

Nominal mass and amino acid changes genetically governed by single base changes in the nucleotide codon

This table shows the amino acid residue changes and the corresponding nominal molecular weight (mass) changes (Da) that are genetically determined by single mutations in the nucleotide codon (coding triplet).

In the context of the human hemoglobin α - and β -chains that contain no isoleucine, there are 141 ways of producing a single amino acid mutation. Of these, 127 (90%) produce a mass change of more than 6 Da and hence can be resolved in normal-variant heterozygotes by analyzing the intact α - and β -chains from human blood samples by electrospray ionization mass spectrometry and deconvoluting the data by MaxEnt™, the maximum entropy based software described in Technical Note 202 and Application Note 212.

Mass change	Amino acid change	Mass change	Amino acid change	Mass change	Amino acid change	Mass change	Amino acid change
0	Gln ↔ Lys Ile ↔ Leu	16	Ala ↔ Ser Phe ↔ Tyr Pro ↔ Leu Ser ↔ Cys Val ↔ Asp	30	Ala ↔ Thr Arg ↔ Trp Gly ↔ Ser Thr ↔ Met Val ↔ Glu	53	Cys ↔ Arg
1	Asn ↔ Asp Gln ↔ Glu Ile ↔ Asn Lys ↔ Glu	18	Ile ↔ Met Leu ↔ Met	31	Pro ↔ Gln	55	Thr ↔ Arg
3	Lys ↔ Met	19	His ↔ Arg	32	Val ↔ Met	58	Ala ↔ Glu Gly ↔ Asp
4	Pro ↔ Thr	22	Asp ↔ His	34	Ile ↔ Phe Leu ↔ Phe	59	Pro ↔ Arg
9	Gln ↔ His	23	Asn ↔ His	40	Pro ↔ His	60	Cys ↔ Tyr Ser ↔ Phe
10	Ser ↔ Pro	24	Leu ↔ His	42	Gly ↔ Val	69	Ser ↔ Arg
12	Thr ↔ Ile	25	Met ↔ Arg	43	Ile ↔ Arg Leu ↔ Arg	72	Gly ↔ Glu
13	Thr ↔ Asn	26	Ala ↔ Pro His ↔ Tyr Ser ↔ Ile Ser ↔ Leu	44	Ala ↔ Asp Cys ↔ Phe	73	Leu ↔ Trp
14	Asn ↔ Lys Asp ↔ Glu Gly ↔ Ala Ser ↔ Thr Val ↔ Ile Val ↔ Leu	27	Ser ↔ Asn Thr ↔ Lys	46	Gly ↔ Cys	76	Ser ↔ Tyr
15	Ile ↔ Lys Leu ↔ Gln	28	Ala ↔ Val Gln ↔ Arg Lys ↔ Arg	48	Asp ↔ Tyr Val ↔ Phe	83	Cys ↔ Trp
				49	Asn ↔ Tyr	99	Gly ↔ Arg Ser ↔ Trp
						129	Gly ↔ Trp



**MALDI
ELECTROSPRAY
MS
MS-MS
Mass-Informatics™**

Waters



WATERS CORPORATION
USA Milford, MA Tel: 508 478 2000
EUROPE France Tel: 1 3048 7200

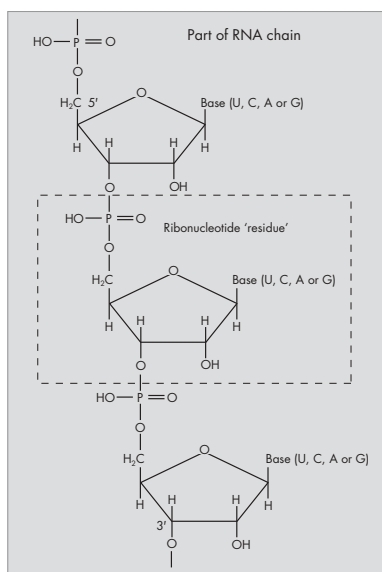
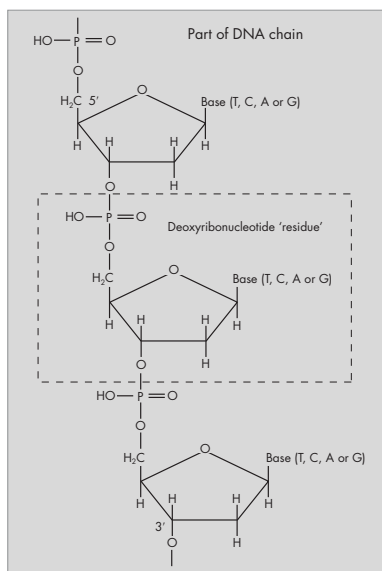


©2003 Waters Corporation January 2003
02/00484 WCH16/DAM Version 2
720000540EN

www.waters.com/micromass

The Genetic Code

The primary source of the genetic code, DNA, is a chain of deoxyribonucleotides (deoxyribonucleic acids interconnected by phosphodiester bonds), which occur with four different structures defined by the bases thymine (T), cytosine (C), adenine (A) and guanine (G). Transcription copies DNA into messenger RNA, which is a chain of ribonucleotides of similar structure to DNA except that thymine is replaced by uracil (U).

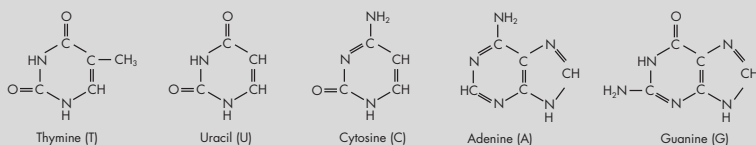


The notation for chains of nucleotides are the letters T, C, A, G for DNA and U, C, A, G for RNA, written left to right from the 5' end to the 3' end of a chain. Each group of three consecutive (and in frame) DNA or RNA nucleotides (codon or coding triplet) encodes one amino acid in a protein. The table below lists the DNA codons that encode the twenty common amino acids in proteins. To apply the table to RNA, replace T by U.

The DNA codons for the twenty commonly occurring amino acids

Amino Acid	Codon	Amino Acid	Codon	Amino Acid	Codon
Alanine Ala, A	GCT GCC GCA GCG	Glycine Gly, G	GGT GGC GGA GGG	Proline Pro, P	CCT CCC CCA CCG
Arginine Arg, R	CGT CGC CGA CGG AGA AGG	Histidine His, H	CAT CAC	Serine Ser, S	TCT TCC TCA TCG AGT AGC
		Isoleucine Ile, I	ATT ATC ATA		
Asparagine Asn, N	AAT AAC	Leucine Leu, L	TTA TTG CTT CTC CTA CTG	Threonine Thr, T	ACT ACC ACA ACG
Aspartic Acid Asp, D	GAT GAC			Tryptophan Trp, W	TGG
Cysteine Cys, C	TGT TGC	Lysine Lys, K	AAA AAG		
Glutamine Gln, Q	CAA CAG			Methionine Met, M	ATG
Glutamic Acid Glu, E	GAA GAG	Phenylalanine Phe, F	TTT TTC		
ATG also serves as a chain initiation codon. For RNA, replace T by U.				Chain termination	TAA TAG TGA

The five major bases



Data for the calculation of the masses of oligonucleotides for use in mass spectrometry

The molecular weight (mass) of an oligodeoxyribonucleotide (DNA) or oligoribonucleotide (RNA) may be calculated by summing the masses of the appropriate nucleotide 'residues' from the table below and making an allowance for the terminal groups as shown in the table.

Nucleotide 'residue'				
	Nucleotide	Elemental composition	Monoisotopic mass	Average mass
DNA	Thymine (T)	$C_{10}H_{13}N_2O_7P$	304.04604	304.1963
	Cytosine (C)	$C_9H_{12}N_3O_6P$	289.04637	289.1847
	Adenine (A)	$C_{10}H_{12}N_5O_5P$	313.05761	313.2097
	Guanine (G)	$C_{10}H_{12}N_5O_6P$	329.05252	329.2091
RNA	Uracil (U)	$C_9H_{11}N_2O_6P$	306.02530	306.1688
	Cytosine (C)	$C_9H_{12}N_3O_7P$	305.04129	305.1841
	Adenine (A)	$C_{10}H_{12}N_5O_6P$	329.05252	329.2091
	Guanine (G)	$C_{10}H_{12}N_5O_7P$	345.04744	345.2085
Terminal groups				
Both hydroxyl		H minus PO_2	-61.95577	-61.9646
Phosphate/hydroxyl		H_2O	18.01056	18.0153
Both phosphate		H_3PO_4	97.97690	97.9952

The monoisotopic masses were calculated using the following atomic masses of the most abundant isotope of the elements:
C=12.0000000, H=1.0078250, N=14.0030740, O=15.9949146, P=30.9737634.

The average masses were calculated using the following atomic weights of the elements: C=12.011, H=1.00794, N=14.00674, O=15.9994, P=30.97376.
Atomic Weights of the Elements 1991, IUPAC Commission on atomic weights and isotopic abundances, Pure and Appl. Chem., **64** (10), 1519-1534 (1992).