Anexo

Enlaces de hidrógeno entre el dominio SAM de SCM y el dominio PNT de dL(3)MBT: La cadena A simboliza el dominio SAM y la cadena B, simboliza el dominio PNT.

Cadena principal - Cadena principal:

DONOR				ACCEPTOR				PARAMETERS				
POS	CHAIN	RES	ATOM	POS	CHAIN	RES	ATOM	MO	Dd-a	Dh-a	A(d-H-N)	A(a-O=C)
838	A	ALA	N	1361	B	LEU	O	-	3.41	3.75	62.62	147.44

Dd-a = Distance Between Donor and Acceptor
Dh-a = Distance Between Hydrogen and Acceptor
A(d-H-N) = Angle Between Donor-H-N
A(a-O=C) = Angle Between Acceptor-O=C
MO = Multiple Occupancy
Note that angles that are undefined are written as 999.99

Cadena principal - Cadena lateral:

DONOR				ACCEPTOR				PARAMETERS				
POS	CHAIN	RES	ATOM	POS	CHAIN	RES	ATOM	MO	Dd-a	Dh-a	A(d-H-N)	A(a-O=C)
837	A	LYS	NZ	1362	B	ASN	O	-	2.72	9.99	999.99	144.31
837	A	LYS	NZ	1363	B	LEU	OXT	-	2.88	9.99	999.99	92.73
843	A	ASN	ND2	1335	B	LEU	O	1	2.74	1.98	126.38	131.06
843	A	ASN	ND2	1335	B	LEU	O	2	2.74	2.81	75.15	131.06
1362	B	ASN	OD1	833	A	GLU	O	1	3.49	2.72	129.08	158.69
1362	B	ASN	OD1	833	A	GLU	O	2	3.49	4.42	26.23	158.69
1362	B	ASN	ND2	833	A	GLU	O	1	2.99	2.02	152.83	149.93
1362	B	ASN	ND2	833	A	GLU	O	2	2.99	3.67	42.75	149.93

Dd-a = Distance Between Donor and Acceptor
Dh-a = Distance Between Hydrogen and Acceptor
A(d-H-N) = Angle Between Donor-H-N
A(a-O=C) = Angle Between Acceptor-O=C
MO = Multiple Occupancy
Note that angles that are undefined are written as 999.99

Cadena lateral – Cadena lateral:

DONOR				ACCEPTOR				PARAMETERS				
POS	CHAIN	RES	ATOM	POS	CHAIN	RES	ATOM	MO	Dd-a	Dh-a	A(d-H-N)	A(a-O=C)
835	A	ASP	OD1	1362	B	ASN	OD1	1	2.96	3.45	54.34	999.99
835	A	ASP	OD1	1362	B	ASN	OD1	2	2.96	2.68	93.82	999.99
843	A	ASN	OD1	1336	B	MET	SD	1	3.59	3.06	111.09	999.99
843	A	ASN	OD1	1336	B	MET	SD	2	3.59	4.32	41.12	999.99
843	A	ASN	ND2	1336	B	MET	SD	1	3.44	2.89	113.02	999.99
843	A	ASN	ND2	1336	B	MET	SD	2	3.44	4.07	46.39	999.99
850	A	TYR	OH	1341	B	GLU	OE2	-	2.78	9.99	999.99	999.99
1340	B	LYS	NZ	850	A	TYR	OH	-	2.86	9.99	999.99	999.99
1358	B	SER	OG	833	A	GLU	OE1	-	2.89	9.99	999.99	999.99
1362	B	ASN	OD1	835	A	ASP	OD1	1	2.96	3.16	69.50	999.99
1362	B	ASN	OD1	835	A	ASP	OD1	2	2.96	2.82	86.63	999.99

Dd-a = Distance Between Donor and Acceptor
Dh-a = Distance Between Hydrogen and Acceptor
A(d-H-N) = Angle Between Donor-H-N
A(a-O=C) = Angle Between Acceptor-O=C
MO = Multiple Occupancy
Note that angles that are undefined are written as 999.99

Enlaces de hidrógeno entre el dominio SAM de SCM y el dominio BTB de PSQ-A: La cadena A simboliza el dominio SAM, y la cadena C, el dominio BTB.

Cadena principal – Cadena principal:

DONOR				ACCEPTOR				PARAMETERS				
POS	CHAIN	RES	ATOM	POS	CHAIN	RES	ATOM	MO	Dd-a	Dh-a	A(d-H-N)	A(a-O=C)
838	A	ALA	N	1361	B	LEU	O	-	3.41	3.75	62.62	147.44
855	A	GLU	N	100	C	THR	O	-	3.25	2.31	156.31	115.63
98	C	ASP	N	852	A	GLY	O	-	3.46	3.87	58.34	150.71
99	C	VAL	N	852	A	GLY	O	-	3.23	3.66	56.10	111.17

Dd-a = Distance Between Donor and Acceptor
Dh-a = Distance Between Hydrogen and Acceptor
A(d-H-N) = Angle Between Donor-H-N
A(a-O=C) = Angle Between Acceptor-O=C
MO = Multiple Occupancy
Note that angles that are undefined are written as 999.99

Cadena principal – Cadena lateral:

DONOR				ACCEPTOR				PARAMETERS				
POS	CHAIN	RES	ATOM	POS	CHAIN	RES	ATOM	MO	Dd-a	Dh-a	A(d-H-N)	A(a-O=C)
827	A	ASP	OD1	55	C	ALA	O	1	3.33	3.54	69.82	93.57
827	A	ASP	OD1	55	C	ALA	O	2	3.33	2.41	142.13	93.57
830	A	ARG	NH1	55	C	ALA	O	1	2.68	3.06	59.03	135.19
830	A	ARG	NH1	55	C	ALA	O	2	2.68	1.75	149.86	135.19
831	A	LYS	NZ	95	C	GLY	O	-	2.67	9.99	999.99	139.06
837	A	LYS	NZ	1362	B	ASN	O	-	3.33	9.99	999.99	125.07
843	A	ASN	ND2	1335	B	LEU	O	1	2.91	2.05	136.69	124.08
843	A	ASN	ND2	1335	B	LEU	O	2	2.91	3.24	62.50	124.08
850	A	TYR	OH	1336	B	MET	O	-	3.34	9.99	999.99	173.86
855	A	GLU	OE1	100	C	THR	O	1	3.21	2.93	95.75	62.99
855	A	GLU	OE1	100	C	THR	O	2	3.21	3.79	50.71	62.99
855	A	GLU	OE1	100	C	THR	OXT	1	2.67	2.36	94.13	86.83
855	A	GLU	OE1	100	C	THR	OXT	2	2.67	3.68	17.50	86.83
855	A	GLU	OE2	100	C	THR	O	1	3.42	3.17	94.18	49.95
855	A	GLU	OE2	100	C	THR	O	2	3.42	4.10	44.97	49.95
855	A	GLU	OE2	100	C	THR	OXT	1	1.74	1.13	104.31	139.50
855	A	GLU	OE2	100	C	THR	OXT	2	1.74	2.38	42.31	139.50
1362	B	ASN	ND2	833	A	GLU	O	1	3.46	3.47	80.54	162.06
1362	B	ASN	ND2	833	A	GLU	O	2	3.46	2.72	129.90	162.06
58	C	THR	N	816	A	GLU	OE2	-	2.78	2.26	115.07	142.34
59	C	TYR	N	816	A	GLU	OE1	-	2.94	2.98	78.12	86.52
59	C	TYR	N	816	A	GLU	OE2	-	2.92	2.35	117.85	87.60

Dd-a = Distance Between Donor and Acceptor
Dh-a = Distance Between Hydrogen and Acceptor
A(d-H-N) = Angle Between Donor-H-N
A(a-O=C) = Angle Between Acceptor-O=C
MO = Multiple Occupancy
Note that angles that are undefined are written as 999.99

Cadena lateral – Cadena lateral:

DONOR				ACCEPTOR				PARAMETERS				
POS	CHAIN	RES	ATOM	POS	CHAIN	RES	ATOM	MO	Dd-a	Dh-a	A(d-H-N)	A(a-O=C)
831	A	LYS	NZ	96	C	GLU	OE1	-	2.56	9.99	999.99	999.99
831	A	LYS	NZ	96	C	GLU	OE2	-	2.62	9.99	999.99	999.99
832	A	HIS	ND1	1357	B	TYR	OH	-	2.92	2.09	152.90	999.99
835	A	ASP	OD1	1362	B	ASN	OD1	1	3.35	3.35	80.67	999.99
835	A	ASP	OD1	1362	B	ASN	OD1	2	3.35	3.43	76.72	999.99
835	A	ASP	OD1	1362	B	ASN	ND2	1	3.01	3.51	54.26	999.99
835	A	ASP	OD1	1362	B	ASN	ND2	2	3.01	2.39	114.21	999.99
837	A	LYS	NZ	1362	B	ASN	OD1	-	2.56	9.99	999.99	999.99
843	A	ASN	OD1	1336	B	MET	SD	1	3.89	3.28	117.20	999.99
843	A	ASN	OD1	1336	B	MET	SD	2	3.89	4.62	40.66	999.99
843	A	ASN	ND2	1336	B	MET	SD	1	3.69	3.04	120.12	999.99
843	A	ASN	ND2	1336	B	MET	SD	2	3.69	4.30	47.47	999.99
845	A	GLU	OE1	1336	B	MET	SD	1	3.19	3.61	58.37	999.99
845	A	GLU	OE1	1336	B	MET	SD	2	3.19	2.26	142.36	999.99
849	A	LYS	NZ	1341	B	GLU	OE1	-	2.85	9.99	999.99	999.99
849	A	LYS	NZ	1341	B	GLU	OE2	-	2.87	9.99	999.99	999.99
850	A	TYR	OH	1341	B	GLU	OE2	-	2.79	9.99	999.99	999.99
854	A	LYS	NZ	84	C	ASP	OD1	-	2.63	9.99	999.99	999.99
854	A	LYS	NZ	84	C	ASP	OD2	-	2.59	9.99	999.99	999.99
1357	B	TYR	OH	832	A	HIS	ND1	-	2.92	9.99	999.99	999.99
1357	B	TYR	OH	846	A	MET	SD	-	3.88	9.99	999.99	999.99
1358	B	SER	OG	833	A	GLU	OE1	-	2.88	9.99	999.99	999.99
1362	B	ASN	OD1	835	A	ASP	OD1	1	3.35	3.16	90.76	999.99
1362	B	ASN	OD1	835	A	ASP	OD1	2	3.35	4.05	41.91	999.99
1362	B	ASN	ND2	835	A	ASP	OD1	1	3.01	2.79	91.32	999.99
1362	B	ASN	ND2	835	A	ASP	OD1	2	3.01	3.50	53.29	999.99
58	C	THR	OG1	816	A	GLU	OE1	-	2.75	9.99	999.99	999.99
58	C	THR	OG1	816	A	GLU	OE2	-	2.80	9.99	999.99	999.99
62	C	LYS	NZ	816	A	GLU	OE1	-	2.66	9.99	999.99	999.99