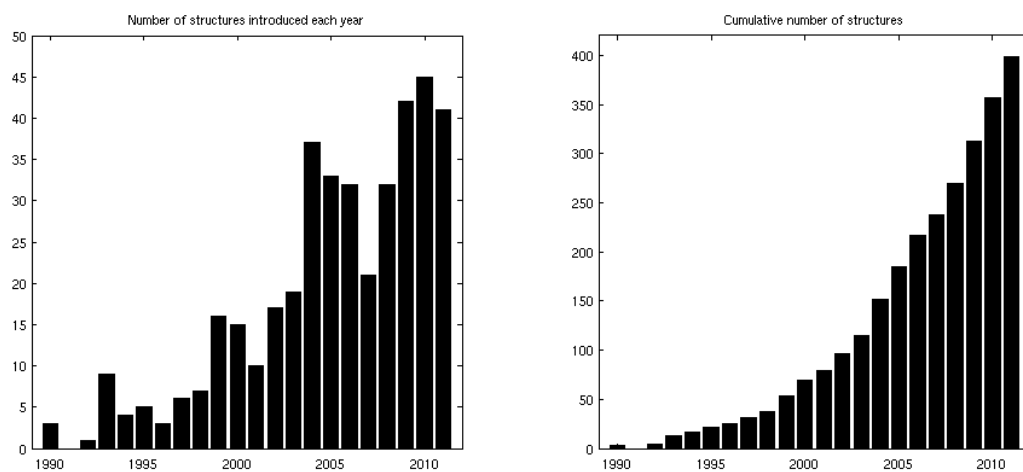


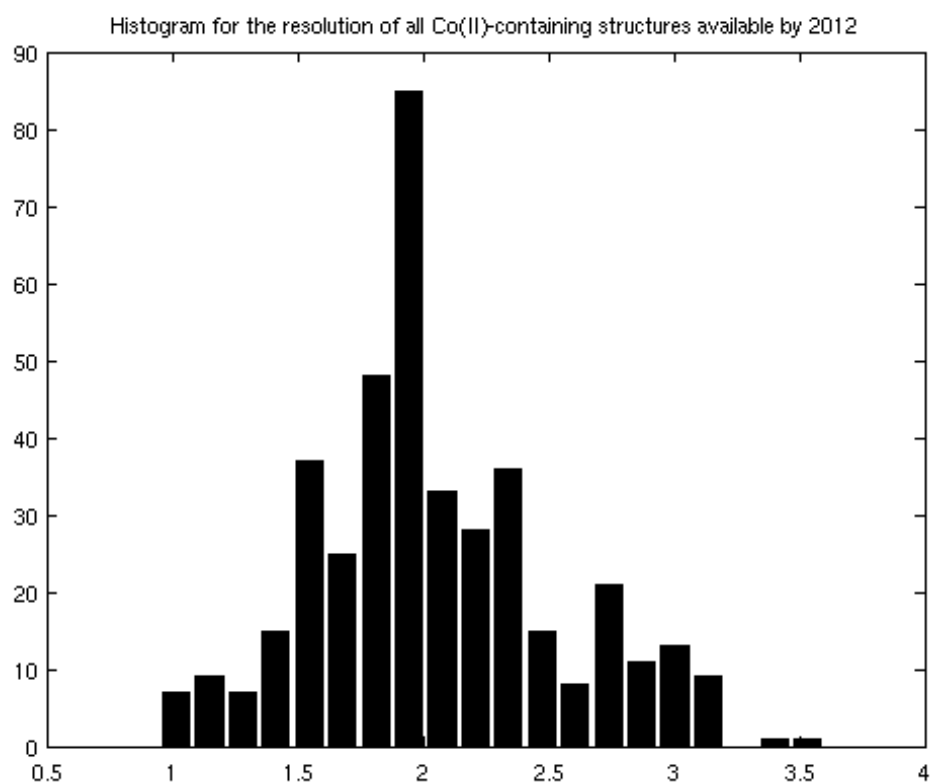
## Supporting Information

### Investigation of non-corrin Co(II)-containing sites in protein structures of the Protein Data Bank

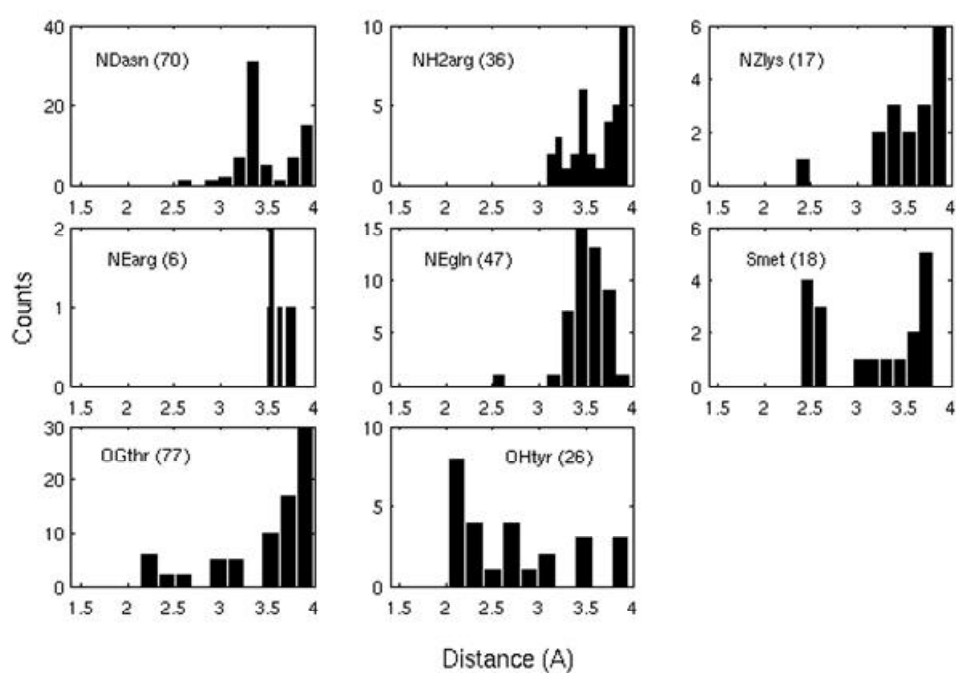
Luciano A. Abriata



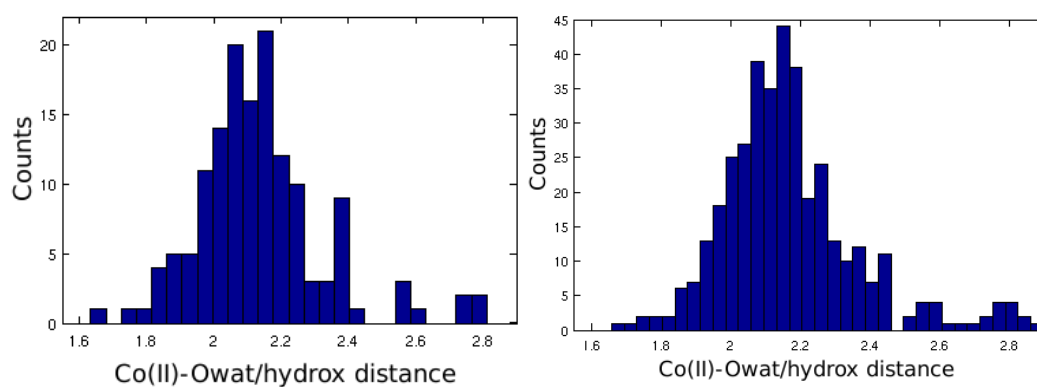
**Figure S1. Number of structures released** by the Protein Data Bank over time for proteins with non-corrin Co(II) sites.



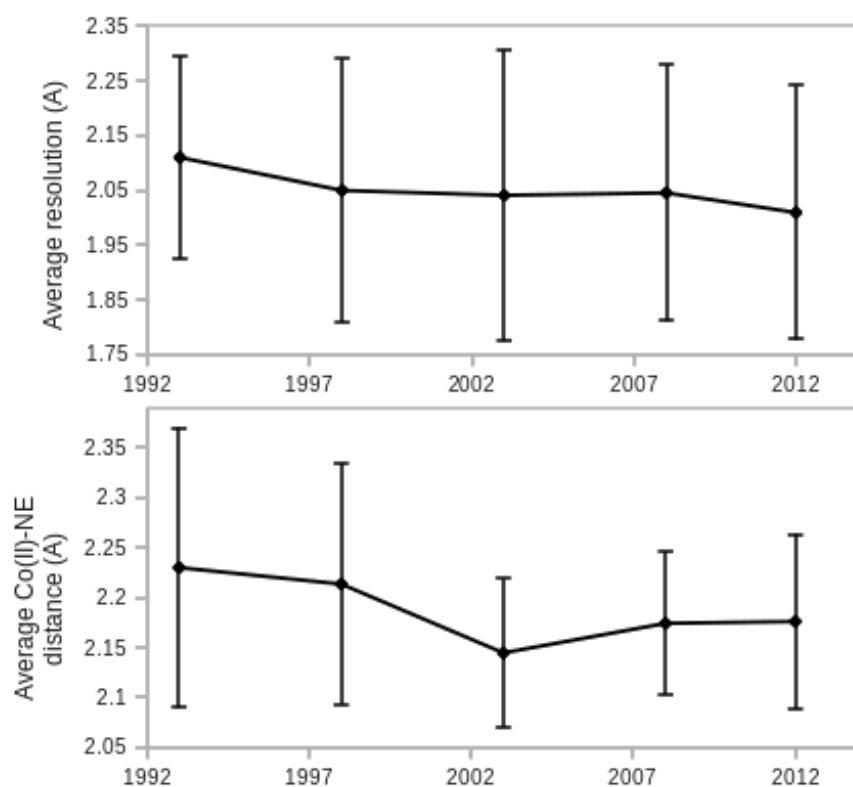
**Figure S2. Distribution of structure resolutions.**



**Figure S3 Histogram of Co(II)-donor distances for donor atoms in group (iii) of the main text, *i.e.* those with no clear group of distances below 3 Å.**



**Figure S4 Histograms of Co(II)-Owat distances built from protein structure data solved at resolutions better than 1.5 or 1.75 Å (left and right, respectively)**



**Figure S5 Average structure resolution (top) and computed Co(II)-NEhis bond lengths (bottom) over 5-year windows**

**Table S1.** PDB entries analyzed in this work (See xls file in Supporting Information)

<b>PDB ID</b>	<b>Structure Title</b>
1A0C	Xylose Isomerase From Thermoanaerobacterium Thermosulfurigenes
1A0E	Xylose Isomerase From Thermotoga Neapolitana
1B59	Complex Of Human Methionine Aminopeptidase-2 Complexed With Ovalicin
1B6A	Human Methionine Aminopeptidase 2 Complexed With Tnp-470
1C0W	Crystal Structure Of The Cobalt-Activated Diphtheria Toxin Repressor-Dna Complex Reveals A Metal Binding Sh-Like Domain
1C4G	Phosphoglucomutase Vanadate Based Transition State Analog Complex
1COB	Crystal Structure Solution And Refinement Of The Semisynthetic Cobalt Substituted Bovine Erythrocyte Enzyme Superoxide Dismutase At 2.0 Angstroms Resolution
1EPY	T4 Lysozyme Mutant T21h/C54t/C97a/Q141h/T142h
1FA6	Crystal Structure Of The Co(II)-Bound Glyoxalase I Of Escherichia Coli
1FOF	Crystal Structure Of The Class D Beta-Lactamase Oxa-10
1FX7	Crystal Structure Of The Iron-Dependent Regulator (Ider) From Mycobacterium Tuberculosis
1G16	Crystal Structure Of Sec4-Gdp
1GWM	Carbohydrate Binding Module Family29 Complexed With Glucohexaose
1H0O	Cobalt Substitution Of Mouse R2 Ribonucleotide Reductase To Model The Reactive Diferrous State
1H41	Pseudomonas Cellulosa E292a Alpha-D-Glucuronidase Mutant Complexed With Aldotriuronic Acid
1IAB	Crystal Structures Spectroscopic Features And Catalytic Properties Of Cobalt(II) Copper(II) Nickel(II) And Mercury(II) Derivatives Of The Zinc Endopeptidase Astacin. A Correlation Of Structure And Proteolytic Activity
1IN4	Thermotoga Maritima Ruvb Holliday Junction Branch Migration Motor
1JN1	Structure Of 2C-Methyl-D-Erythritol 2,4-Cyclodiphosphate Synthase From Haemophilus Influenzae (HI0671)
1K1E	Structure Of The Cobalt-Bound Form Of The Deoxy-D-Mannose-Octulosonate 8-Phosphate Phosphatase (Yrbi) From Haemophilus Influenzae (HI1679)
1KEJ	Crystal Structure Of Murine Terminal Deoxynucleotidyl Transferase Complexed With Ddatp
1L8X	Crystal Structure Of Ferrochelataase From The Yeast Saccharomyces Cerevisiae With Cobalt(II) As The Substrate Ion
1LNA	A Structural Analysis Of Metal Substitutions In Thermolysin
1M38	Structure Of Inorganic Pyrophosphatase
1OF8	Double Complex Of The Tyrosine Sensitive Dahp Synthase From S. Cerevisiae With Co2+ Pep And The E4p Analogoue G3p
1OVV	CRYSTAL STRUCTURE OF FOUR-HELIX BUNDLE MODEL Di-Co(II)-DF1-L13A (Form II)
1QK0	Cel6a In Complex With M-Iodobenzyl Beta-D-Glucopyranosyl-Beta(14)-D-Xylopyranoside
1QRE	A Closer Look At The Active Site Of Gamma-Carbonic Anhydrases: High Resolution Crystallographic Studies Of The Carbonic Anhydrase From Methanosarcina Thermophila
1QRF	A Closer Look At The Active Site Of Gamma-Carbonic Anhydrases: High Resolution Crystallographic Studies Of The Carbonic Anhydrase From Methanosarcina Thermophila
1QXY	Crystal Structure Of S. Aureus Methionine Aminopeptidase In Complex With A Ketoheterocycle 618
1R0H	Cobalt-Substituted Rubredoxin
1R6X	The Crystal Structure Of A Truncated Form Of Yeast ATP Sulfurylase Lacking The C-Terminal APS Kinase-Like Domain In Complex With Sulfate
1R8K	Pdxa Protein; Nad-Dependent Dehydrogenase/Carboxylase; Subunit Of Pyridoxine Phosphate Biosynthetic Protein Pdxj-Pdxa [Salmonella Typhimurium]
1RL4	Plasmodium Falciparum Peptide Deformylase Complex With Inhibitor
1RMQ	Crystal Structure Of Apha Class B Acid Phosphatase/Phosphotransferase With

Osmiate Mimicking The Catalytic Intermediate

1RQB Propionibacterium Shermanii Transcarboxylase 5S Subunit

1RRK Crystal Structure Analysis Of The Bb Segment Of Factor B  
Crystal Structure Of Class II Fructose-Bisphosphate Aldolase From Thermus

1RVG Aquaticus In Complex With Y  
High-Resolution Structures Of Single-Metal-Substituted Concanavalin A: The Coca-

1SCS Protein At 1.6 Angstroms And The Nica-Protein At 2.0 Angstroms  
Two Distinctly Different Metal Binding Modes Are Seen In X-Ray Crystal Structures

1STG Of Staphylococcal Nuclease-Cobalt(II)-Nucleotide Complexes  
A Dual Inhibitor Of The Leukocyte Proteases Cathepsin G And Chymase With

1T31 Therapeutic Efficacy In Animals Models Of Inflammation

1T5K Crystal Structure Of Amicyanin Substituted With Cobalt

1TU4 Crystal Structure Of Rab5-GDP Complex  
Crystal Structure Of An Ider-DNA Complex Reveals A Conformational Change In

1U8R Activated Ider For Base-Specific Interactions

1UGP Crystal Structure Of Co-Type Nitrile Hydratase Complexed With N-Butyric Acid  
Crystal Structure Of Medium-Chain Acyl-CoA Dehydrogenase From Thermus

1UKW Thermophilus HB8

1V29 Crystal Structure Of Nitrile Hydratase From A Thermophile Bacillus Smithii

1V9B Crystal Structure Of Pyrococcus Horikoshii Cuta1 Complexed With Co<sup>2+</sup>

1VLX Structure Of Electron Transfer (Cobalt-Protein)  
Crystal Structure Of Topaquinoxone-Containing Amine Oxidase Activated By Cobalt

1WMN Ion

1WN1 Crystal Structure Of Dipeptidase From Pyrococcus Horikoshii OT3  
High Resolution Crystals Structure Of Cobalt- Peptide Deformylase Bound To

1XEO Formate

1XGS Methionine Aminopeptidase From Hyperthermophile Pyrococcus Furiosus

1XIM Arginine Residues As Stabilizing Elements In Proteins  
Structure Of Co(II) Reconstituted Methane Monooxygenase Hydroxylase From M.

1XMH Capsulatus (Bath)

1XUH TRYPSIN-KETO-BABIM-CO<sub>2</sub> Ph 8.2  
Structure Of E. Coli Alkaline Phosphatase In Presence Of Cobalt At 1.60 A

1Y6V Resolution  
Crystal Structure Analysis Of Product Bound Methionine Aminopeptidase Type 1c

1YJ3 From Mycobacterium Tuberculosis

1ZJC Aminopeptidase S From S. Aureus

2AMX Crystal Structure Of Plasmodium Yoelii Adenosine Deaminase (PY02076)  
Crystal Structure Of Human Methionine Aminopeptidase Type I With A Third Cobalt

2B3H In The Active Site

2BDI Human Kallikrein 4 Complex With Cobalt And P-Aminobenzamidine

2BO7 Dissection Of Mannosylglycerate Synthase: An Archetypal Mannosyltransferase  
The Structure Of A Family 4 Acetyl Xylan Esterase From Clostridium Thermocellum

2C79 In Complex With A Cobalt Ion.

2DDS Crystal Structure Of Sphingomyelinase From Bacillus Cereus With Cobalt Ion

2DPP Crystal Structure Of Thermostable Bacillus Sp. Raps8 Nitrile Hydratase

2DTR Structure Of Diphtheria Toxin Repressor

2EFF Crystal Structure Analysis Of The Complex Between Cyay And Co(II)

2EW5 Structure Of Helicobacter Pylori Peptide Deformylase In Complex With Inhibitor  
Crystal Structure Of Monomeric Uncomplexed Form Of Xenopus Dishevelled PDZ

2F0A Domain

2F7N Structure Of D. Radiodurans Dps-1

2F7V Structure Of Acetylcitrulline Deacetylase Complexed With One Co  
Crystal Structure Of Alkb In Complex With Co(II) 2-Oxoglutarate And Methylated

2FDF Trinucleotide T-Mea-T  
Crystal Structure Of B.Subtilis Luxs In Complex With (2S)-2-Amino-4-[(2R3S)-23-

2FQT Dihydroxy-3-N-Hydroxycarbamoyl-Propylmercapto]Butyric Acid

2FUA L-Fucose 1-Phosphate Aldolase Crystal Form T With Cobalt

2GGC Novel Bacterial Methionine Aminopeptidase Inhibitors

2GLI Five-Finger Gli/Dna Complex  
 Crystal Structure Of 2-Deoxy-Scyllo-Inosose Synthase Complexed With  
 2GRU Carbaglucose-6-Phosphate NAD<sup>+</sup> And Co<sub>2</sub><sup>+</sup>  
 Crystal Structure Of Alpha-Amino-Beta-Carboxymuconate-Epsilon-Semialdehyde-  
 2HBX Decarboxylase (ACMSD)  
 Crystal Structure Of A Cora Soluble Domain From A. Fulgidus In Complex With  
 2HN1 Co<sub>2</sub><sup>+</sup>  
 Crystal Structure Of Uridylate Kinase From Sulfolobus Solfataricus In Complex With  
 2J4J Ump And Ampcp To 2.1 Angstrom Resolution  
 2JF5 Crystal Structure Of Lys63-Linked Di-Ubiquitin  
 2OPC Structure Of Melampsora Lini Avirulence Protein Avr1567-A  
 Structures Of Actinonin Bound Peptide Deformylases From E. Faecalis And S.  
 2OS3 Pyogenes  
 Crystal Structure Of The 5'-Deoxynucleotidase Yfbr Mutant E72A Complexed With  
 2PAR Co(2<sup>+</sup>) And TMP  
 X-Ray Crystallographic Characterization Of The Co(II)-Substituted Tris-Bound Form  
 2PRQ Of The Aminopeptidase From Aeromonas Proteolytica  
 Structure And Metal Binding Properties Of Znua A Periplasmic Zinc Transporter  
 2PS9 From Escherichia Coli  
 Crystal Structure Of Spc42p A Critical Component Of Spindle Pole Body In Budding  
 2Q6Q Yeast  
 2QB7 Saccharomyces Cerevisiae Cytosolic Exopolyphosphatase Phosphate Complex  
 2R5V Hydroxymandelate Synthase Crystal Structure  
 2UZP Crystal Structure Of The C2 Domain Of Human Protein Kinase C Gamma.  
 2V3I Hypocrea Jecorina Cel7a In Complex With (R)-Dihydroxy-Phenanthrenolol  
 Structural Basis For Natural Lactonase And Promiscuous Phosphotriesterase  
 2VC7 Activities  
 2VKE Tet Repressor Class D Complexed With Cobalt And Tetracycline  
 2VOS Mycobacterium Tuberculosis Folylpolyglutamate Synthase Complexed With Adp  
 Crystal Structure Of The Actinomyces R39 Dd-Peptidase Inhibited By 6-Beta-  
 2WKE Iodopenicillanate.  
 2WYR 3-D Structure Of Phtet1-12s Dodecamer In The Asymmetric Unit  
 2XDB A Processed Non-Coding Rna Regulates A Bacterial Antiviral System  
 2XJM Crystal Structure Of Streptococcus Suis Dpr With Cobalt  
 2XPH Crystal Structure Of Human SENP1 With The Bound Cobalt  
 Crystal Structure Of The Sulfane Dehydrogenase Soxcd From Paracoccus  
 2XTS Pantotrophus  
 Cobalt Chelataze Cbik (Periplasmic) From Desulfovibrio Vulgaris Hildenborough  
 2XVY (Co-Crystallised With Cobalt And Shc)  
 2Y3B Co-Bound Form Of Cupriavidus Metallidurans Ch34 Cnrxs  
 2Y8U A. Nidulans Chitin Deacetylase  
 Crystal Structure Of Selenophosphate Synthetase From Aquifex Aeolicus  
 2YYE Complexed With AMPCPP  
 Crystal Structure Of Uncharacterized Conserved Protein From Thermus  
 2Z06 Thermophilus  
 Crystal Structure Of Mannosyl-3-Phosphoglycerate Synthase From Pyrococcus  
 2ZU9 Horikoshii  
 379D The Structural Basis Of Hammerhead Ribozyme Self-Cleavage  
 3A4J Arpte (K185R/D208G/N265D/T274N)  
 Crystal Structure Of Homocitrate Synthase From Thermus Thermophilus Complexed  
 3A9I With Lys  
 3ALQ Crystal Structure Of TNF-TNFR2 Complex  
 Refined Crystal Structure Of Type Iii Chloramphenicol Acetyltransferase At 1.75  
 3CLA Angstroms Resolution  
 1.9A Structure Of Glycerophosphodiesterase (Gpdq) From Enterobacter  
 3D03 Aerogenes  
 3DWC Trypanosoma Cruzi Metalloprotease 1  
 3G5P Structure And Activity Of Human Mitochondrial Peptide Deformylase

3GB4 Crystal Structure Of Dicamba Monooxygenase With Non-Heme Cobalt And Dicamba  
 Crystal Structure Of SAM-Dependent Methyltransferase (YP\_325210.1) From  
 3GGD ANABAENA VARIABILIS ATCC 29413 At 2.11 Å Resolution  
 Crystal Structure Of The Bacteriophage Phi29 Gene Product 12 N-Terminal  
 3GQA Fragment In Complex With Cobalt Ions  
 D71G/E101G Mutant In Organophosphorus Hydrolase From Deinococcus  
 3GTX Radiodurans  
 3H2W Structure Of A. Acidocaldarius Cellulase Cels In Complex With Cellobiose  
 3H7J Crystal Structure Of BacB An Enzyme Involved In Bacilysin Synthesis  
 3HDI Crystal Structure Of Bacillus Halodurans Metallo Peptidase  
 3I11 Cobalt-Substituted Metallo-Beta-Lactamase From Bacillus Cereus  
 Crystal Structures Of Leishmania Mexicana Phosphoglycerate Mutase At Low  
 3IGZ Cobalt Concentration  
 3ISQ Crystal Structure Of Human 4-Hydroxyphenylpyruvate Dioxygenase  
 3IUH Co<sup>2+</sup>-Bound Form Of Pseudomonas Stutzeri L-Rhamnose Isomerase  
 3IVS Homocitrate Synthase Lys4  
 3KA8 Frog M-Ferritin EQH Mutant With Cobalt  
 3KHB Crystal Structure Of Escherichia Coli AlkB With Co(II) And 2-OG  
 Crystal Structure Of Escherichia Coli AlkB In Complex With Ssdna Containing A 1-  
 3KHC Methylguanine Lesion  
 3KOL Crystal Structure Of A Glyoxalase/Dioxygenase From Nostoc Punctiforme  
 3KON Crystal Structure Of Cobalt (II) Human Carbonic Anhydrase II At Ph 11.0  
 Structural Insights Into Substrate Specificity And The Anti Beta-Elimination  
 3KRG Mechanism Of Pectate Lyase  
 Crystal Structures Of Zinc Cobalt And Iron Containing Adenylate Kinase From Gram-  
 3LOS Negative Bacteria Desulfovibrio Gigas  
 3L48 Crystal Structure Of The C-Terminal Domain Of The PapC Usher  
 Crystal Structure Of The DIP2311 Protein From Corynebacterium Diphtheriae  
 3LMM Northeast Structural Genomics Consortium Target Cdr35  
 3M4Z Crystal Structure Of B. Subtilis Ferrochelata With Cobalt Bound At The Active Site  
 Crystal Structure Of NADH Dehydrogenase Subunit C (Tfu\_2693) From  
 3MCR THERMOBIFIDA FUSCA YX-ER1 At 2.65 Å Resolution  
 3MF3 Cobalt(II)-Substituted Haemophilus Influenzae B-Carbonic Anhydrase  
 3MGP Binding Of Cobalt Ions To The Nucleosome Core Particle  
 3MGW Thermodynamics And Structure Of A Salmon Cold-Active Goose-Type Lysozyme  
 3MZ7 Crystal Structure Of D101L Co<sup>2+</sup> HDAC8 Complexed With M344  
 Crystal Structure Of L-N-Carbamoylase From Geobacillus Stearothermophilus  
 3N5F CECT43  
 3NVL Crystal Structure Of Phosphoglycerate Mutase From Trypanosoma Brucei  
 3NYK The Structure Of Cobalt-Substituted Pseudoazurin From Alcaligenes Faecalis  
 3NZH Crystal Structure Of Anti-Emmprin Antibody 5F6 FAB  
 Crystal Structure Of Fumarate Lyase:Delta Crystallin From Brucella Melitensis  
 3OCE Bound To Cobalt  
 Structure Of Co-Substituted Homoprotocatechuate 23-Dioxygenase In Complex With  
 3OJK 4-Nitrocatechol At 1.68 Å Resolution  
 3P0F Structure Of Hupp2 In An Inactive Conformation With Bound 5-Benzylacetylcholine  
 3PJL The Crystal Structure Of Tp34 Bound To Co (II) Ion At Ph 7.5  
 3QQ7 Crystal Structure Of The P97 N-Terminal Domain  
 3R61 Structure Of The Mntr Co<sup>2+</sup> Complex  
 Crystal Structure Of D-Mannosate Dehydratase From Chromohalobacter Saalexigens  
 3RGT Complexed With D-Arabinohydroxamate  
 3RMU Crystal Structure Of Human Methylmalonyl-CoA Epimerase  
 Crystal Structures Of Falcilysin A M16 Metalloprotease From The Malaria Parasite  
 3S5H Plasmodium Falciparum  
 Crystal Structure Of A Papaya Latex Serine Protease Inhibitor (PPI) At 1.7Å  
 3S8K Resolution  
 Human DNA Polymerase Eta - DNA Ternary Complex With The 5'T Of A CPD In  
 3SI8 The Active Site (TT2)

3SXX	Hansenula Polymorpha Copper Amine Oxidase-1 In Complex With Co(II) Cobalt Bound Structure Of An Archaeal Member Of The Ligd 3'-Phosphoesterase
3TA5	DNA Repair Enzyme Family
3THJ	Crystal Structure Of The Co <sub>2</sub> +2-HAI-L-Orn Complex
3TR3	Structure Of A Bola Protein Homologue From Coxiella Burnetii Structure Of The Thioalkalivibrio Paradoxus Cytochrome C Nitrite Reductase In
3TTB	Complex With Sulfite
3TW3	Crystal Structure Of Rtca.ATP.Co Ternary Complex
3UT1	Crystal Structure Of The 3-MBT Repeat Domain Of L3MBTL3
3V1D	Crystal Structure Of De Novo Designed MID1-Cobalt
3ZR9	Structure Of New Delhi Metallo-Beta-Lactamase 1 (Ndm-1) Protein Crystallization And Microgravity: Glucose Isomerase Crystals Grown During
4A8I	The Pcdf-Protein Mission