.281	901234567	89012345	678901 0.50		8901234567890	
ATOM	32	345678901 N AARG CA AARG	A -3 A -3	57890123456789 3 11.281 3 12.353	901234567 86.699	89012345 94.383	678903 0.50 0.50	35.88	8901234567890 N	
ATOM ATOM	32 33	345678901 N AARG CA AARG	A -3 A -3 A -3	57890123456789 3 11.281 3 12.353 3 13.559	901234567 86.699 85.696	89012345 94.383 94.456	678903 0.50 0.50 0.50	35.88 36.67	8901234567890 N C	
ATOM ATOM ATOM	32 33 34	345678901 N AARG CA AARG C AARG	A -3 A -3 A -3	57890123456789 3 11.281 3 12.353 3 13.559 3 13.753	901234567 86.699 85.696 86.257	89012345 94.383 94.456 95.222	678903 0.50 0.50 0.50 0.50	35.88 36.67 37.37	8901234567890 N C C	
ATOM ATOM ATOM ATOM	32 33 34 35	345678901 N AARG CA AARG C AARG O AARG	A -3 A -3 A -3 A -3	57890123456789 3 11.281 3 12.353 3 13.559 3 13.753 3 12.774	901234567 86.699 85.696 86.257 87.471	89012345 94.383 94.456 95.222 95.270	678903 0.50 0.50 0.50 0.50 0.50	35.88 36.67 37.37 37.74	8901234567890 N C C O	
ATOM ATOM ATOM ATOM ATOM	32 33 34 35 36	345678901 N AARG CA AARG C AARG O AARG CB AARG	A -3 A -3 A -3 A -3 A -3	57890123456789 3 11.281 3 12.353 3 13.559 3 13.753 3 12.774 4 11.754	901234567 86.699 85.696 86.257 87.471 85.306	89012345 94.383 94.456 95.222 95.270 93.039	678903 0.50 0.50 0.50 0.50 0.50	35.88 36.67 37.37 37.74 37.25	8901234567890 N C C O C	
ATOM ATOM ATOM ATOM ATOM ATOM	32 33 34 35 36 37	345678901 N AARG CA AARG C AARG O AARG CB AARG CG AARG	A -3 A -3 A -3 A -3 A -3 A -3 A -3	57890123456789 3 11.281 3 12.353 3 13.559 3 13.753 4 12.774 6 11.754 6 11.698	901234567 86.699 85.696 86.257 87.471 85.306 84.432	89012345 94.383 94.456 95.222 95.270 93.039 92.321	678903 0.50 0.50 0.50 0.50 0.50 0.50	35.88 36.67 37.37 37.74 37.25 38.44	8901234567890 N C C O C	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	32 33 34 35 36 37 38	345678901 N AARG CA AARG C AARG O AARG CB AARG CG AARG CD AARG	A -3 A -3 A -3 A -3 A -3 A -3 A -3	57890123456789 3 11.281 4 12.353 5 13.559 6 13.753 6 12.774 7 11.754 7 11.698 7 12.984	901234567 86.699 85.696 86.257 87.471 85.306 84.432 84.678	89012345 94.383 94.456 95.222 95.270 93.039 92.321 90.815	678903 0.50 0.50 0.50 0.50 0.50 0.50 0.50	35.88 36.67 37.37 37.74 37.25 38.44 38.51	8901234567890 N C C O C C C	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	32 33 34 35 36 37 38 39	345678901 N AARG CA AARG C AARG O AARG CB AARG CG AARG CD AARG NE AARG	A -3 A -3 A -3 A -3 A -3 A -3 A -3 A -3	37890123456789 3 11.281 3 12.353 3 13.559 3 13.753 4 12.774 5 11.754 6 11.698 6 12.984 7 13.202	901234567 86.699 85.696 86.257 87.471 85.306 84.432 84.678 84.447	89012345 94.383 94.456 95.222 95.270 93.039 92.321 90.815 90.163	678903 0.50 0.50 0.50 0.50 0.50 0.50 0.50	35.88 36.67 37.37 37.74 37.25 38.44 38.51 39.94	8901234567890 N C C O C C C C	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	32 33 34 35 36 37 38 39	345678901 N AARG CA AARG C AARG O AARG CB AARG CG AARG CD AARG NE AARG CZ AARG	A -3 A -3 A -3 A -3 A -3 A -3 A -3 A -3	3789012345678 3 11.281 4 12.353 5 13.559 6 13.753 7 12.774 7 11.754 11.698 12.984 13.202 12.218	901234567 86.699 85.696 86.257 87.471 85.306 84.432 84.678 84.447 84.534	89012345 94.383 94.456 95.222 95.270 93.039 92.321 90.815 90.163 88.850	67890: 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.	35.88 36.67 37.37 37.74 37.25 38.44 38.51 39.94 40.03	8901234567890 N C C O C C C C N	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	32 33 34 35 36 37 38 39 40 41	345678901 N AARG CA AARG C AARG O AARG CB AARG CG AARG CD AARG NE AARG CZ AARG NH1AARG	A -3 A -3 A -3 A -3 A -3 A -3 A -3 A -3	57890123456789 3 11.281 4 12.353 5 13.559 6 13.753 6 12.774 7 11.754 7 11.698 7 12.984 7 13.202 7 12.218	901234567 86.699 85.696 86.257 87.471 85.306 84.432 84.678 84.447 84.534 84.840	89012345 94.383 94.456 95.222 95.270 93.039 92.321 90.815 90.163 88.850 88.007	678903 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.	35.88 36.67 37.37 37.74 37.25 38.44 38.51 39.94 40.03 40.76	8901234567890 N C C O C C C C N C	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	32 33 34 35 36 37 38 39 40 41 42	345678901 N AARG CA AARG C AARG O AARG CB AARG CG AARG CD AARG NE AARG CZ AARG NH1AARG NH2AARG	A -3 A -3 A -3 A -3 A -3 A -3 A -3 A -3	7890123456789 11.281 12.353 13.559 13.753 12.774 11.754 11.698 12.984 13.202 12.218 14.421 11.296	901234567 86.699 85.696 86.257 87.471 85.306 84.432 84.678 84.447 84.534 84.840 84.308	89012345 94.383 94.456 95.222 95.270 93.039 92.321 90.815 90.163 88.850 88.007 88.373	678903 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.	35.88 36.67 37.37 37.74 37.25 38.44 38.51 39.94 40.03 40.76 40.45	8901234567890 N C C O C C C C N C	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	32 33 34 35 36 37 38 39 40 41 42 43	345678901 N AARG CA AARG C AARG O AARG CB AARG CC AARG CD AARG NE AARG CZ AARG NH1AARG NH2AARG N BARG	A -3 A -3 A -3 A -3 A -3 A -3 A -3 A -3	77890123456789 11.281 12.353 13.559 13.753 12.774 11.754 11.698 12.984 13.202 12.218 14.421 11.296 12.333	901234567 86.699 85.696 86.257 87.471 85.306 84.432 84.678 84.447 84.534 84.840 84.308 86.721	89012345 94.383 94.456 95.222 95.270 93.039 92.321 90.815 90.163 88.850 88.007 88.373 94.521	678903 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.	35.88 36.67 37.37 37.74 37.25 38.44 38.51 39.94 40.03 40.76 40.45 35.60	8901234567890 N C C O C C C N C N N	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	32 33 34 35 36 37 38 39 40 41 42 43 44	N AARG CA AARG C AARG O AARG CB AARG CC AARG CD AARG NE AARG CZ AARG NH1AARG NH2AARG N BARG CA BARG	A -3 A -3 A -3 A -3 A -3 A -3 A -3 A -3	7890123456789 11.281 12.353 13.559 13.753 12.774 11.754 11.698 12.984 13.202 12.218 14.421 11.296 12.333 12.759	901234567 86.699 85.696 86.257 87.471 85.306 84.432 84.678 84.447 84.534 84.534 84.308 86.721 85.862	89012345 94.383 94.456 95.222 95.270 93.039 92.321 90.815 90.163 88.850 88.007 88.373 94.521 95.041	678903 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50	35.88 36.67 37.37 37.74 37.25 38.44 38.51 39.94 40.03 40.76 40.45 35.60 36.42	8901234567890 N C C O C C C N C N N N	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	32 33 34 35 36 37 38 39 40 41 42 43 44 45	N AARG CA AARG C AARG O AARG CB AARG CC AARG CD AARG NE AARG CZ AARG NH1AARG NH2AARG N BARG CA BARG C BARG	A -3 A -3 A -3 A -3 A -3 A -3 A -3 A -3	7890123456789 11.281 12.353 13.559 13.753 12.774 11.754 11.698 12.984 13.202 12.218 14.421 11.296 12.333 12.759 12.924	901234567 86.699 85.696 86.257 87.471 85.306 84.432 84.678 84.447 84.534 84.534 84.721 85.862 86.721	89012345 94.383 94.456 95.222 95.270 93.039 92.321 90.815 90.163 88.850 88.007 88.373 94.521 95.041 96.365	678903 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50	35.88 36.67 37.37 37.74 37.25 38.44 38.51 39.94 40.03 40.76 40.45 35.60 36.42 36.39	8901234567890 N C C O C C N C N N C O C	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	32 33 34 35 36 37 38 39 40 41 42 43 44 45 46	N AARG CA AARG C AARG O AARG CB AARG CC AARG CC AARG NE AARG NE AARG NH1AARG NH1AARG NH2AARG N BARG CA BARG C BARG O BARG	A -3 A -3 A -3 A -3 A -3 A -3 A -3 A -3	7890123456789 11.281 12.353 13.559 13.753 12.774 11.698 11.754 11.698 12.984 13.202 12.218 14.421 11.296 12.333 12.759 12.924 13.428	901234567 86.699 85.696 86.257 87.471 85.306 84.432 84.678 84.447 84.534 84.840 84.308 86.721 85.862 86.530 87.757	89012345 94.383 94.456 95.222 95.270 93.039 92.321 90.815 90.163 88.850 88.007 88.373 94.521 95.041 96.365 96.420	678903 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50	35.88 36.67 37.37 37.74 37.25 38.44 38.51 39.94 40.03 40.76 40.45 35.60 36.42 36.39 37.26	8901234567890 N C C O C C N C N N C O C	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47	N AARG CA AARG C AARG O AARG CB AARG CC AARG CD AARG NE AARG CZ AARG NH1AARG NH2AARG N BARG CA BARG C BARG O BARG CB BARG	A -3 A -3 A -3 A -3 A -3 A -3 A -3 A -3	57890123456789 3 11.281 4 12.353 3 13.559 3 12.774 3 11.754 3 11.698 4 13.202 3 12.218 4 14.421 3 12.333 4 12.924 3 13.428 3 12.866	901234567 86.699 85.696 86.257 87.471 85.306 84.432 84.678 84.447 84.534 84.840 84.308 86.721 85.862 86.530 87.757 85.746	89012345 94.383 94.456 95.222 95.270 93.039 92.321 90.815 90.163 88.850 88.007 88.373 94.521 95.041 96.365 96.420 93.980	678903 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50	35.88 36.67 37.37 37.74 37.25 38.44 38.51 39.94 40.03 40.76 40.45 35.60 36.42 36.39 37.26 36.60	8901234567890 N C C O C C N C N N C O C	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48	N AARG CA AARG C AARG O AARG CB AARG CC AARG CD AARG NE AARG CZ AARG NH1AARG NH2AARG N BARG CA BARG C BARG C BARG C BARG CB BARG CB BARG	A -3 A -3 A -3 A -3 A -3 A -3 A -3 A -3	57890123456789 3 11.281 4 12.353 3 13.559 3 12.774 4 11.754 3 11.698 4 13.202 3 12.218 4 421 3 12.333 4 12.333 3 12.759 4 13.428 3 12.866 3 13.374	901234567 86.699 85.696 86.257 87.471 85.306 84.432 84.678 84.447 84.534 84.840 84.308 86.721 85.862 86.530 87.757 85.746 85.172	89012345 94.383 94.456 95.222 95.270 93.039 92.321 90.815 90.163 88.850 88.007 88.373 94.521 95.041 96.365 96.420 93.980 92.651	678903 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50	35.88 36.67 37.37 37.74 37.25 38.44 38.51 39.94 40.03 40.76 40.45 35.60 36.42 36.39 37.26 36.60 37.31	8901234567890 N C C O C C N C N N C O C	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49	N AARG CA AARG C AARG O AARG CB AARG CC AARG CD AARG NE AARG CZ AARG NH1AARG NH2AARG N BARG CA BARG C BARG	A -3 A -3 A -3 A -3 A -3 A -3 A -3 A -3	37890123456789 38 11.281 39 12.353 31 13.559 31 13.753 31 12.774 31 11.698 31 12.984 31 12.218 31 12.218 31 12.333 31 12.759 31 12.866 31 13.374 32 12.644	901234567 86.699 85.696 86.257 87.471 85.306 84.432 84.678 84.447 84.534 84.940 84.308 86.721 85.862 86.530 87.757 85.746 85.172 85.886	89012345 94.383 94.456 95.222 95.270 93.039 92.321 90.815 90.163 88.850 88.007 88.373 94.521 95.041 96.365 96.420 93.980 92.651 91.406	678903 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50	35.88 36.67 37.37 37.74 37.25 38.44 38.51 39.94 40.03 40.76 40.45 35.60 36.42 36.39 37.26 36.60 37.31 37.66	8901234567890 N C C O C C N C N N C C O C	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50	N AARG CA AARG C AARG O AARG CB AARG CC AARG CD AARG NE AARG CZ AARG NH1AARG NH2AARG C BARG C	A -3 A -3 A -3 A -3 A -3 A -3 A -3 A -3	57890123456789 3 11.281 4 12.353 5 13.559 6 13.753 7 12.774 7 11.698 8 12.984 8 12.218 8 12.218 9 12.333 12.759 12.924 13.428 12.866 13.374 12.644 13.114	901234567 86.699 85.696 86.257 87.471 85.306 84.432 84.678 84.447 84.534 84.840 84.308 86.721 85.862 86.530 87.757 85.746 85.172 85.886 85.487	89012345 94.383 94.456 95.222 95.270 93.039 92.321 90.815 90.163 88.850 88.007 88.373 94.521 95.041 96.365 96.420 93.980 92.651 91.406 90.195	678903 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50	35.88 36.67 37.37 37.74 37.25 38.44 38.51 39.94 40.03 40.76 40.45 35.60 36.42 36.39 37.26 36.60 37.31 37.66 38.24	8901234567890 N C C O C C N C N N C C O C	

ANISOU

Overview

The ANISOU records present the anisotropic temperature factors.

Record Format

COLUMNS	DATA TYPE	FIELD	DEFINITION