Unsupervised 3D Ring Template Searching as an Ideas Generator for Scaffold Hopping: Use of the LAMDA, RigFit and FBSS Methods

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List of CSD Refcodes for dataset containing 200 structures:

ACNPHB
AFUTDZ10
ALPMIA
AMOXAP
ARFMAD
AZHPXB
BAFROP
BALSOW
BCMBTH
BCUNDL
BECNUS02
BERHEL
BEVPIB
BHYPOR
BIKQER
BILXAV
BOCCUR
BOHMIU
BUFDIP
BUGDOW
BZAZOA
BZAZOB
CAZPXT
CBMURD
CBYPZT
CIKNIT
CIQMOE
CITREC01
CIXYEN
CIZQAD01
COCXUN
COGYAY
CPBDTP
CUQPIN
CUVVIY
CUIYKI
DEMWUN
DICRAI01
DIGLAG
DIGMEL

DIHATO10
DISXEI
DOCJOU10
DOFNOB
DOJVAZ
DOQYUD
DOXTEP
DOZPEN
DPHACT05
DPOBCO
DUPRIP
FADWIQ
FASQOF
FAWREA
FEYLUQ
FINMAQ
FOGFUC
FUGROO
FUNKEE
GALVEU
GANGUX
GESCAI
GIQMEY
GUCTAZ
GUFXIO
HARGEM
HAVJOD
HAWTAA
HEPQIC01
HEWCER
HICQOZ
HIXVOZ
HNOBCH
HOPJOL
HYDTZA
ICEPAM
JAWVOS
JEJRIZ
JEWDIY
JEWSEJ
JITPIL
JIZREP
JOFSAY
JUFKIE
JUGCIX
JUISEM
JUYNAS
KAFVIW
KAWYEM
KEQLAT
KERXEK
KETHUM
KOQKIK
KORBAU
KOXCAB
KOYVEZ

LAJNUF
LEBGOO
LIDYEC
LIHTIF
LINRUV
LIWDIE
LODZUZ
MABYPN
MAEPTZ
MATEST
MPBZPO
NAJLOZ
NAPNUN
NECZOK
NEFKIS
NEYZOG
NIXWIA
NOFCIU
NOPGEE
NPHPSB
NUDHUP
OPHSLA
OXTZDX10
PABDIF
PAPJAR
PBZZOC
PCLPAZ
PELZIP
PEMBEO
PEXDAX
PHTRPL03
PIYQOD
PMPZOL
POGJEA
POYJOC
QACYIC
RAYXOE
REFLOD
REGLOE
RERDEX
RIBFUD
RIWTEW
RULRUL
SALWOR
SALXUY
SAPBUG
SATGUP
SAZDEC
SEGPUP
SELZIS
SIKGIC
SIQVOD
SITQIV
SOSKUG
SOSLAN
TAPJUP

TAVDAV
TBTXAN
TEKJIC
TEZWIE
THZOLA
TINCIC
TIWCOR
TOTDEL
TPFPCP
VAGXEG
VEBPUN
VEPKAC
VEVCAA
VEXPIX
VICXUA
VIMPEN
VINCAM
VIXRID
VIXTOL
VIYBOU
VOFGUS
VUHSIA
VUKBOS
VUMNAS
WEJFEW
WEJJAW
WEXJUE
WEYNOD
WIVFOW
WIZCUD
WOBQOT
WOPJIU
XAMSEJ
YITBAE
YORYUZ
YUFMUH
YUGBOR
YUKDUD
YUWSIS
ZAQDUQ
ZERLEN
ZIDLED
ZIGZEU
ZIHQEM
ZOHVEX
ZOWWAJ
ZUKRUS
ZZZGCW01