

# ! Topology definitions for anandamide (AEA)

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RESI AEA          0.00 !
GROUP            !
ATOM C5   CTL2   0.05 !
ATOM H51  HAL2   0.09 !
ATOM H52  HAL2   0.09 !
ATOM OH1  OHL   -0.66 !
ATOM HO1  HOL    0.43 !
GROUP            !
ATOM N1   NH1   -0.47 !
ATOM HN1  H      0.31 !
ATOM C1   CTL2  -0.22 !
ATOM H11  HAL2   0.09 !
ATOM H12  HAL2   0.09 !
ATOM C21  CL    0.79 !
ATOM O22  OBL   -0.55 !
ATOM C22  CTL2  -0.22 !
ATOM H2R  HAL2   0.09 !
ATOM H2S  HAL2   0.09 !
GROUP            !
ATOM C23  CTL2  -0.18 !
ATOM H3R  HAL2   0.09 !
ATOM H3S  HAL2   0.09 !
GROUP            !
ATOM C24  CTL2  -0.18 !
ATOM H4R  HAL2   0.09 !
ATOM H4S  HAL2   0.09 !
GROUP            !
ATOM C25  CEL1  -0.15 !
ATOM H5R  HEL1   0.15 !
GROUP            !
ATOM C26  CEL1  -0.15 !
ATOM H6R  HEL1   0.15 !
GROUP            !
ATOM C27  CTL2  -0.18 !
ATOM H7R  HAL2   0.09 !
ATOM H7S  HAL2   0.09 !
GROUP            !
ATOM C28  CEL1  -0.15 !
ATOM H8R  HEL1   0.15 !
GROUP            !
ATOM C29  CEL1  -0.15 !
ATOM H9R  HEL1   0.15 !
GROUP            !
ATOM C210 CTL2  -0.18 !
ATOM H10R HAL2   0.09 !
ATOM H10S HAL2   0.09 !
GROUP            !
ATOM C211 CEL1  -0.15 !

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OH1---HO1  
 |  
 H52---C5---H51  
 |  
 H12---C1---H11  
 |  
 N1---HN1  
 /  
 /  
 O22==C21  
 |  
 H2R---C22---H2S  
 |  
 H3R---C23---H3S  
 |  
 H4R---C24---H4S  
 |  
 H5R---C25  
 ||  
 H6R---C26  
 |  
 H7R---C27--H7S  
 |  
 H8R---C28  
 ||  
 H9R---C29  
 |  
 H10R---C210--H10S  
 |

ATOM	H11R	HEL1	0.15	!	H11R---	C211		
GROUP				!				
ATOM	C212	CEL1	-0.15	!				
ATOM	H12R	HEL1	0.15	!	H12R---	C212		
GROUP				!				
ATOM	C213	CTL2	-0.18	!				
ATOM	H13R	HAL2	0.09	!	H13R---	C213--H13S		
ATOM	H13S	HAL2	0.09	!				
GROUP				!				
ATOM	C214	CEL1	-0.15	!				
ATOM	H14R	HEL1	0.15	!	H14R---	C214		
GROUP				!				
ATOM	C215	CEL1	-0.15	!				
ATOM	H15R	HEL1	0.15	!	H15R---	C215		
GROUP				!				
ATOM	C216	CTL2	-0.18	!				
ATOM	H16R	HAL2	0.09	!	H16R---	C216--H16S		
ATOM	H16S	HAL2	0.09	!				
GROUP				!				
ATOM	C217	CTL2	-0.18	!				
ATOM	H17R	HAL2	0.09	!	H17R---	C217--H17S		
ATOM	H17S	HAL2	0.09	!				
GROUP				!				
ATOM	C218	CTL2	-0.18	!				
ATOM	H18R	HAL2	0.09	!	H18R---	C218--H18S		
ATOM	H18S	HAL2	0.09	!				
GROUP				!				
ATOM	C219	CTL2	-0.18	!				
ATOM	H19R	HAL2	0.09	!	H19R---	C219--H19S		
ATOM	H19S	HAL2	0.09	!				
GROUP				!				
ATOM	C220	CTL3	-0.27	!				
ATOM	H20R	HAL3	0.09	!	H20R---	C220--H20S		
ATOM	H20S	HAL3	0.09	!				
ATOM	H20T	HAL3	0.09	!		H20T		
BOND	C1	H11	C1	H12	C1	C5	C1	N1
BOND	C5	H51	C5	H52				
BOND	C5	OH1	OH1	HO1				
BOND	N1	HN1	N1	C21				
DOUBLE	C21	O22						
BOND	C21	C22						
BOND	C22	C23	C22	H2R	C22	H2S		
BOND	C23	C24	C23	H3R	C23	H3S		
BOND	C24	C25	C24	H4R	C24	H4S		
DOUBLE	C25	C26						
BOND	C25	H5R						
BOND	C26	C27	C26	H6R				
BOND	C27	C28	C27	H7R	C27	H7S		
DOUBLE	C28	C29						
BOND	C28	H8R						
BOND	C29	C210	C29	H9R				
BOND	C210	C211	C210	H10R	C210	H10S		



IC	C214	C212	*C213	H13R	1.5192	121.35	-124.15	108.68	1.1135
IC	C214	C212	*C213	H13S	1.5192	121.35	123.34	106.97	1.1128
IC	C212	C213	C214	C215	1.5067	111.57	180.00	126.10	1.3471
IC	C215	C213	*C214	H14R	1.3453	125.97	-176.85	115.39	1.1011
IC	C213	C214	C215	C216	1.5090	126.10	0.00	125.86	1.5091
IC	C216	C214	*C215	H15R	1.5097	125.28	178.19	119.65	1.1004
IC	C214	C215	C216	C217	1.3471	125.86	180.00	113.25	1.5428
IC	C217	C215	*C216	H16R	1.5192	121.35	-124.15	108.68	1.1135
IC	C217	C215	*C216	H16S	1.5192	121.35	123.34	106.97	1.1128
IC	C215	C216	C217	C218	1.5091	113.25	180.00	115.19	1.5395
IC	C218	C216	*C217	H17R	1.5192	121.35	-124.15	108.68	1.1135
IC	C218	C216	*C217	H17S	1.5192	121.35	123.34	106.97	1.1128
IC	C216	C217	C218	C219	1.5428	115.19	180.00	113.95	1.5345
IC	C219	C217	*C218	H18R	1.5192	121.35	-124.15	108.68	1.1135
IC	C219	C217	*C218	H18S	1.5192	121.35	123.34	106.97	1.1128
IC	C217	C218	C219	C220	1.5395	113.95	180.00	112.95	1.5309
IC	C220	C218	*C219	H19R	1.5192	121.35	-124.15	108.68	1.1135
IC	C220	C218	*C219	H19S	1.5192	121.35	123.34	106.97	1.1128
IC	C218	C219	C220	H20T	1.5345	112.95	180.00	110.39	1.1115
IC	H20T	C219	*C220	H20R	1.5192	121.35	-124.15	108.68	1.1135
IC	H20T	C219	*C220	H20S	1.5192	121.35	123.34	106.97	1.1128

PATCHING FIRST NONE LAST NONE