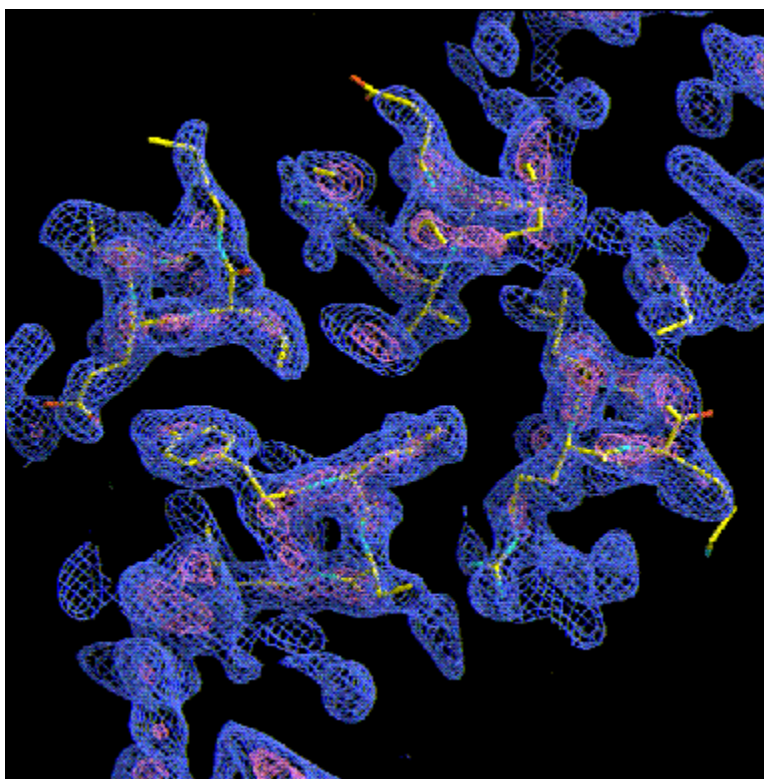


Tools of Crystallography



Christian Laing.
April 2002.

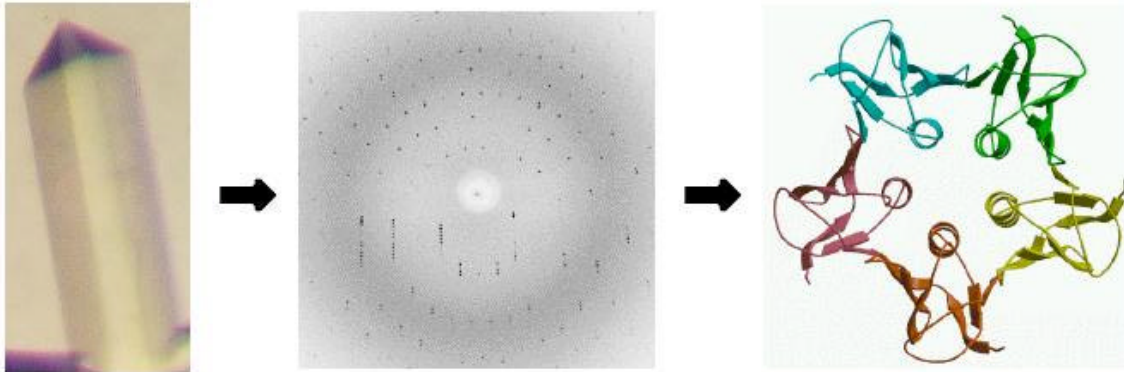
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Introduction

Most of the information that we have on protein structure comes from X-ray crystallography.

According to [R], X-ray crystallography is an experimental technique that exploits the fact that X-rays are diffracted by crystals (see figure below). It is not an imaging technique. X-rays have the proper wavelength (in the Ångström range, $\sim 10^{-8}$ cm) to be scattered by the electron cloud of an atom of comparable size. Based on the diffraction pattern obtained from X-ray scattering off the periodic assembly of molecules or atoms in the crystal, the electron density can be reconstructed. Additional phase information must be extracted either from the diffraction data or from supplementing diffraction experiments to complete the reconstruction (the phase problem in crystallography). A model is then progressively built into the experimental electron density, refined against the data and the result is a quite accurate molecular structure.



On the following work, I intent to show some of the mathematical and computer tools to crystallography as well as some applications.

On the first section we give an informal explanation about what we understand for crystal, such work was written based on [S] also we talk about the possible software that help to understand the groups, lattices and patterns.

On the second section we talk about the technique to obtain such crystals information, based on Bragg's Law, the X-ray diffraction is the main topic on this section.

For the third section we refer mostly to the Fourier analysis, we talk about some computational tools and we give references about the mathematical concepts that rule such a powerful technique.

On the section four we show the database of macromolecules obtained from crystallography called Protein Data Bank. Also we mention another databases.

On the fifth, another important section for bioinformatics we talk shortly about the software to model these macromolecules. We explain how to use these and give some examples.

Finally on the last section we give our conclusions, as well as the references.

1. Definition of a crystal and lattice

Crystals frequently have characteristic polyhedral shapes, bounded by flat faces, and much of the beauty of crystals is due to this face development. Many of the earliest contributions to crystals were based on observations of shapes, and the study of morphology is still important for recognizing and identifying specimens. However, faces can be ground away or destroyed, and they are not essential to a modern definition of a crystal. Furthermore, crystals are often too small to be seen without a high-powered microscope, and many substances consist of thousands of tiny crystals (polycrystalline). Metals are crystalline, but the individual crystals are often very small, and faces are not apparent. The following definition provides a more precise criterion for distinguishing crystalline matter.

A crystal consists of atoms arranged in a pattern that repeats periodically in three dimensions.

The pattern referred to in this definition can consist of a single atom, a group of atoms, a molecule, or a group of molecules. The important feature of a crystal is the periodicity or regularity of the arrangement of these patterns. The atoms in benzene, for example, are arranged in patterns with six carbons at the vertices of a regular hexagon and one oxygen atom attached to each carbon atom, but in liquid benzene there is no regularity in the arrangement of these patterns.

The fact that benzene is a liquid rather than a gas at room temperature is evidence of the existence of attractive forces between molecules. In the case of benzene these are relatively weak van der Waals' forces, and thermal agitation keeps the molecules from associating into ordered clusters. If benzene is cooled below its freezing point of 5.5°C , the kinetic energy of the molecules is no longer sufficient to overcome the intermolecular attractions. The molecules assume fixed orientations and positions with respect to each other, and solidification occurs.

As each molecule joins the growing solid particle, it is oriented so as to minimize the forces acting upon it. Each molecule entering the solid phase is influenced in almost exactly the same way as the preceding molecule, and the solid particle consists of a three-dimensional ordered array of molecules; that is, it is a crystal.

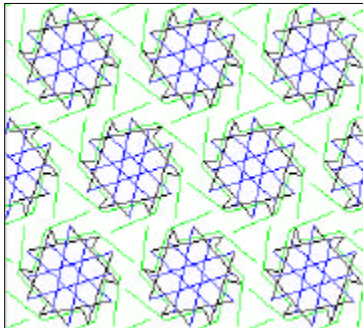
When a crystal is formed, we get a lattice. A lattice in the three dimensional space is the set of integer combination of the three base vectors. If the lattice is L , then we have three vectors a , b and c so that L is the set of all vectors $ha + kb + lc$ where h , k and l are integers.

The origin of a lattice can be put at any point in the crystal. If the origin is placed at a given atom in the structure, then every lattice point will be on exactly the same atom in the structure.

A crystal will not actually extend infinitely in all directions like a lattice does, but assuming that it does, then you can translate the crystal by vectors a , b or c and the crystal will remain unchanged.

In the pbd file for a crystal structure (see appendix), you can find the lengths of the vectors a , b and c and the angles between them.

1.1 Related Software



To construct your own patterns of lattices, here is [kali](http://www.scienceu.com/geometry/handson/kali/).

<http://www.scienceu.com/geometry/handson/kali/>

The figure on the left is one example of it.

Another similar program is [Escher](http://www-sphys.unil.ch/escher/):

<http://www-sphys.unil.ch/escher/>

Once we have a pattern we can use the [Reciprocal Lattice Calculator](http://www-sphys.unil.ch/x-ray/rlattice/):

<http://www-sphys.unil.ch/x-ray/rlattice/>

Which is a wonderful java program where you can find the lattices from patterns that they have, it is easy to use and gives a nice idea about the lattice.

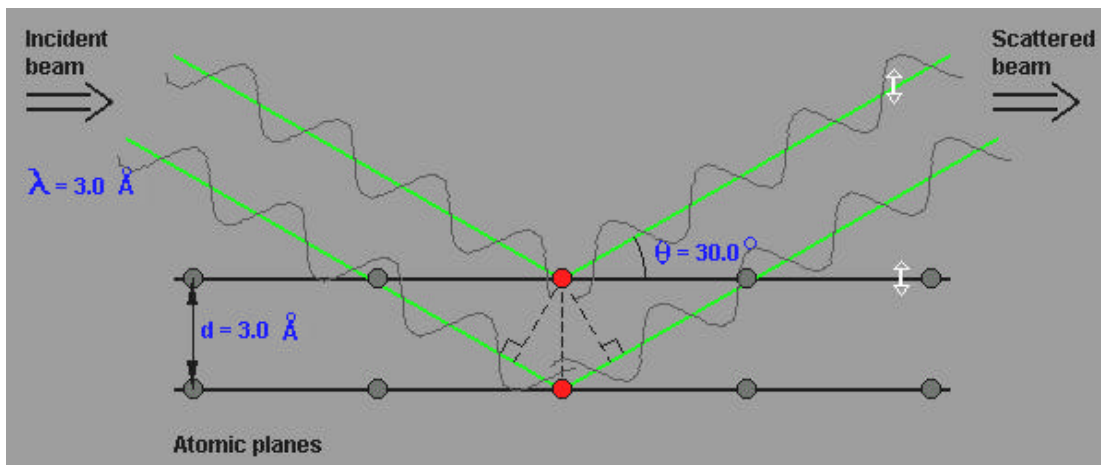
2. X-ray Crystallography

2.1 Bragg's Law

Bragg's Law refers to the simple equation:

$$n\lambda = 2d \sin\theta$$

Which derived by W.H. Bragg in 1913 to explain why the cleavage faces of crystals appear to reflect X-ray beams at certain angles of incidence (θ). The variable d is the distance between atomic layers in a crystal, and the variable λ is the wavelength of the incident X-ray beam (figure below); n is an integer.



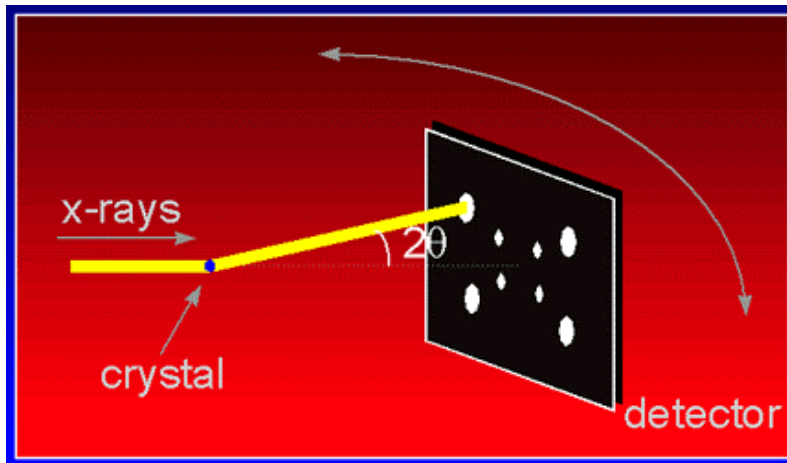
This observation is an example of X-ray wave interference, commonly known as X-ray diffraction (XRD), and was direct evidence for the periodic atomic structure of crystals postulated for several centuries. Although Bragg's law was used to explain the interference pattern of X-rays scattered by crystals, diffraction has been developed to study the structure of all states of matter with any beam, e.g., ions, electrons, neutrons, and protons, with a wavelength similar to the distance between the atomic or molecular structures of interest.

The image above was obtained from [L]. This website have an applet design to modified the values of lambda, the distance and the angle, and everything obeys to this Law. Also you can see the mathematical and the geometrical ideas behind of this Law.

2.2. X-ray diffraction

The following information was obtained from [R].

In a macromolecular X-ray diffraction experiment a small protein crystal is placed into an intense X-ray beam and the diffracted X-rays are collected with an area detector (it is advantageous to cool the crystals to low temperatures, primarily to prevent radiation damage). The diffraction pattern consists of reflections of different intensity, and a lot of patterns need to be collected to cover all necessary crystal orientations.



The diffracted X-rays are scattered by the crystal at a certain angle. The further backwards the x-rays scatter, the higher we say is the resolution if the data set the extent to which the crystal diffracts determines how fine a detail we can actually distinguish in our final model of the

structure. High resolution is thus desirable. Knowing the wavelength and the diffraction angle of a reflection, its resolution d can be easily calculated from Bragg's law.

The description of the required X-ray Diffraction Equipment is omitted from this work, but to learn about it, a good source is in [R].

3. Fourier Analysis and the Electron density function.

Fourier analysis arises because of the electron density function is periodic.

Section partially obtained by [Q].

Although the information about protein structure is given in the form of a file containing the coordinates of each atom, in reality what the crystallographer sees is the electron density. The atom is not located at one point in the space. The X-ray interacts with the cloud of electrons surrounding the nucleus.

To describe an electron cloud, at each point in the crystal a number is assigned which gives the density of electrons at that point. The electron density is a non-negative number giving the amount of charge per unit volume at that point.

Suppose that a structure is crystallized into a lattice consisting of all integer combinations of vectors a , b and c . Let $f(x,y,z)$ be the electron density at the point $xa + by + cz$. The function f is called the *electron density function*. Since the crystal is unchanged if it is translated by a , b or c , the electron density has period 1 in each variable,

$$f(x,y,z) = f(x+1,y,z) = f(x,y+1,z) = f(x,y,z+1)$$

The function f can be approximated by a three variable Fourier series.

On the Kevin Cowtan's Book of Fourier, webpage whose reference is shown as [C], we can appreciate the role that the Fourier transform plays on crystallography, mainly on the transformations from atoms, lattices, molecules and more.

4. Databases

In this section we will show some of the great amount of databases all over the Internet. We discuss only one of the most important databases and show the links for other data sites.

- [Protein Data Bank](#)

This is perhaps one of the most important data bases related to macromolecules. From this website you can get a file with extension "pdb" which contain information of the geometry of the macromolecule, such as the number of atoms, the angles between them, the coordinates of such atoms and much more.

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[BETA TEST new features](#)

Current Holdings

17869 Structures
 Last Update: 16-Apr-2002
[PDB Statistics](#)



Molecule of the Month:
[Anthrax Toxin](#)

The Protein Data Bank (PDB) is operated by Rutgers, The State University of New Jersey; the San Diego Supercomputer Center at the University of California, San Diego; and the National Institute of Standards and Technology -- three members of the Research

PROTEIN DATA BANK

Welcome to the PDB, the single worldwide repository for the processing and distribution of 3-D biological macromolecular structure data.

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To work on this database just find the name of your favorite molecule, and by following a very simple instruction; you can download the file as a text or html file. On the index there is an example of the Myoglobin 1HEW. Also on this website you can see some crystallographic information about how this molecule was obtain, information about temperatures and techniques. Another very nice thing about the pbd files is that from this files you are able to plot the macromolecule, this will be discussed on the next section.

Another Database sites:

- [Cambridge Crystallographic Data Centre](#)

<http://www.ccdc.cam.ac.uk/>

- [World Database of Crystallographers](#)

<http://www.iucr.ac.uk/iucr-top/wdc/index.html>

- [BMCD - The Biological Macromolecule Crystallization Database and the Nasa Archive for Protein Crystal Growth](#)

<http://ibm4.carb.nist.gov:4400/bmcd/bmcd.html>

- [Proteins Motions Database](#)

<http://molmovdb.mbb.yale.edu/MolMovDB/>

- [MOOSE Macromolecular Structure Database at San Diego Super Computer Center](http://db2.sdsc.edu/moose/)

<http://db2.sdsc.edu/moose/>

5. Graphic software

Rasmol

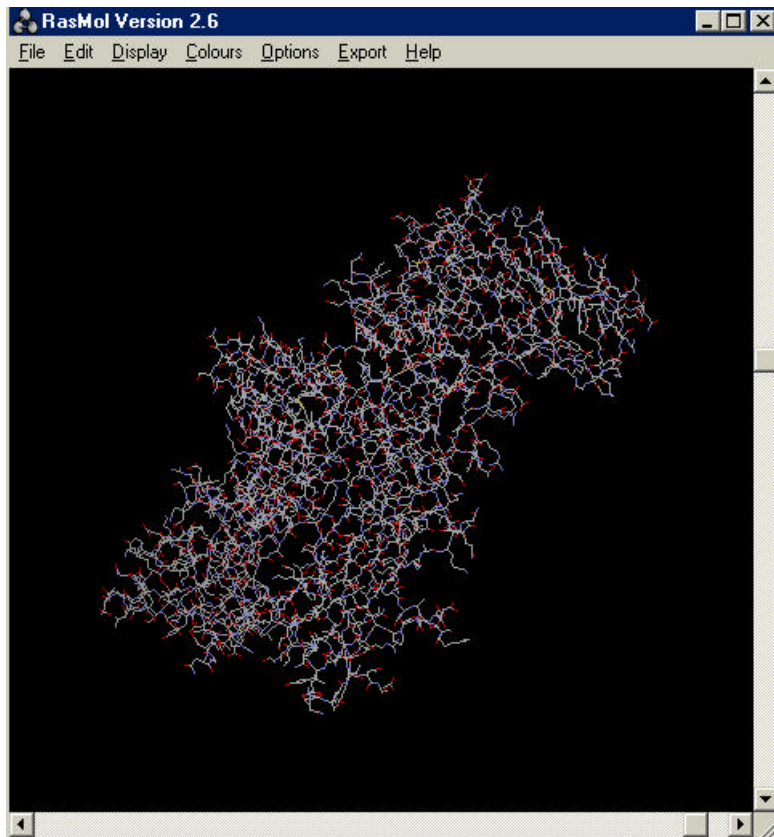
Rasmol is perhaps one of the most popular software for macromolecules.

By like the authors said is an easy-to-use and powerful software for looking at macromolecular structure and its relation to function. And its free!!!!. To download it just go to this web page:
<http://www.umass.edu/microbio/rasmol/>.

As an example, lets take the file 1ACC.pdb which is related to the anthrax toxin and that you can get from the Protein Data Bank from this website:

<http://www.rcsb.org/pdb/cgi/explore.cgi?job=download;pdbId=1ACC;page=;pid=54731017360146&opt=show&format=PDB&pre=1>

Now open Rasmol program, and from file/open choose your 1ACC.pdb file. The program will show the following structure:



Notice that you can inspect this structure by rotate this with your mouse. The file that we are reading is, like we said previously, a pdb file that contains the coordinates of every one of the atoms of this really big molecule (see the fragment of a pdb on the Appendix.)

What can we do with RasMol? You can have different views of this molecule, just go to “display” and try any of the options (like wireframe, backbone, sticks, etc...). Another nice tool is labeling, just go on options/label, such option label the atoms that you have there, and of course this is a useful tool when your molecule is small. There is also an option to color regions according to some properties, for example click on color/temperature and there you can see the changes in the macromolecule.

To learn more about this software, here is a nice tutorial:

<http://www.umass.edu/microbio/rasmol/index2.htm>

Another useful software:

- [GRASP \(Graphical Representation and Analysis of Structural Properties\)](http://trantor.bioc.columbia.edu/grasp/)
<http://trantor.bioc.columbia.edu/grasp/>
- VRML (Virtual Reality Modeling Language)
<http://www.cristal.org/vrml/intvrml.html>
- [Ribbons](http://www.cmc.uab.edu/ribbons/)
<http://www.cmc.uab.edu/ribbons/>
- [Shake-and-Bake Program SnB](http://www.hwi.buffalo.edu/SnB/)
<http://www.hwi.buffalo.edu/SnB/>

6. Conclusions

The knowledge of accurate molecular structures is a prerequisite for rational drug design and for structure based functional studies to aid the development of effective therapeutic agents and drugs. Crystallography can reliably provide the answer to many structure related questions, from global folds to atomic details of bonding. In contrast to NMR, which is an indirect spectroscopic method, no size limitation exists for the molecule or complex to be studied. The price for the high accuracy of crystallographic structures is that a good crystal must be found, and that only limited information about the molecule's dynamic behavior is available from one single diffraction experiment.

Because of the exponential increased of information in crystallography, we urged to use more and more updated databases, computer software, books and any other tool as much as possible. The future of computer graphics goes without any doubt to the Virtual Reality models and fast databases.

7. Appendix

A fragment of the pbd file of Myoglobin 1HEW

```
HEADER  HYDROLASE(O-GLYCOSYL)          20-JAN-92  1HEW  1HEW  2
COMPND  LYSOZYME (E.C.3.2.1.17) COMPLEXED WITH THE INHIBITOR  1HEW  3
COMPND  2 TRI-N-ACETYLCHITOTRIOSE          1HEW  4
SOURCE  HEN (GALLUS GALLUS) EGG WHITE      1HEW  5
AUTHOR  J.C.CHEETHAM,P.J.ARTYMIUK,D.C.PHILLIPS  1HEW  6
REVDAT  1 31-JAN-94 1HEW  0                1HEW  7
JRNL    AUTH  J.C.CHEETHAM,P.J.ARTYMIUK,D.C.PHILLIPS  1HEW  8
JRNL    TITL  REFINEMENT OF AN ENZYME COMPLEX WITH INHIBITOR  1HEW  9
JRNL    TITL  2 BOUND AT PARTIAL OCCUPANCY. HEN EGG-WHITE  1HEW 10
JRNL    TITL  3 LYSOZYME AND TRI-N-ACETYLCHITOTRIOSE AT 1.75  1HEW 11
JRNL    TITL  4 ANGSTROMS RESOLUTION          1HEW 12
JRNL    REF  J.MOL.BIOL. V. 224 613 1992  1HEW 13
JRNL    REF  ASTM JMOBAM UK ISSN 0022-2836  070 1HEW 14
REMARK  1 REFERENCE 1                1HEW 15
REMARK  1 REFERENCE 1                1HEW 16
REMARK  1 AUTH  L.N.JOHNSON,J.C.CHEETHAM,P.J.MC*LAUGHLIN,  1HEW 17
REMARK  1 AUTH  2 K.R.ACHARYA,D.BARFORD,D.C.PHILLIPS  1HEW 18
REMARK  1 TITL  PROTEIN-OLIGOSACCHARIDE INTERACTIONS: LYSOZYME,  1HEW 19
REMARK  1 TITL  2 PHOSPHORYLASE, AMYLASES  1HEW 20
REMARK  1 REF  CURR.TOP.MICROBIOL.IMMUNOL. V. 139 81 1988  1HEW 21
REMARK  1 REF  ASTM CTMIA3 GW ISSN 0070-217X  761 1HEW 22
REMARK  1 REFERENCE 2                1HEW 23
REMARK  1 AUTH  C.C.F.BLAKE,L.N.JOHNSON,G.A.MAIR,A.C.T.NORTH,  1HEW 24
REMARK  1 AUTH  2 D.C.PHILLIPS,V.R.SARMA  1HEW 25
REMARK  1 TITL  CRYSTALLOGRAPHIC STUDIES OF THE ACTIVITY OF HEN  1HEW 26
REMARK  1 TITL  2 EGG-WHITE LYSOZYME  1HEW 27
REMARK  1 REF  PROC.R.SOC.LONDON,SER.B V. 167 378 1967  1HEW 28
REMARK  1 REF  ASTM PRLBA4 UK ISSN 0080-4649  338 1HEW 29
REMARK  1 REFERENCE 3                1HEW 30
REMARK  1 AUTH  C.C.F.BLAKE,G.A.MAIR,A.C.T.NORTH,D.C.PHILLIPS,  1HEW 31
REMARK  1 AUTH  2 V.R.SARMA  1HEW 32
REMARK  1 TITL  ON THE CONFORMATION OF THE HEN EGG-WHITE LYSOZYME  1HEW 33
REMARK  1 TITL  2 MOLECULE  1HEW 34
REMARK  1 REF  PROC.R.SOC.LONDON,SER.B V. 167 365 1967  1HEW 35
REMARK  1 REF  ASTM PRLBA4 UK ISSN 0080-4649  338 1HEW 36
REMARK  2 RESOLUTION. 1.75 ANGSTROMS.  1HEW 37
REMARK  2 RESOLUTION. 1.75 ANGSTROMS.  1HEW 38
REMARK  3 REFERENCE 3                1HEW 39
REMARK  3 REFINEMENT.  1HEW 40
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REMARK  3 AUTHORS  KONNERT,HENDRICKSON  1HEW 42
REMARK  3 R VALUE  0.229  1HEW 43
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REMARK  3  1HEW 46
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REMARK  3  1HEW 48
REMARK  3 NUMBER OF PROTEIN ATOMS  1001  1HEW 49
REMARK  3 NUMBER OF SOLVENT ATOMS  103  1HEW 50
REMARK  4  1HEW 51
REMARK  4 PROTEIN DATA BANK ADVISORY NOTICE:  1HEW 52
REMARK  4 THERE ARE A FEW WATER MOLECULES ASSOCIATED WITH SYMMETRY  1HEW 53
REMARK  4 RELATED PROTEIN MOLECULES.  1HEW 54
REMARK  5  1HEW 55
REMARK  5 THE THREE SUGAR UNITS OF THE INHIBITOR MOLECULE ARE BOUND  1HEW 56
REMARK  5 IN THE UPPER THREE SITES (A TO C) OF THE LYSOZYME ACTIVE  1HEW 57
REMARK  5 SITE CLEFT. NAG MOLECULES, NUMBERED 203, 202, AND 201, ARE  1HEW 58
REMARK  5 BOUND IN SITES A, B, AND C, RESPECTIVELY.  1HEW 59
SEQRES  1 129 LYS VAL PHE GLY ARG CYS GLU LEU ALA ALA MET LYS  1HEW 60
SEQRES  2 129 ARG HIS GLY LEU ASP ASN TYR ARG GLY TYR SER LEU GLY  1HEW 61
SEQRES  3 129 ASN TRP VAL CYS ALA ALA LYS PHE GLU SER ASN PHE ASN  1HEW 62
SEQRES  4 129 THR GLN ALA THR ASN ARG ASN THR ASP GLY SER THR ASP  1HEW 63
SEQRES  5 129 TYR GLY ILE LEU GLN ILE ASN SER ARG TRP TRP CYS ASN  1HEW 64
SEQRES  6 129 ASP GLY ARG THR PRO GLY SER ARG ASN LEU CYS ASN ILE  1HEW 65
SEQRES  7 129 PRO CYS SER ALA LEU LEU SER SER ASP ILE THR ALA SER  1HEW 66
SEQRES  8 129 VAL ASN CYS ALA LYS LYS ILE VAL SER ASP GLY ASN GLY  1HEW 67
SEQRES  9 129 MET ASN ALA TRP VAL ALA TRP ARG ASN ARG CYS LYS GLY  1HEW 68
SEQRES 10 129 THR ASP VAL GLN ALA TRP ILE ARG GLY CYS ARG LEU  1HEW 69
HET NAG  201  15  N-ACETYL-D-GLUCOSAMINE  1HEW 70
HET NAG  202  14  N-ACETYL-D-GLUCOSAMINE  1HEW 71
HET NAG  203  14  N-ACETYL-D-GLUCOSAMINE  1HEW 72
FORMUL  2 NAG  3(C8 H15 N1 O6)  1HEW 73
FORMUL  3 HOH  *103(H2 O1)  1HEW 74
HELIX  1 A ARG  5 HIS  15 1  1HEW 75
HELIX  2 B LEU  25 GLU  35 1  1HEW 76
HELIX  3 C CYS  80 LEU  84 5  1HEW 77
HELIX  4 D THR  89 ILE  98 1  1HEW 78
HELIX  5 E VAL 109 ASN 113 1  1HEW 79
SHEET  1 S12 LYS  1 PHE  3 0  1HEW 80
SHEET  2 S12 PHE  38 THR  40 -1 N THR  40 O LYS  1 1HEW 81
SHEET  1 S23 ALA  42 ASN  46 0  1HEW 82
SHEET  2 S23 SER  50 GLY  54 -1 O SER  50 N ASN  46 1HEW 83
```

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TURN	3	T3	LEU	17	TYR	20		TYPE II					1HEW	87
TURN	4	T4	ASN	19	GLY	22		DISTORTED TYPE II					1HEW	88
TURN	5	T5	TYR	20	TYR	23		TYPE I'					1HEW	89
TURN	6	T6	SER	24	ASN	27		TYPE III					1HEW	90
TURN	7	T7	LEU	25	TRP	28		TYPE III					1HEW	91
TURN	8	T8	SER	36	ASN	39		TYPE III'					1HEW	92
TURN	9	T9	ASN	46	GLY	49		TYPE I					1HEW	93
TURN	10	T10	GLY	54	GLN	57		TYPE I					1HEW	94
TURN	11	T11	THR	69	SER	72		TYPE I					1HEW	95
TURN	12	T12	ASN	74	ASN	77		TYPE I					1HEW	96
TURN	13	T13	PRO	79	ALA	82		TYPE III					1HEW	97
TURN	14	T14	CYS	80	LEU	83		TYPE III					1HEW	98
TURN	15	T15	SER	81	LEU	84		TYPE I					1HEW	99
TURN	16	T16	CYS	94	LYS	97		TYPE III					1HEW	100
TURN	17	T17	ILE	98	ASP	101		TYPE I					1HEW	101
TURN	18	T18	ASN	103	ASN	106		TYPE II'					1HEW	102
TURN	19	T19	MET	105	TRP	108		TYPE III					1HEW	103
TURN	20	T20	TRP	108	TRP	111		TYPE III					1HEW	104
TURN	21	T21	CYS	115	THR	118		TYPE II					1HEW	105
TURN	22	T22	ASP	119	ALA	122		TYPE III					1HEW	106
TURN	23	T23	VAL	120	TRP	123		TYPE III					1HEW	107
TURN	24	T24	GLN	121	ILE	124		TYPE III					1HEW	108
SSBOND	1	CYS	6	CYS	127								1HEW	109
SSBOND	2	CYS	30	CYS	115								1HEW	110
SSBOND	3	CYS	64	CYS	80								1HEW	111
SSBOND	4	CYS	76	CYS	94								1HEW	112
CRYST1	78.860	78.860	38.250	90.00	90.00	90.00	P	43	21	2	8	1HEW	113	
ORIGX1	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000							1HEW	114
ORIGX2	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000							1HEW	115
ORIGX3	0.000000	0.000000	1.000000	0.000000	0.000000	0.000000							1HEW	116
SCALE1	0.012681	0.000000	0.000000	0.000000	0.000000	0.000000							1HEW	117
SCALE2	0.000000	0.012681	0.000000	0.000000	0.000000	0.000000							1HEW	118
SCALE3	0.000000	0.000000	0.026144	0.000000	0.000000	0.000000							1HEW	119
ATOM	1	N	LYS	1		3.398	9.981	10.408	1.00	30.48			1HEW	120
ATOM	2	CA	LYS	1		2.459	10.365	9.364	1.00	28.03			1HEW	121
ATOM	3	C	LYS	1		2.458	11.880	9.149	1.00	21.93			1HEW	122
ATOM	4	O	LYS	1		2.481	12.672	10.100	1.00	14.10			1HEW	123
ATOM	5	CB	LYS	1		1.026	9.935	9.695	1.00	30.54			1HEW	124
ATOM	6	CG	LYS	1		0.028	10.169	8.558	1.00	37.93			1HEW	125
ATOM	7	CD	LYS	1		-1.415	10.089	9.048	1.00	33.23			1HEW	126
ATOM	8	CE	LYS	1		-2.357	10.822	8.082	1.00	32.17			1HEW	127
ATOM	9	NZ	LYS	1		-3.661	10.090	8.025	1.00	31.92			1HEW	128
ATOM	10	N	VAL	2		2.429	12.232	7.880	1.00	17.30			1HEW	129
ATOM	11	CA	VAL	2		2.395	13.653	7.465	1.00	14.47			1HEW	130
ATOM	12	C	VAL	2		0.977	13.868	6.903	1.00	17.58			1HEW	131
ATOM	13	O	VAL	2		0.642	13.368	5.826	1.00	32.65			1HEW	132
ATOM	14	CB	VAL	2		3.533	14.012	6.536	1.00	22.88			1HEW	133
ATOM	15	CG1	VAL	2		3.463	15.446	6.029	1.00	17.60			1HEW	134
ATOM	16	CG2	VAL	2		4.896	13.752	7.185	1.00	25.10			1HEW	135
ATOM	17	N	PHE	3		0.202	14.602	7.679	1.00	24.88			1HEW	136
ATOM	18	CA	PHE	3		-1.182	14.930	7.362	1.00	25.54			1HEW	137
ATOM	19	C	PHE	3		-1.323	16.027	6.307	1.00	44.91			1HEW	138
ATOM	20	O	PHE	3		-0.451	16.906	6.207	1.00	27.79			1HEW	139
ATOM	21	CB	PHE	3		-1.912	15.431	8.640	1.00	24.13			1HEW	140
ATOM	22	CG	PHE	3		-2.504	14.407	9.541	1.00	18.68			1HEW	141
ATOM	23	CD1	PHE	3		-1.727	13.761	10.505	1.00	18.71			1HEW	142
ATOM	24	CD2	PHE	3		-3.860	14.088	9.439	1.00	19.15			1HEW	143
ATOM	25	CE1	PHE	3		-2.303	12.797	11.353	1.00	26.64			1HEW	144
ATOM	26	CE2	PHE	3		-4.441	13.143	10.262	1.00	22.36			1HEW	145
ATOM	27	CZ	PHE	3		-3.659	12.495	11.226	1.00	17.81			1HEW	146
ATOM	28	N	GLY	4		-2.430	15.953	5.586	1.00	17.72			1HEW	147
ATOM	29	CA	GLY	4		-2.751	16.990	4.552	1.00	31.68			1HEW	148
ATOM	30	C	GLY	4		-3.547	18.053	5.370	1.00	17.02			1HEW	149
ATOM	31	O	GLY	4		-4.114	17.681	6.421	1.00	17.27			1HEW	150
ATOM	32	N	ARG	5		-3.566	19.276	4.911	1.00	23.79			1HEW	151
ATOM	33	CA	ARG	5		-4.263	20.383	5.589	1.00	19.38			1HEW	152
ATOM	34	C	ARG	5		-5.696	20.017	5.939	1.00	29.92			1HEW	153
ATOM	35	O	ARG	5		-6.048	19.981	7.141	1.00	28.65			1HEW	154
ATOM	36	CB	ARG	5		-4.202	21.690	4.772	1.00	15.01			1HEW	155
ATOM	37	CG	ARG	5		-4.673	22.912	5.555	1.00	7.22			1HEW	156
ATOM	38	CD	ARG	5		-4.468	24.256	4.862	1.00	32.04			1HEW	157
ATOM	39	NE	ARG	5		-4.855	24.191	3.491	1.00	39.10			1HEW	158
ATOM	40	CZ	ARG	5		-6.080	24.419	3.022	1.00	21.11			1HEW	159
ATOM	41	NH1	ARG	5		-7.143	24.794	3.846	1.00	36.18			1HEW	160
ATOM	42	NH2	ARG	5		-6.355	24.278	1.759	1.00	47.30			1HEW	161
ATOM	43	N	CYS	6		-6.494	19.744	4.929	1.00	31.37			1HEW	162
ATOM	44	CA	CYS	6		-7.927	19.378	5.088	1.00	32.81			1HEW	163
ATOM	45	C	CYS	6		-8.096	18.138	5.922	1.00	19.65			1HEW	164
ATOM	46	O	CYS	6		-8.951	18.087	6.840	1.00	24.72			1HEW	165
ATOM	47	CB	CYS	6		-8.579	19.336	3.697	1.00	25.91			1HEW	166
ATOM	48	SG	CYS	6		-8.763	21.096	3.142	1.00	29.62			1HEW	167
ATOM	49	N	GLU	7		-7.275	17.144	5.630	1.00	19.41			1HEW	168
ATOM	50	CA	GLU	7		-7.285	15.889	6.363	1.00	27.46			1HEW	169
ATOM	51	C	GLU	7		-7.215	16.114	7.871	1.00	28.60			1HEW	170
ATOM	52	O	GLU	7		-8.012	15.554	8.648	1.00	20.67			1HEW	171
ATOM	53	CB	GLU	7		-6.066	15.041	5.997	1.00	16.86			1HEW	172
ATOM	54	CG	GLU	7		-6.092	13.584	6.483	1.00	32.99			1HEW	173
ATOM	55	CD	GLU	7		-4.912	12.777	5.999	1.00	31.30			1HEW	174
ATOM	56	OE1	GLU	7		-3.945	13.298	5.403	1.00	36.16			1HEW	175
ATOM	57	OE2	GLU	7		-5.039	11.570	6.267	1.00	35.15			1HEW	176

ATOM	58	N	LEU	8	-6.242	16.934	8.265	1.00	20.93	1HEW177
ATOM	59	CA	LEU	8	-6.013	17.248	9.682	1.00	18.37	1HEW178
ATOM	60	C	LEU	8	-7.184	17.999	10.289	1.00	12.20	1HEW179
ATOM	61	O	LEU	8	-7.616	17.691	11.414	1.00	20.78	1HEW180
ATOM	62	CB	LEU	8	-4.660	17.985	9.810	1.00	18.37	1HEW181
ATOM	63	CG	LEU	8	-4.268	18.305	11.264	1.00	20.77	1HEW182
ATOM	64	CD1	LEU	8	-3.830	17.042	12.004	1.00	18.41	1HEW183
ATOM	65	CD2	LEU	8	-3.155	19.339	11.230	1.00	20.24	1HEW184
ATOM	66	N	ALA	9	-7.660	18.968	9.529	1.00	17.56	1HEW185
ATOM	67	CA	ALA	9	-8.796	19.804	9.923	1.00	18.32	1HEW186
ATOM	68	C	ALA	9	-9.964	18.897	10.316	1.00	13.30	1HEW187
ATOM	69	O	ALA	9	-10.573	19.060	11.379	1.00	23.27	1HEW188
ATOM	70	CB	ALA	9	-9.180	20.746	8.795	1.00	13.96	1HEW189
ATOM	71	N	ALA	10	-10.228	17.946	9.435	1.00	16.02	1HEW190
ATOM	72	CA	ALA	10	-11.317	16.976	9.620	1.00	26.28	1HEW191
ATOM	73	C	ALA	10	-11.109	16.094	10.836	1.00	18.11	1HEW192
ATOM	74	O	ALA	10	-12.067	15.806	11.580	1.00	19.85	1HEW193
ATOM	75	CB	ALA	10	-11.470	16.138	8.347	1.00	36.67	1HEW194
ATOM	76	N	ALA	11	-9.863	15.675	11.030	1.00	18.46	1HEW195
ATOM	77	CA	ALA	11	-9.506	14.804	12.157	1.00	18.53	1HEW196
ATOM	78	C	ALA	11	-9.631	15.520	13.489	1.00	30.31	1HEW197
ATOM	79	O	ALA	11	-10.005	14.871	14.489	1.00	27.18	1HEW198
ATOM	80	CB	ALA	11	-8.095	14.238	11.970	1.00	27.90	1HEW199
ATOM	81	N	MET	12	-9.311	16.812	13.470	1.00	31.55	1HEW200
ATOM	985	O	ARG	128	-14.970	18.015	5.178	1.00	42.56	1HEW1104
ATOM	986	CB	ARG	128	-15.082	18.354	2.368	1.00	31.05	1HEW1105
ATOM	987	CG	ARG	128	-15.481	18.611	0.934	1.00	35.45	1HEW1106
ATOM	988	CD	ARG	128	-16.984	18.628	0.788	1.00	54.63	1HEW1107
ATOM	989	NE	ARG	128	-17.467	17.307	0.324	1.00	55.58	1HEW1108
ATOM	990	CZ	ARG	128	-18.032	16.412	1.146	1.00	83.67	1HEW1109
ATOM	991	NH1	ARG	128	-17.728	16.390	2.450	1.00	85.64	1HEW1110
ATOM	992	NH2	ARG	128	-18.918	15.515	0.676	1.00	62.69	1HEW1111
ATOM	993	N	LEU	129	-15.873	20.060	5.495	1.00	26.02	1HEW1112
ATOM	994	CA	LEU	129	-16.186	19.851	6.911	1.00	30.59	1HEW1113
ATOM	995	C	LEU	129	-17.661	20.003	7.247	1.00	43.61	1HEW1114
ATOM	996	O	LEU	129	-18.388	20.459	6.336	1.00	39.83	1HEW1115
ATOM	997	CB	LEU	129	-15.324	20.866	7.700	1.00	15.32	1HEW1116
ATOM	998	CG	LEU	129	-13.824	20.675	7.712	1.00	22.28	1HEW1117
ATOM	999	CD1	LEU	129	-13.088	22.029	7.721	1.00	41.00	1HEW1118
ATOM	1000	CD2	LEU	129	-13.441	19.891	8.982	1.00	29.73	1HEW1119
ATOM	1001	OXT	LEU	129	-17.993	19.662	8.407	1.00	31.81	1HEW1120
TER	1002	LEU	129							1HEW1121
HETATM	1003	C1	NAG	201	5.991	25.237	25.980	1.00	32.10	1HEW1122
HETATM	1004	C2	NAG	201	4.850	24.302	26.455	1.00	29.05	1HEW1123
HETATM	1005	C3	NAG	201	4.046	24.991	27.538	1.00	14.31	1HEW1124
HETATM	1006	C4	NAG	201	5.038	25.548	28.618	1.00	41.63	1HEW1125
HETATM	1007	C5	NAG	201	6.314	26.233	28.108	1.00	38.82	1HEW1126
HETATM	1008	C6	NAG	201	7.340	26.466	29.190	1.00	50.43	1HEW1127
HETATM	1009	C7	NAG	201	3.635	22.668	25.008	1.00	19.61	1HEW1128
HETATM	1010	C8	NAG	201	2.737	22.563	23.828	1.00	14.43	1HEW1129
HETATM	1011	N2	NAG	201	4.007	23.939	25.299	1.00	30.31	1HEW1130
HETATM	1012	O1	NAG	201	6.692	24.491	24.991	1.00	46.64	1HEW1131
HETATM	1013	O3	NAG	201	3.150	24.098	28.216	1.00	28.14	1HEW1132
HETATM	1014	O4	NAG	201	4.196	26.571	29.463	1.00	46.30	1HEW1133
HETATM	1015	O5	NAG	201	6.936	25.335	27.116	1.00	32.95	1HEW1134
HETATM	1016	O6	NAG	201	7.944	25.194	29.718	1.00	38.95	1HEW1135
HETATM	1017	O7	NAG	201	3.999	21.786	25.641	1.00	24.37	1HEW1136
HETATM	1018	C1	NAG	202	3.885	26.427	30.899	1.00	24.54	1HEW1137
HETATM	1019	C2	NAG	202	3.803	27.923	31.574	1.00	38.18	1HEW1138
HETATM	1020	C3	NAG	202	3.501	27.760	33.097	1.00	40.28	1HEW1139
HETATM	1021	C4	NAG	202	2.221	26.848	33.126	1.00	31.56	1HEW1140
HETATM	1022	C5	NAG	202	2.479	25.410	32.459	1.00	25.00	1HEW1141
HETATM	1023	C6	NAG	202	1.289	24.518	32.681	1.00	41.21	1HEW1142
HETATM	1024	C7	NAG	202	5.120	29.996	31.136	1.00	36.27	1HEW1143
HETATM	1025	C8	NAG	202	6.500	30.566	31.143	1.00	25.48	1HEW1144
HETATM	1026	N2	NAG	202	5.055	28.671	31.420	1.00	47.13	1HEW1145
HETATM	1027	O3	NAG	202	3.281	29.063	33.664	1.00	44.52	1HEW1146
HETATM	1028	O4	NAG	202	1.717	26.573	34.467	1.00	37.56	1HEW1147
HETATM	1029	O5	NAG	202	2.607	25.693	31.010	1.00	56.77	1HEW1148
HETATM	1030	O6	NAG	202	0.147	25.114	31.890	1.00	29.51	1HEW1149
HETATM	1031	O7	NAG	202	4.177	30.616	30.914	1.00	77.29	1HEW1150
HETATM	1032	C1	NAG	203	0.550	26.901	35.270	1.00	31.25	1HEW1151
HETATM	1033	C2	NAG	203	0.590	26.520	36.747	1.00	50.86	1HEW1152
HETATM	1034	C3	NAG	203	-0.756	26.737	37.362	1.00	27.28	1HEW1153
HETATM	1035	C4	NAG	203	-1.366	28.109	36.946	1.00	62.31	1HEW1154
HETATM	1036	C5	NAG	203	-1.210	28.461	35.452	1.00	37.66	1HEW1155
HETATM	1037	C6	NAG	203	-1.512	29.931	35.193	1.00	49.19	1HEW1156
HETATM	1038	C7	NAG	203	2.074	24.558	37.356	1.00	64.76	1HEW1157
HETATM	1039	C8	NAG	203	2.050	23.092	37.620	1.00	56.03	1HEW1158
HETATM	1040	N2	NAG	203	0.971	25.033	36.747	1.00	55.71	1HEW1159
HETATM	1041	O3	NAG	203	-0.603	26.737	38.795	1.00	49.98	1HEW1160
HETATM	1042	O4	NAG	203	-2.807	28.096	37.222	1.00	75.30	1HEW1161
HETATM	1043	O5	NAG	203	0.146	28.266	35.043	1.00	55.96	1HEW1162
HETATM	1044	O6	NAG	203	-0.695	30.486	34.118	1.00	68.92	1HEW1163
HETATM	1045	O7	NAG	203	2.947	25.248	37.653	1.00	66.12	1HEW1164
HETATM	1046	O	HOH	1	-16.295	29.471	0.511	1.00	18.64	1HEW1165
HETATM	1047	O	HOH	2	-1.660	14.995	1.659	1.00	45.86	1HEW1166
HETATM	1048	O	HOH	3	-2.284	23.422	1.995	1.00	35.24	1HEW1167
HETATM	1049	O	HOH	4	12.023	0.759	1.575	1.00	40.57	1HEW1168
HETATM	1050	O	HOH	5	-5.649	19.629	2.249	1.00	22.05	1HEW1169
HETATM	1051	O	HOH	6	10.088	9.701	1.835	1.00	38.86	1HEW1170
HETATM	1052	O	HOH	7	-11.738	18.468	1.989	1.00	28.37	1HEW1171
HETATM	1053	O	HOH	8	-5.783	17.025	2.791	1.00	15.46	1HEW1

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