

Viewing the 2xgf ligands from its Summary page

Macromolecular structures contain a variety of small molecule compounds. In the PDB archive these are defined as **heterogens** or as **ligands**. Some of them are covalently linked to a macromolecule chain and some are incorporated as modified residues. Even if not directly included in this way, they all get a **three-letter** code and a chain identifier equivalent to a **residue**. To see the small molecule content of a PDB entry you can visit the **Ligand** summary page from the entry's main **Summary** page. As shown in screenshot 1 you click either on the Ligand link (circled in red) or directly on the green **PDBePrints** ligand logo (the benzene ring symbol, arrowed).

Usefully, ligands only turn the **PDBeMotif** symbol green if they are bound to the macromolecule rather than being modified residues that are incorporated into the backbone of the molecule.

PDB entry 2xgf

STRUCTURE OF THE BACTERIOPHAGE T4 LONG TAIL FIBRE NEEDLE-SHAPED RECEPTOR-BINDING TIP

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Quaternary

The structure was published by Bartual, S.G., Otero, J.M., Garcia-Doval, C., et al., Kahn, R., Fox, G.C., and Van Raaij, M.J., in 2010 in a paper entitled "Structure of the Bacteriophage T4 Long Tail Fiber Receptor-Binding Tip" ([abstract](#)).

This crystal structure was determined using X-ray diffraction at a resolution of 2.2 Å and deposited in 2010.

The [experimental data](#) on which the structure is based was also deposited.

This PDB entry contains multiple copies of the structure of LONG TAIL FIBER PROTEIN P37.

It also contains one or more heterogenic compounds (e.g., ligands, co-factors, ions, modified amino acids, etc.); see [here](#) for a complete list.

The molecule most likely forms homotrimers.

The following tables show cross-reference information to other databases (to obtain a list of all PDB entries sharing the same property or classification, click on the magnifying glass icon):

Chain Name	UniProt	Name of source organism	% of UniProt sequence present in the sample	Residues in the sample molecules	% of residues observed
A, B, C	LONG TAIL FIBER PROTEIN P37	P03744 (Q037_BPT4) Enterobacteria phage T4	< 90%	242	89%

This entry contains 1 unique UniProt protein:

UniProt accession	Name	Organism	PDB
P03744	LONG TAIL FIBER PROTEIN P37	Enterobacteria phage T4	Related PDB UniProt coverage

B-factors and symmetry contacts

- This image shows the backbone of the macromolecules.
- The thickness reflects the B-values (thin = low, thick = high).
- The colour varies from blue to red corresponding to a B-factor range of 10 to 100 Å².

screenshot 1

Ligands in the 2xgf structure from its Summary page.

Click on the green Ligand logo in the PDBePrints (arrowed) or on the Ligands link (circled in red).

The list of ligands in 2xgf

This **Ligand** summary page for the phage receptor-binding **gp47** structure shows that it contains one instance of the ligand **CO3** (bicarbonate) and seven instances of **FE2** (iron, Fe²⁺, ion). You will know from the accompanying **Quips** article that seven iron ions are integral structural components of the **gp47** central needle domain structure. In general metal ions can be bound by protein sidechains and prosthetic groups. To examine the environment that these seven iron ions are bound in by the **gp47** protein you can browse the analysis from the **PDBeMotif** service. This is precalculated for most PDB entries. To view this information click on the '**binding site details**' link under the 'Formula Fe' line for the FE2 ligand (arrowed in screenshot 2).

The screenshot shows the PDBe website interface for PDB entry 2xgf. The header includes the PDBe logo and the title '2xgf Ligands'. A sidebar on the left contains navigation links such as Summary, Details, Experiment, EDS, Structure, Taxonomy, Citation, Ligands, Cross references, Visualisation, and Downloads. The main content area is titled 'PDB entry 2xgf' and 'STRUCTURE OF THE BACTERIOPHAGE T4 LONG TAIL FIBRE NEEDLE-SHAPED RECEPTOR-BINDING TIP'. It displays a table of ligands. The first ligand is CO3 (CARBONATE ION) with a chemical structure diagram and a link to 'binding site details'. The second ligand is FE2 (FE (II) ION) with the chemical formula Fe²⁺ and a link to 'binding site details' that is being pointed to by a mouse cursor. The text 'screenshot 2' is visible in the bottom right corner of the image.

The list of ligands in PDB entry 2xgf.

To examine the environment around the Fe²⁺, click on 'binding site details' link (arrowed).

'Almost' covalent links to the Fe²⁺ ions

Metal ions are coordinated by sidechains through donation of electrons to the ions. This **coordination** chemistry gives an association that is not as strong as that from the usual covalent bonds. PDBeMotif analyses the environment around the metal ions and also help you explore other similar examples in the PDB archive.

The standard **PDBeMotif** analysis in fact recognizes only one of the seven sites as having a complete set of 'almost covalent' bonds. You can see these shown in red in screenshot 3. For other environments you will also see examples of interactions shown by the colours listed at the top.

Click on the FE2 for the octahedral **2030A** site to see the full analysis for it. Notice that the iron ion has a residue number offset from those of the protein residues, but that it has inherited a protein chain id -'A'. For ligands this chain will be that closest in space or with a direct contact or bond.

www.ebi.ac.uk/pdbe-site/pdbemotif/?tab=boundmolecule&pdb=2xgf&ligandCode3letter=FE2

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Classification: viral protein | **release date:** Thu, Jun 3, 2010
Title: structure of the bacteriophage t4 long tail fibre needle- shaped receptor-binding tip
Authors: A.L.LLAMAS-SALZ, C.GARCIA-DOVAL, J.M.OTERO, M.J.VAN RAAIJ, R.KAHN, S.G.BARTUAL
Method: X-RAY DIFFRACTION (resolution: 2.20Å)

Small molecules: [CQ3](#) [FE2](#)

Ligand bond colours: [covalent](#) [ionic](#) [hydrogen](#) [electrostatic](#) [van-der-waals](#) [plane-atom](#) [plane-plane](#) [undefined](#) - [Click here](#)

Assembly 1 View the assembly/model: ([PDB](#) [3D](#))

bound molecules	
No. Motif/Active site Ligand	Environment
1 FE2 2033A	[SQUARE_PYRAMIDAL] HIS 929C HIS 929A HIS 929B HIS 931C HIS 931E
2 FE2 2032A	
3 FE2 2031A	
4 FE2 2030A	[OCTAHEDRAL] HIS 980A HIS 980C HIS 980B HIS 982A HIS 982B HIS 982C
5 FE2 2029A	
6 FE2 2028A	
7 FE2 2027A	

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screenshot 3

Motifs and Sites analysis of Fe2+ ions environment in 2xgf

The results from the standard **PDBeMotif** analysis have only two of the Fe2+ sites displayed. In one case only five out of the six His residues are listed. To view the complete octahedral site click on the FE2 2030A link (arrowed).

The iron octahedral coordination site in detail

Clicking on the FE2 2030A example of the **gp37** sites gives a fuller analysis (screenshot 4). This shows that it is bound by two histidines from each of the three protein chains (boxed in green). The bond length to each are shown (boxed in blue). You can rotate the view of the site. This page can also be used to search for similar environments in other structures in the PDB archive.

Octahedrally-coordinated iron ions are of course common in the PDB, but much more commonly they are held in the centre of a porphyrin ring which provides four nitrogen atoms in a plane. The out-of-plane contacts to the iron in porphyrins are provided by protein sidechains. This is the basic structure of haem in proteins such as cytochromes and haemoglobin.

PDBe HOME **Motifs and Sites** pdbe.org/pdbemotif

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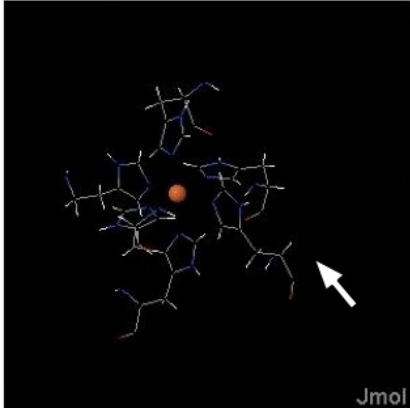
Classification: viral protein | **release date:** Thu, Jun 3, 2010
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Authors: A.L.LLAMAS-SALZ, C.GARCIA-DOVAL, J.M.OTERO, M.J.VAN RAAIJ, R.KAHN, S.G.BARTUAL
Method: X-RAY DIFFRACTION (resolution: 2.20Å)

Ligand bond colours: [covalent](#) [ionic](#) [hydrogen](#) [electrostatic](#) [van-der-waals](#) [plane-atom](#) [plane-plane](#) [undefined](#) - [Click here](#)

Assembly 1 View the assembly/model: ([PDB](#) [Jmol](#))

Ligands

[FE2 2030A \[OCTAHEDRAL\]](#)



Protein chain	Atom	Bond	Neighbour
Protein chain A	HIS980	2.23Å	NE2.HIS 980A
	HIS982	2.26Å	NE2.HIS 982A
Protein chain B	HIS980	2.20Å	NE2.HIS 980B
	HIS982	2.31Å	NE2.HIS 982B
Protein chain C	HIS980	2.37Å	NE2.HIS 980C
	HIS982	2.37Å	NE2.HIS 982C

screenshot 4

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Looking at the best octahedral Fe²⁺ ion (residue 2030A).

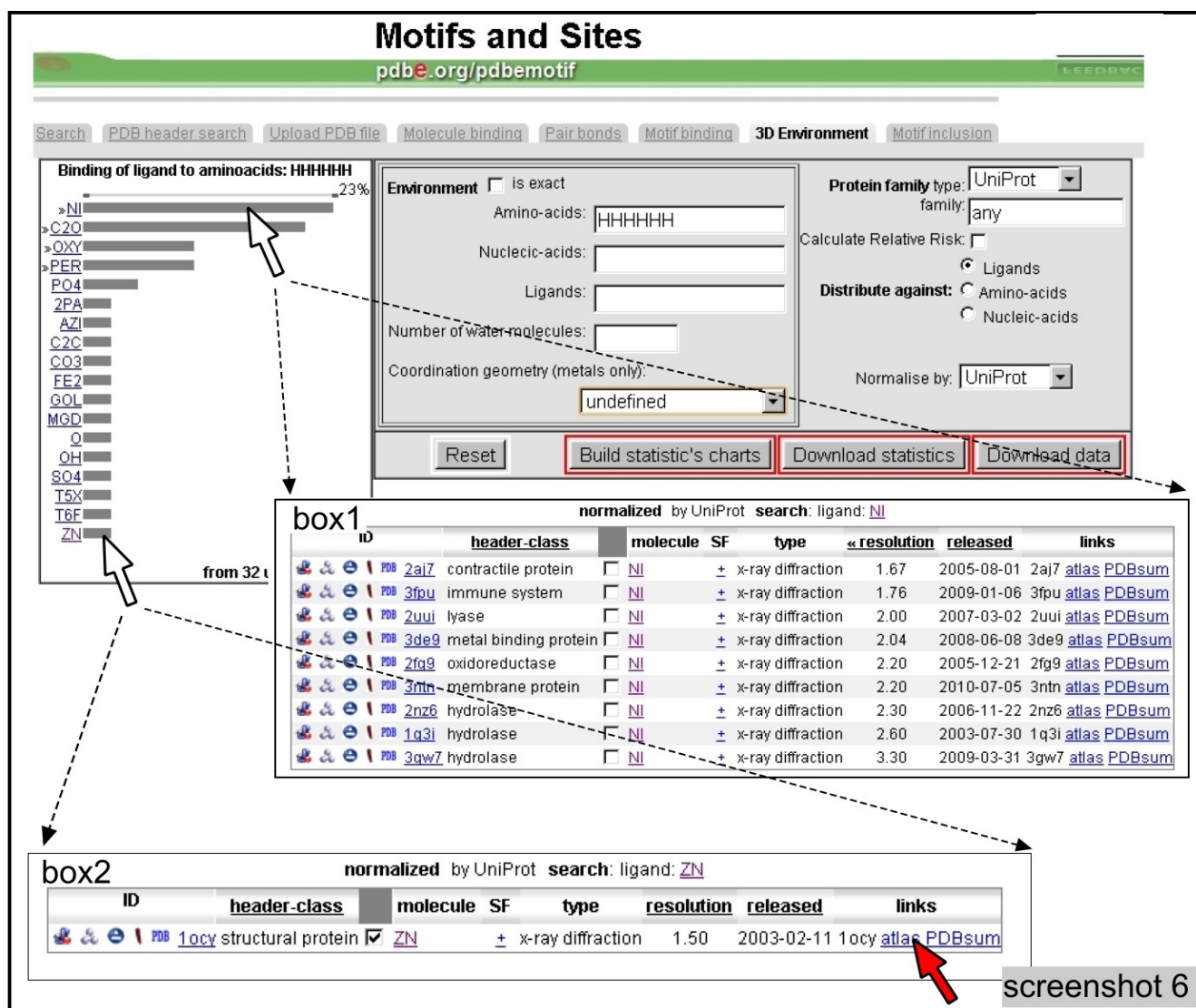
The PDBeMotif analysis of the environment of Fe²⁺ 2030A. The notionally covalent bonds to a pair of His residues from each protein chain are listed (boxed in green *) and the bond-lengths are indicated (boxed in blue *). An interactive graphics window shows the arrangement around the iron - you can rotate this with the mouse (arrowed).

A less restrictive view of the 2xgf sites

You can relax the definition of the length of bonds shown by PDBeMotif. Press the '**click here to show 5 Å bonds**' (circled in red, screenshot 5) to see all of the His residues around each of the seven iron ion.

The results are shown in the screenshot below.

code to see what they are, and click on each bar in the chart (arrowed) to see the list of entries. In fact there are only three metals listed: Ni, Fe, and Zn. The Ni and Fe were explored above, so now explore the Zn binding site by clicking on the 'atlas' link (red arrow) to visit its Summary page.



PDBeMotif summary for the HHHHHH environment

These statistics relate to all ligands that are bound by an environment containing six Histidines. Click on the bar in the chart to see the list for each ligand (arrows). Ni is bound in a number of entries (box 1) but Zn is bound only in a single entry (box 2). Click on that atlas link to see details of this (red arrow).

Zn bound by six His residues in the phage T4 short fibre protein

Zn bound by six His residues is observed in PDB entry **1ocy**. This is the short fibre of phage T4. As described in the accompanying **Quips** article this is a trimeric protein with a structural similarity to the extended Fe-binding domain of the long fibre **gp37** protein.

PDB

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1ocy Summary

pdb.org/1ocy

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PDB entry 1ocy

X-RAY

STRUCTURE OF THE RECEPTOR-BINDING DOMAIN OF THE BACTERIOPHAGE T4 SHORT TAIL FIBRE

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Similar structures

Quaternary

The structure was published by Thomassen, E., Gielen, G., Schuetz, M., et al., Abrahams, J.P., Miller, S., and Van Raaij, M.J., in 2003 in a paper entitled "The Structure of the Receptor-Binding Domain of the Bacteriophage T4 Short Tail Fibre Reveals a Knitted Trimeric Metal-Binding Fold" ([abstract](#)).

This crystal structure was determined using X-ray diffraction at a resolution of 1.5 Å and deposited in 2003.

The [experimental data](#) on which the structure is based was also deposited.

The PDB entry contains the structure of BACTERIOPHAGE T4 SHORT TAIL FIBRE. This molecule has the UniProt identifier [Q38160 \(Q38160_BPT2\)](#). The sample contained 198 residues which is < 90% of the natural sequence. Out of 198 residues 198 were observed and are deposited in the PDB.

It also contains one or more heterogenic compounds (e.g., ligands, co-factors, ions, modified amino acids, etc.), see [here](#) for a complete list.

The molecule most likely forms homotrimers.

The following tables show cross-reference information to other databases (to obtain a list of all PDB entries sharing the same property or classification, click on the magnifying glass icon):

Chain Name	UniProt	Name of source organism	% of UniProt sequence present in the sample	Residues in the sample molecules	% of residues observed
A	Q38160 (Q38160_BPT2)	Enterobacteria phage T4	< 90%	198	100%

1ocy

HomoTrimeric Assembly

- This assembly is defined by the author and software (PQS).
- This assembly consists of 3 molecules (1 type):
 - 3 copies of bacteriophage t4 short tail fibre

screenshot 7

The summary page for the structure with Zn bound to six Histidines
The entry 2ocy is the structure of the short fibre receptor binding region of bacteriophage T4.