Protein Data Bank Contents Guide:

Atomic Coordinate Entry Format Description

Version 3.1, July 19, 2007 Version 3.1, February 11, 2008

1. Introduction

The Protein Data Bank (PDB) is an archive of experimentally determined threedimensional structures of biological macromolecules that serves a global community of researchers, educators, and students. The data contained in the archive include atomic coordinates, bibliographic citations, primary and secondary structure, information, and crystallographic structure factors and NMR experimental data.

This guide describes the "PDB format" used by the members of the worldwide Protein Data Bank (Berman, H.M., Henrick, K. and Nakamura, H. (2003) Announcing the worldwide Protein Data Bank. Nat Struct Biol, 10, 980). Questions should be sent to info@wwpdb.org

Version 3.1 of the PDB file format introduces a small number of changes and extensions supporting the annotation practices adopted by the wwPDB beginning in August 2007. These annotation practices are described in detail in the documentation section of the wwPDB website. Format version 3.1 also incorporates all of the revisions of format version 3.0 which was used by the wwPDB to integrate uniformity and remediation data into a single set of archival data files. This document describes the small number of differences between version 3.1 and the preceding version 2.3 formats. All changes of the changes described in the version 3.0 Format Guide are incorporated into this version 3.1 format description. The complete details of the PDB format version 2.3 can be found at http://www.wwpdb.org/docs.html.

Version 3.1, July 19, 2007 Initial version Version 3.1, February 11, 2008 minor changes in remark 350 and revdat, add cutoff limits for close contacts

2. Title Section

This section contains records used to describe the experiment and the biological macromolecules present in the entry: HEADER, OBSLTE, TITLE, CAVEAT, COMPND, SOURCE, KEYWDS, EXPDTA, AUTHOR, REVDAT, SPRSDE, JRNL, and REMARK records. The changes in records in this section are described below.

REVDAT

REVDAT records contain a history of the modifications made to an entry since its release.

Record Format

COLUMNS	DATA TYPE	FIELD	DEFINITION
1 - 6 8 - 10 11 - 12 14 - 22	Record name Integer Continuation Date	"REVDAT" modNum continuation modDate	Modification number. Allows concatenation of multiple records Date of modification (or release for new entries). This is not repeated on continuation lines.
24 - 28	String(5)	modId	Identifies this particular modification. It links to the archive used internally by PDB. This is not repeated on continuation lines
32	Integer	modType	An integer identifying the type of modification. In case of revisions with more than one possible modType, the highest value applicable will be assigned
40 - 45 47 - 52 54 - 59 61 - 66	LString(6) LString(6) LString(6) LString(6)	record	Modification detail. Modification detail. Modification detail. Modification detail.

Each time revisions are made to the entry, a modification number is assigned in increasing (by 1) numerical order. REVDAT records appear in descending order (most recent modification appears first). New entries have a REVDAT record with modNum equal to 1 and modType equal to 0. Allowed modTypes are:

- 0 Initial released entry.
- 1 Other modification.

Each revision may have more than one REVDAT record, and each revision has a separate continuation field.

Modification details are typically PDB record names such as SOURCE, TITLE, or COMPND. A special modification detail VERSN indicates that the file has undergone a change in version. The current version will be specified in REMARK 4.

Verification/Validation/Value Authority Control

The modType must be one of the defined types, and the given record type must be valid. If modType is 0, the modId must match the entry's ID code in the HEADER record.

Relationships to Other Record Types

In the case of a version revision, the current will be specified in REMARK 4.

Template

```
1 2 3 4 5 6 7
1234567890123456789012345678901234567890123456789012345678901234567890

REVDAT 2 15-OCT-99 1ABC 1 REMARK

REVDAT 1 09-JAN-89 1ABC 0

1 2 3 4 5 6 7
123456789012345678901234567890123456789012345678901234567890

REVDAT 2 11-MAR-08 2ABC 1 JRNL VERSN

REVDAT 1 09-DEC-03 2ABC 0
```

REMARK 0

REMARK 0 identifies entries in which a re-refinement has been performed using the data from existing entry.

Template

```
REMARK 0
REMARK 0 THIS ENTRY YYYY REFLECTS AN ALTERNATIVE MODELING OF THE
REMARK 0 STRUCTURAL DATA IN RXXXXSF (or XXXX.MR).
REMARK 0 IN PDB ENTRY YYYY INFORMATION IN REMARK 200 (or 210)
REMARK 0 SERIES IS BASED ON THE EXPERIMENT DESCRIBED IN PDB ENTRY XXXX
REMARK 0 ORIGINAL DATA DETERMINED BY AUTHOR:
REMARK 0 AUTHOR INITIALS, AUTHOR LAST NAME ...
```

Note: In entries where REMARK 0 is included as described above, remarks REMARK 1, REMARK 200/210 and REMARK 900 will also reflect the reuse of existing experimental data.

REMARK 4

Remark 4 indicates the version of the PDB file format used to generate the file.

Version 3.1 files include a version remark like the following:

```
1 2 3 4 5 6 7
12345678901234567890123456789012345678901234567890
REMARK 4
REMARK 4 1ABC COMPLIES WITH FORMAT V. 3.1, 1-AUG-2007
```

Version 3.0 files include a version remark like the following:

```
REMARK 4
REMARK 4 1ABC COMPLIES WITH FORMAT V. 3.0, 1-DEC-2006
REMARK 4
REMARK 4 THIS IS THE REMEDIATED VERSION OF THIS PDB ENTRY.
REMARK 4 REMEDIATED DATA FILE REVISION 3.XXX (YYYY-MM-DD)
```

REMARK 40

Pre-submission validation and similar software used before deposition, may be listed in a REMARK 40. This remark will list the software name, authors and function of the program. Results of these software methods will not be listed. This free text remark is optional.

Template

REMARK 40 FREE TEXT DESCRIPTION

REMARKs 102-199 Nucleic Acids

The text remarks for nucleic acids will reflect the standardization of nomenclature for the polymer nucleotides described in later sections. In particular, the polymeric deoxyribonucleotides are represented by 2-letter codes DC, DG, DA, and DT to distinguish these from their ribonucletide counterparts. The asterisk character in the in saccharide atom names is replaced by the single prime character. The text of REMARK 105 is correspondingly changed as follows.

REMARK 105

Remark 105 is mandatory if nucleic acids exist in an entry.

Template

1 2 3 4 5 6 7
123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890
REMARK 105
REMARK 105 THE PROTEIN DATA BANK HAS ADOPTED THE SACCHARIDE CHEMISTS
REMARK 105 NOMENCLATURE FOR ATOMS OF THE DEOXYRIBOSE/RIBOSE MOIETY
REMARK 105 RATHER THAN THAT OF THE NUCLEOSIDE CHEMISTS. THE RING
REMARK 105 OXYGEN ATOM IS LABELLED 04' INSTEAD OF 01'.

REMARK 200, X-ray Diffraction Experimental Details

The following example illustrates the how REMARK 200 will be used in cases in which multiple data collections are described. In this example, data items corresponding to different data collection sessions are separated by semi-colons. Multiple data values within a single session (e.g wavelength) are separated by commas.

```
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200 EXPERIMENT TYPE : X-RAY DIFFRACTION REMARK 200 DATE OF DATA COLLECTION : 17-MAR-2002; 17-MAR-2002
REMARK 200 TEMPERATURE (KELVIN): 100; 100
REMARK 200 NUMBER OF CRYSTALS USED : 2
REMARK 200
REMARK 200
REMARK 200
REMARK 200 SYNCHROTRON (Y/N): Y; Y
REMARK 200 RADIATION SOURCE : APS; APS
REMARK 200 BEAMLINE : 17ID; 17ID
REMARK 200 X-RAY GENERATOR MODEL
REMARK 200 MONOCHROMATIC OR LAUE (M/L): M; M
REMARK 200 WAVELENGTH OR RANGE (A): 1.5545; 1.0720, 1.0723,
REMARK 200 MONOCHROMATOR : SI (111): SI (111)
REMARK 200 MONOCHROMATOR
                                                             : SI (111); SI (111)
REMARK 200
                                                              : NULL
                 OPTICS
REMARK 200
REMARK 200 DETECTOR TYPE : CCD; CCD
REMARK 200 DETECTOR MANUFACTURER : ADSC QUANTUM 210; ADSC
REMARK 200 QUANTUM 210
REMARK 200
REMARK 200
                                                                OUANTUM 210
REMARK 200 INTENSITY-INTEGRATION SOFTWARE : DENZO
REMARK 200 DATA SCALING SOFTWARE : HKL
REMARK 200
REMARK 200 NUMBER OF UNIQUE REFLECTIONS : 29132
REMARK 200 RESOLUTION RANGE HIGH (A) : 1.900
REMARK 200 RESOLUTION RANGE LOW (A) : 30.000
REMARK 200 REJECTION CRITERIA (SIGMA(I)) : 0.000
REMARK 200
REMARK 200 OVERALL.
REMARK 200 COMPLETENESS FOR RANGE
                                                       (%) : 98.3
REMARK 200 DATA REDUNDANCY
REMARK 200 R MERGE
                                                             : 19.800
                                                         (I) : NULL
REMARK 200 R SYM
                                                         (I) : 0.07500
REMARK 200 <I/SIGMA(I) > FOR THE DATA SET : 17.0000
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A): 1.90
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A): 1.97
REMARK 200 COMPLETENESS FOR SHELL (%): 83.4
REMARK 200 DATA REDUNDANCY IN SHELL : 3.00
REMARK 200 R MERGE FOR SHELL (I): NULL
REMARK 200 R SYM FOR SHELL (I): 0.65000
REMARK 200 <I/SIGMA(I) > FOR SHELL : 1.500
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH; MAD
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MAD
REMARK 200 SOFTWARE USED: SOLVE 2.02
REMARK 200 STARTING MODEL: NULL
REMARK 200
REMARK 200 REMARK: NULL
```

REMARK 300, Biomolecule

Description of the biologically functional molecule (biomolecule) in free text.

Remark 300 is mandatory if Remark 350 is provided. Template

```
1 2 3 4 5 6 7
123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890
REMARK 300
REMARK 300 BIOMOLECULE: 1
REMARK 300 SEE REMARK 350 FOR THE AUTHOR PROVIDED AND/OR PROGRAM
REMARK 300 GENERATED ASSEMBLY INFORMATION FOR THE STRUCTURE IN
REMARK 300 THIS ENTRY. THE REMARK MAY ALSO PROVIDE INFORMATION ON
REMARK 300 BURIED SURFACE AREA.
REMARK 300 free text ...
```

Example - Icosahedral virus

```
REMARK 300
REMARK 300 BIOMOLECULE: 1
REMARK 300 SEE REMARK 350 FOR THE AUTHOR PROVIDED AND/OR PROGRAM
REMARK 300 GENERATED ASSEMBLY INFORMATION FOR THE STRUCTURE IN
REMARK 300 THIS ENTRY. THE REMARK MAY ALSO PROVIDE INFORMATION ON
REMARK 300 BURIED SURFACE AREA.
REMARK 300 DETAILS: THE ASSEMBLY REPRESENTED IN THIS ENTRY HAS REGULAR
REMARK 300 ICOSAHEDRAL POINT SYMMETRY (SCHOENFLIES SYMBOL = I).
```

Example - Helical viruses

```
REMARK 300 BIOMOLECULE: 1
REMARK 300 SEE REMARK 350 FOR THE AUTHOR PROVIDED AND/OR PROGRAM
REMARK 300 GENERATED ASSEMBLY INFORMATION FOR THE STRUCTURE IN
REMARK 300 THIS ENTRY. THE REMARK MAY ALSO PROVIDE INFORMATION ON
REMARK 300 BURIED SURFACE AREA.
REMARK 300 DETAILS: THE ASSEMBLY REPRESENTED IN THIS ENTRY HAS REGULAR
REMARK 300 HELICAL SYMMETRY WITH THE FOLLOWING PARAMETERS:
REMARK 300 ROTATION PER SUBUNIT (TWIST) = -33.23 DEGREES
REMARK 300 RISE PER SUBUNIT (HEIGHT) = 16.00 ANGSTROMS
REMARK 300 IN ADDITION, THERE IS 5-FOLD CIRCULAR
REMARK 300 SYMMETRY AROUND THE HELIX AXIS
```

REMARK 350, Generating the Biomolecule

Remark 350 presents all transformations, both crystallographic and noncrystallographic, needed to generate the biomolecule. These transformations operate on the coordinates in the entry. Both author and computational descriptions of assemblies are provided if these are available.

Example – Author and computed assembly predictions agree

```
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
```

```
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
REMARK 350 GIVEN BELOW. BOTH NON-CRYSTALLOGRAPHIC AND
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK 350
REMARK 350 BIOMOLECULE: 1
REMARK 350 AUTHOR DETERMINED BIOLOGICAL UNIT: DODECAMERIC
REMARK 350 SOFTWARE DETERMINED QUATERNARY STRUCTURE: DODECAMERIC
REMARK 350 SOFTWARE USED: PISA
REMARK 350 TOTAL BURIED SURFACE AREA: 2990 ANGSTROM**2
REMARK 350 TOTAL SURFACE AREA FOR THE COMPLEX: 9330 ANGSTROM**2
REMARK 350 GAIN IN SOLVENT FREE ENERGY: -40 KCAL/MOL
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A, B, C, D, E, F, G, H, I,
REMARK 350
                                               J, K, L
REMARK 350 BIOMT1 1 1.000000 0.000000 0.000000 REMARK 350 BIOMT2 1 0.000000 1.000000 0.000000 REMARK 350 BIOMT3 1 0.000000 0.000000 1.000000
                                                                     0.00000
                                                                     0.00000
                                                                     0.00000
```

Note: The value for the average buried surface area will be round to the nearest 10.

Example – Author and computed assembly predictions differ

```
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
REMARK 350 GIVEN BELOW. BOTH NON-CRYSTALLOGRAPHIC AND
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK 350
REMARK 350 BIOMOLECULE: 1
REMARK 350 AUTHOR DETERMINED BIOLOGICAL UNIT: HEXAMERIC
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A, B, C, D, E, F
REMARK 350 BIOMT1 1 1.000000 0.000000 0.000000 0.000000 REMARK 350 BIOMT2 1 0.000000 1.000000 0.000000 0.000000 REMARK 350 BIOMT3 1 0.000000 0.000000 1.000000 0.000000
REMARK 350
REMARK 350 BIOMOLECULE: 2
REMARK 350 AUTHOR DETERMINED BIOLOGICAL UNIT: HEXAMERIC
REMARK 350 APPLY THE FOLLOWING TO CHAINS: G, H, I, J, K, L
REMARK 350 BIOMT1 1 1.000000 0.000000 0.000000 REMARK 350 BIOMT2 1 0.000000 1.000000 0.000000
                                                                  0.00000
                                                                 0.00000
REMARK 350 BIOMT3 1 0.000000 0.000000 1.000000
                                                                 0.00000
REMARK 350
REMARK 350 BIOMOLECULE: 3
REMARK 350 SOFTWARE DETERMINED QUATERNARY STRUCTURE: DODECAMERIC
REMARK 350 SOFTWARE USED: PISA
REMARK 350 TOTAL BURIED SURFACE AREA: 2990 ANGSTROM**2
REMARK 350 TOTAL SURFACE AREA FOR THE COMPLEX: 9330 ANGSTROM**2
REMARK 350 GAIN IN SOLVENT FREE ENERGY: -40 KCAL/MOL
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A, B, C, D, E, F, G, H, I,
REMARK 350
                                       J, K, L
REMARK 350 BIOMT1 1 1.000000 0.000000 0.000000
REMARK 350 BIOMT2 1 0.000000 1.000000 0.000000
                                                                 0.00000
REMARK 350 BIOMT3 1 0.000000 0.000000 1.000000
                                                                 0.00000
```

Example - No experimental information about assembly provided

```
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING
REMARK 350 OLIGOMERIZATION STATE(S) OF THE
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
REMARK 350 GIVEN BELOW. BOTH NON-CRYSTALLOGRAPHIC AND
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK 350
REMARK 350 BIOMOLECULE:
REMARK 350 SOFTWARE DETERMINED QUATERNARY STRUCTURE: MONOMERIC
REMARK 350 SOFTWARE USED: PISA
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A
REMARK 350 BIOMT1 1 1.000000 0.000000 0.000000
REMARK 350 BIOMT2 1 0.000000 1.000000 0.000000
                                                         0.00000
REMARK 350 BIOMT3 1 0.000000 0.000000 1.000000
                                                          0.00000
REMARK 350
```

REMARK 475, Residues modeled with zero occupancy

REMARK 475 enumerates residues modeled with zero occupancy.

Example -

```
REMARK 475
```

REMARK 480, Polymer atoms modeled with zero occupancy

REMARK 480 enumerates atoms in residues modeled with zero occupancy.

Example -

```
REMARK 480
REMARK 480 ZERO OCCUPANCY ATOM
REMARK 480 THE FOLLOWING RESIDUES HAVE ATOMS MODELED WITH ZERO
REMARK 480 OCCUPANCY. THE LOCATION AND PROPERTIES OF THESE ATOMS
REMARK 480 MAY NOT BE RELIABLE. (M=MODEL NUMBER; RES=RESIDUE NAME;
REMARK 480 C=CHAIN IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE):
REMARK 480 M RES C SSEQI ATOMS
REMARK 480 DC D 3 C4' O4' C1' C3' O3'
```

REMARK 500, Geometry and Stereochemistry

Remark 500 provides further details on the stereochemistry of the structure. This remark is generated by PDB and may incorporate comments provided by the author. This remark is currently divided into the subtopics:

CLOSE CONTACTS IN SAME ASYMMETRIC UNIT. CLOSE CONTACTS. COVALENT BOND LENGTHS, COVALENT BOND ANGLES. TORSION ANGLES. NON-CIS & NON-TRANS. PLANAR GROUPS, MAIN CHAIN PLANARITY, CHIRAL CENTERS.

Additional subtopics may be added as needed. For close contacts, the cutoff limit is 2.2 angstrom for non hydrogen atoms and is 1.6 angstrom for H and D atoms. These distances are listed in the REMARK 500 for close contacts symmetry.

The calculation of bond and angle deviations for protein entries will be based on the updated Engh & Huber amino acid target values¹. For nucleic acids, the Parkinson et al., statistics will be used for these calculations². All bonds and angles that deviate more than 6 times from their standard target values will be flagged as a deviation. The PHI/PSI values are based on Kleywegt's calculations³.

Template

3 5 REMARK 500 REMARK 500 GEOMETRY AND STEREOCHEMISTRY REMARK 500 SUBTOPIC: REMARK 500 REMARK 500 FREE TEXT GOES HERE.

¹ Structure quality and target parameters. R. A. Engh and R. Huber. International Tables for Crystallography (2006). Vol. F, ch. 18.3, pp. 382-392

² "New Parameters for the Refinement of Nucleic Acid Containing Structures." Gary Parkinson, Jaroslav Vojtechovsky, Lester Clowney, Axel Brunger*, and Helen M. Berman. (1996) Acta Cryst. D 52, 57-64

[&]quot;PHI/PSI- Chology: Ramachandran revisited. "GJ Kleywegt and TA Jones (1996) Structure 4, 1395-1400.

Example – Close Contacts in the same asymmetric unit

REMARK REMARK		GEOMET	'RY AN	ID S	STEREO	CHE	MISTF	RY			
REMARK	500	SUBTOPIC: CLOSE CONTACTS IN SAME ASYMMETRIC UNIT									
REMARK	500										
REMARK	500	THE FO	LLOWI	NG	ATOMS	AR	E IN	CLOSI	Ξ C	CONTACT.	
REMARK	500										
REMARK	500	ATM1	RES	C	SSEQI		ATM2	RES	C	SSEQI	DISTANCE
REMARK	500	N	PHE	1	8	-	OD2	ASP	1	31	2.17
REMARK	500	OD2	ASP	1	31	-	N	PHE	1	8	2.17
REMARK	500										
REMARK	500	THIS E	NTRY	HAS	3 :	104	CLOS	SE COI	ATV	CTS	
REMARK	500										
REMARK	500	REMARK	: NUI	ιL							

Example – Close Contacts

	500 500	GEOMET SUBTOP		~	CHEMISTR CACTS	ĽΥ				
REMARK	500	THE FO	LLOWING	ATOMS	THAT AF	E REI	LAT	ED BY C	RYSTALLO	GRAPHIC
REMARK	500	SYMMET	RY ARE	IN CLOS	SE CONTA	CT.	ΑN	ATOM L	OCATED W	ITHIN 0.15
REMARK	500	ANGSTR	OMS OF	A SYMME	ETRY REI	ATED	ΑT	OM IS A	SSUMED TO	D BE ON A
		SPECIAL POSITION AND IS, THEREFORE, LISTED IN REMARK 375								
REMARK		INSTEAD OFREMARK 500. ATOMS WITH NON-BLANK ALTERNATE								
		LOCATION INDICATORS ARE NOT INCLUDED IN THE CALCULATIONS.								
REMARK			~= ~==~							
		DISTAN		•						
REMARK									HYDROGEN	
		1.6 AN	GSTROMS	FOR CO	NTACTS	INVOI	LVI	NG HYDR	OGEN ATON	MS
REMARK										
REMARK		ATM1	RES C	SSEQI	ATM2	RES	C	SSEQI	SSYMOP	DISTANCE
REMARK										
REMARK	500	OH	TYR 1	90	0	HOH		343	1566	2.09
REMARK	500	OE1	GLU 1	134	CB	LYS	2	135	1556	2.18
REMARK	500									
REMARK	500	THIS E	NTRY HA	S	64 SYMM	IETRY	CO	NTACTS		
REMARK	500									
REMARK	500	REMARK	: NULL							

Example - Covalent bond lengths

```
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X, I3, 1X, A3, 1X, A1, I4, A1, 1X, 2 (A4, A1, 3X), 12X, F5.3)
REMARK 500
REMARK 500 EXPECTED VALUES PROTEIN: ENGH AND HUBER, 1999
REMARK 500 EXPECTED VALUES NUCELIC ACID: CLOWNEY ET AL 1996
REMARK 500
REMARK 500 M RES CSSEOI ATM1 RES CSSEOI ATM2
                                                DEVIATION
                                                 -0.129
REMARK 500 ASP B 117 CB ASP B 117 CG
             CYS J 29 CB CYS J 29 SG
REMARK 500
                                                 -0.111
REMARK 500
REMARK 500 REMARK: NULL
```

Example – Covalent bond angles

```
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND ANGLES
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X, I3, 1X, A3, 1X, A1, I4, A1, 3(1X, A4, 2X), 12X, F5.1)
REMARK 500
REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1999
REMARK 500
                              ATM2
                                     ATM3
REMARK 500
           M RES CSSEQI ATM1
                                            ANGL. DEV. = -12.0 DEGREES
REMARK 500
              VAL A 124 CB - CA - C
                          NE - CZ - NH1 ANGL. DEV. = -3.0 DEGREES
REMARK 500
              ARG B 70
REMARK 500
REMARK 500 REMARK: NULL
```

Example – Torsion angles

```
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: TORSION ANGLES
REMARK 500
REMARK 500
REMARK 500 TORSION ANGLES OUTSIDE THE EXPECTED RAMACHANDRAN REGIONS:
REMARK 500 (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER;
REMARK 500 SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X,I3,1X,A3,1X,A1,I4,A1,4X,F7.2,3X,F7.2)
REMARK 500
REMARK 500 M RES CSSEQI PSI PHI
REMARK 500 ASN A 100 -110.87 -163.72
REMARK 500
REMARK 500
REMARK 500
REMARK 500
REMARK 500
REMARK 500
REMARK: NULL
```

Example - Cis/Trans geometry

```
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: NON-CIS, NON-TRANS
REMARK 500
REMARK 500 THE FOLLOWING PEPTIDE BONDS DEVIATE SIGNIFICANTLY FROM BOTH
REMARK 500 CIS AND TRANS CONFORMATION. CIS BONDS, IF ANY, ARE LISTED
REMARK 500 ON CISPEP RECORDS. TRANS IS DEFINED AS 180 +/- 30 AND
REMARK 500 CIS IS DEFINED AS 0 +/- 30 DEGREES.
                                                      OMEGA
REMARK 500
                                         MODEL
                                                      147.84
REMARK 500 ARG A 413
REMARK 500 ALA B 288
                          ASP A 414
ASN B 289
                                            0
                                               Ω
                                                        -39.12
REMARK 500
REMARK 500 REMARK: NULL
```

Example - Planar groups

```
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: PLANAR GROUPS
REMARK 500
REMARK 500 PLANAR GROUPS IN THE FOLLOWING RESIDUES HAVE A TOTAL
REMARK 500 RMS DISTANCE OF ALL ATOMS FROM THE BEST-FIT PLANE
REMARK 500 BY MORE THAN AN EXPECTED VALUE OF 6*RMSD, WITH AN
REMARK 500 RMSD 0.02 ANGSTROMS, OR AT LEAST ONE ATOM HAS
REMARK 500 AN RMSD GREATER THAN THIS VALUE
REMARK 500 (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER;
REMARK 500 SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 M RES CSSEQI
                              RMS
REMARK 500 TYR A 36
                              0.08
                                     SIDE CHAIN
REMARK 500
             TYR A 104
                              0.08
                                      SIDE CHAIN
REMARK 500
REMARK 500 REMARK: NULL
```

Example – Main chain planarity

```
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: MAIN CHAIN PLANARITY
REMARK 500
REMARK 500 THE FOLLOWING RESIDUES HAVE A PSEUDO PLANARITY
REMARK 500 TORSION, C(I) - CA(I) - N(I+1) - O(I), GREATER
REMARK 500 LO.0 DEGREES. (M=MODEL NUMBER; RES=RESIDUE NAME;
REMARK 500 C=CHAIN IDENTIFIER; SSEQ=SEQUENCE NUMBER;
REMARK 500
REMARK: NULL
```

Example – Chiral centers

```
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: CHIRAL CENTERS
REMARK 500
REMARK 500 UNEXPECTED CONFIGURATION OF THE FOLLOWING CHIRAL
REMARK 500 CENTER(S) (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
```

REMARK 500 STANDARD TABLE:

REMARK 500 FORMAT: (10X,I3,1X,A3,1X,A1,I4,A1,6X,A12)

REMARK 500

REMARK 500 M RES CSSEQI OMEGA REMARK 500 ASP B 405 ALPHA-CARBON 150.48

REMARK 500

REMARK 500 REMARK: NULL

REMARK 525 - Distant Solvent Atoms

REMARK 525 lists solvent atoms more than 5 Angstroms from any polymer chain.

Example -

```
REMARK 525
MOLECULES WHICH ARE MORE THAN 5A AWAY FROM THE REMARK 525
REMARK 525
RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE REMARK 525
```

REMARK 610 – Non-polymer residues with missing atoms

REMARK 610 enumerates non-polymer residues with missing atoms.

Example -

```
REMARK 610
REMARK 610 MISSING HETEROATOM
REMARK 610 THE FOLLOWING RESIDUES HAVE MISSING ATOMS (M=MODEL NUMBER;
REMARK 610 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE NUMBER;
REMARK 610 I=INSERTION CODE):
REMARK 610 M RES C SSEQI
REMARK 610 PPI 438
```

REMARK 615 – Non-polymer residues containing atoms with zero occupancy

REMARK 615 enumerates non-polymer residues containing atoms modeled with zero occupancy.

Example -

```
REMARK 615
REMARK 615 ZERO OCCUPANCY ATOM
REMARK 615 THE FOLLOWING RESIDUES HAVE ATOMS MODELED WITH ZERO
REMARK 615 OCCUPANCY. THE LOCATION AND PROPERTIES OF THESE ATOMS
REMARK 615 MAY NOT BE RELIABLE. (M=MODEL NUMBER; RES=RESIDUE NAME;
REMARK 615 C=CHAIN IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE):
REMARK 615 M RES C SSEQI
REMARK 615 PPI 438
```

REMARK 620 – Metal Coordination

Details of metal coordination are provided in REMARK 620. Coordination angles for any metal coordination and surrounding residues (if present) will be provided this remark.

Template:

```
REMARK 620 METAL COORDINATION REMARK 620 formatted text
```

Example -

```
REMARK 620
REMARK 620 METAL COORDINATION
REMARK 620 (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER;
REMARK 620
             SSEQ=SEQUENCE NUMBER; I=INSERTION CODE):
REMARK 620
REMARK 620 COORDINATION ANGLES FOR: M RES CSSEQI METAL
REMARK 620
                                            F3S A 107
REMARK 620 N RES CSSEQI ATOM
REMARK 620 1 CYS A 39 SG
REMARK 620 2 F3S A 107 FE3 142.2
REMARK 620 3 F3S A 107 FE4 154.3 59.7
REMARK 620 4 F3S A 107 S1 120.2 53.8 55.7
REMARK 620 5 F3S A 107 S2 113.0 103.5 54.3 106.6 REMARK 620 6 F3S A 107 S3 103.8 53.0 101.7 103.2 109.2
REMARK 620 N
REMARK 620
REMARK 620 COORDINATION ANGLES FOR: M RES CSSEQI METAL
                                           F3S A 107 FE3
REMARK 620
REMARK 620 N RES CSSEOI ATOM
REMARK 620 1 F3S A 107 FE1
REMARK 620 2 F3S A 107 FE4 59.0
REMARK 620 3 F3S A 107 S1 52.7 55.1
REMARK 620 4 F3S A 107 S3 52.9 101.0 102.1
REMARK 620 5 CYS A 45 SG 146.5 146.2 115.6 112.8
REMARK 620 6 F3S A 107 S4 103.5 54.5 106.3 109.6 110.0
REMARK 620 N
                                    1
                                          2
                                                3
                                                       4
```

```
REMARK 620
REMARK 620 COORDINATION ANGLES FOR: M RES CSSEQI METAL
REMARK 620
                                  F3S A 107 FE4
REMARK 620 N RES CSSEQI ATOM
REMARK 620 1 F3S A 107 FE1
                         61.3
REMARK 620 2 F3S A 107 FE3
REMARK 620 3 F3S A 107
                      S1
                           53.4 53.9
                          54.4 105.0 104.5
REMARK 620 4 F3S A 107
                      S2
                      SG 142.7 140.2 109.0 114.5
REMARK 620 5 CYS A 20
                     S4 105.1 54.1 104.8 111.7 111.6
REMARK 620 6 F3S A 107
REMARK 620 N
                            1
                                 2 3 4 5
REMARK 620
REMARK 620 COORDINATION ANGLES FOR: M RES CSSEQI METAL
REMARK 620
                                  F3S A 108 FE1
REMARK 620 N RES CSSEQI ATOM
                     S3
SG 120.1
REMARK 620 1 F3S A 108
REMARK 620 2 CYS A 16
REMARK 620 3 F3S A 108 FE3
                          51.4 145.9
REMARK 620 4 F3S A 108 FE4
                          54.3 148.5 59.9
REMARK 620 5 F3S A 108 S1 98.3 110.0 50.6 101.5
REMARK 620 6 F3S A 108 S2 104.2 109.4 104.5 53.3 114.7
REMARK 620 N
                           1 2 3 4
REMARK 620
```

3. Primary Structure Section

The primary structure section of a PDB file contains the sequence of residues in each chain of the macromolecule. Embedded in these records are chain identifiers and sequence numbers that allow other records to link into the sequence.

The changes in the records in this section result from the standardization of nomenclature the standard nucleotides and nucleotide modifications.

DBREF

The DBREF record provides cross-reference links between PDB sequences and the corresponding database entry or entries. There are no character/column format changes in the records in this section. A detailed description of the assignment of sequence database references is presented in Section A of the wwp.db/ Processing Procedures and Policies Document.

SEQADV

The SEQADV record identifies conflicts between sequence information in the SEQRES records of the PDB entry and the sequence database entry given on DBREF. There are no character/column format changes in the records in this section. A detailed description of the assignment of sequence difference records is presented in Section A of the ww.pdb.nih.gov/wwp.be/ Processing Procedures and Policies Document.

SEQRES

SEQRES records contain the amino acid or nucleic acid sequence of residues in each chain of the macromolecule that was studied.

The ribo- and deoxyribonucleotides in the SEQRES records are now distinguished. The deoxy- forms of these residues are now identified with the residue names DA, DC, DG, DT, and DU. Modified nucleotides in the sequence are now identified by separate 3-letter residue codes. The use of the *plus* character prefix to label modified nucleotides (e.g. +A, +C, +T) is no longer used.

MODRES

The MODRES record provides descriptions of modifications (e.g., chemical or post-translational) to protein and nucleic acid residues. Included is a mapping between residue names given in a PDB entry and standard residues.

Modified nucleotides in the sequence are now identified by separate 3-letter residue codes. The use of the *plus* character prefix to label modified nucleotides (e.g. +A, +C, +T) is no longer used.

4. Heterogen Section

The heterogen section of a PDB file contains the complete description of nonstandard residues in the entry. Changes in the detailed chemical descriptions of non-polymer chemical components are described in the PDB Chemical Components dictionary,

http://remediation.wwpdb.org/downloads/Components-rel-alt.cif.

There are no character/column format changes in the records in this section; however, the definition of a PDB HET group is revised owing to the change in nomenclature for the standard deoxyribonucleotides as described in the following section.

HET

HET records are used to describe non-standard residues, such as prosthetic groups, inhibitors, solvent molecules, and ions for which coordinates are supplied. Groups are considered HET if they are not part of a biological polymer described in SEQRES and considered to be a molecule bound to the polymer, or they are a chemical species that constitutes part of a biological polymer that is not one of the following:

- not one of the standard amino acids, and
- not one of the ribonucleic acids (C, G, A, T, U, and I), and
- not one of the deoxyribonucleic acids (DC, DG, DA, DT, DU and DI)
- not an unknown amino acid or nucleic acid where UNK is used to indicate the unknown residue name.

HET records also describe chemical components for which the chemical identity is unknown, in which case the group is assigned the hetID UNL (Unknown Ligand).

5. Secondary Structure Section

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

There are no changes in the formats of the records in this section.

6. Connectivity Annotation Section

The connectivity annotation section allows the depositors to specify the existence and location of disulfide bonds and other linkages.

SSBOND

The disulfide bond distance is included after the symmetry operations at the end of the SSBOND record.

Record Format

COLUMNS	DATA TYPE			FIELD	DEFINITION			
1 - 6		Record name		"SSBOND"				
8 - 10		Integer		serNum	Serial number.			
12 - 14		LString(3)		"CYS"	Residue name.			
16		Character		chainID1	Chain identifier.			
18 - 21		Integer		seqNum1	Residue sequence number.			
22		AChar		icode1	Insertion code.			
26 - 28		LString(3)		"CYS"	Residue name.			
30		Character		chainID2	Chain identifier.			
32 - 35		Integer		seqNum2	Residue sequence number.			
36		AChar		icode2	Insertion code.			
60 - 65		SymOP		sym1	Symmetry op for residue 1.			
67 - 72		SymOP		sym2	Symmetry op for residue 2.			
74 - 78		Real(5.2)		Length	Disulfide bond distance			
Exampl	e –							
SSBOND SSBOND	1 CYS A 2 CYS A 3 CYS A 4 CYS A	30 CYS A	115 80		1555 1555 2.03 1555 1555 2.07 1555 1555 2.06 1555 1555 2.04			

LINK

Link records include the distance associated with the each linkage following the symmetry operations at the end of each record.

Record Format

COLUMNS	DATA TYPE	FIELD	DEFINITION
1 - 6	Record name	"LINK "	
13 - 16	Atom	name1	Atom name.
17 indicator.	Character	altLoc1	Alternate location
18 - 20	Residue name	resName1	Residue name.
22	Character	chainID1	Chain identifier.
23 - 26	Integer	resSeq1	Residue sequence number.
27	AChar	iCode1	Insertion code.
43 - 46	Atom	name2	Atom name.
47 indicator.	Character	altLoc2	Alternate location
48 - 50	Residue name	resName2	Residue name.
52	Character	chainID2	Chain identifier.
53 - 56	Integer	resSeq2	Residue sequence number.
57	AChar	iCode2	Insertion code.
60 - 65	SymOP	sym1	Symmetry operator atom 1.
67 - 72	SymOP	sym2	Symmetry operator atom 2.
74 - 78	Real(5.2)	Length	Link distance
Example -			
LINK OG1 TI		NA NA A6001 NA NA A6001 NA NA A6001 NA NA A6001	1555 1555 2.72

7. Miscellaneous Features Section

The miscellaneous features section may describe features in the molecule such as environments surrounding a non-standard residue or an active site. Other features may be described in the remarks section but are not given a specific record type so far.

There are no changes in the formats of the records in this section.

8. Crystallographic Coordinate Transformation Section

The Crystallographic Section describes the geometry of the crystallographic experiment and the coordinate system transformations.

There are no changes in the formats of the records in this section.

9. Coordinate Section

The Coordinate Section contains the collection of atomic coordinates as well as the MODEL and ENDMDL records.

ATOM/HETATM

The ATOM records present the atomic coordinates for standard residues. 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; segment identifier and charge are optional.

The character/column format of the ATOM/HETATM records is not changed. Changes in ATOM/HETATM records result from the standardization atom and residue nomenclature. This nomenclature is described in electronic form in the PDB Chemical Components Dictionary, which may be downloaded at http://remediation.wwpdb.org/downloads/Components-rel-alt.cif.

A detailed description of the assignment of alternate conformations and the assignment of chain identifiers for non-polymers and solvent is presented in Section A of the wwPDB Processing Procedures and Policies Document.

10. Connectivity Section

This section provides information on chemical connectivity.

There are no changes in the formats of the records in this section.

11. Bookkeeping Section

The Bookkeeping Section provides some final information about the file itself.

There are no changes in the formats of the records in this section.

12. Nomenclature

Atom and residue nomenclature has been standardized in a variety of ways in PDB version 3.0 data files. All changes in nomenclature are documented in the electronic chemical components dictionary,

http://remediation.wwpdb.org/downloads/Components-rel-alt.cif.

The changes in nomenclature include:

- IUPAC nomenclature for standard amino acid and nucleotides. Atoms names follow the recommendations of described in *Pure & Appl. Chem.*, 70, 117-142, 1998. with the exception of the well-established convention for C-terminal atoms OXT and HXT. In this and other cases where an atom name has been changed, the previous name is retained in an alternate name in the PDB Chemical Components dictionary.
- Discrimination of DNA and RNA linking nucleotides and modifications.
 Deoxy- and ribose nucleotides now have separate chemical definitions with
 the DNA forms relabeled as DA, DC, DG, DT, DI and DU. Modified
 nucleotides formerly identified as using the "plus-nucleotide" syntax (e.g. +C,
 +G) have been relabeled with the particular 3-letter code corresponding to the
 full chemical description of the modified nucleotide.
- More conventional atom labeling for non-polymer atoms.
 In the new chemical definitions the following changes have been made to move the atom naming to a more conventional state.
 - Atom names begin with their element symbol
 - Heavy atom names follow the traditional PDB justification rules in which the atom element symbol is right justified in the second character position of the 4-character atom name. 4-character names for atoms with 1-character element symbols have been compressed to 3 characters.
 - Hydrogen atoms names all begin with "H" and are not subject to the justification rule.
- Removal of redundant and deprecated ligands. In cases where the same monomer or ligand had been defined using different identifiers, the most common identifier has been retained and the others have been marked as obsolete. Definitions which were deemed incorrect or better represented in other ways (e.g. metal hydrates) have also been obsoleted.