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| System modeled | Starting pdbID: | modifications made to the original crystal structure | Notes |
| SIRT3/Ac-CS2/ NAD+ | 4FVT | change carba-NAD+ into NAD+; remove waters and other co-crystalized small molecules |  |
| SIRT3/Ac-CS2/ NAD+/NAM | 4FVT | remove carba-NAD+, waters and other co-crystalized small molecules; align with 1YC2:A and superimpose coordinates of NAD+ (AB) and NAM |  |
| SIRT3/AcCS2/ NAD+/isoNAM | 4FVT | remove carba-NAD+, waters and other co-crystalized small molecules; align with 1YC2:A, superimpose coordinates of NAD+ (AB) and NAM and change NAM into isoNAM |  |
| SIRT3/NAD+(AB) | 4FVT | remove Ac-CS2, carba-NAD+, waters and other co-crystalized small molecules; align with 1YC2:A, superimpose coordinates of NAD+ (AB) | Results not used |
| SIRT3/NAD+(AC) | 4FVT | change carba-NAD+ into NAD+; remove Ac-CS2, waters and other co-crystalized small molecules |  |
| SIRT3/Ac-CS2 | 4FVT | remove carba-NAD+, waters and other co-crystalized small molecules |  |
| SIRT3 | 4FVT | remove Ac-CS2, carba-NAD+, waters and other co-crystalized small molecules |  |
| Ac-CS2 | 4FVT | remove SIRT3, carba-NAD+, waters and other co-crystalized small molecules |  |
| NAD+ | 4FVT | change carba-NAD+ into NAD+; remove SIRT3, Ac-CS2, waters and other co-crystalized small molecules |  |
| Sir2TM/Ac-p53/NAD+ | 2H4F | add residues 37-42 using ab initio loop prediction with Prime; remove waters and other co-crystalized small molecules |  |
| Sir2TM/Ac-p53/ NAD+/NAM | 2H4F | add residues 37-42 using ab initio loop prediction with Prime; remove waters and other co-crystalized small molecules; align with 1YC2:A and superimpose coordinates of NAD+ (AB) and NAM |  |
| Sir2TM/NAD+(AC) | 2H4F | add residues 37-42 using ab initio loop prediction with Prime; remove Ac-p53, waters and other co-crystalized small molecules |  |
| Sir2TM | 2H4F | add residues 37-42 using ab initio loop prediction with Prime; remove Ac-p53, NAD+, waters and other co-crystalized small molecules |  |
| Ac-p53 | 2H4F | remove Sir2TM, NAD+, waters and other co-crystalized small molecules |  |