

Structural Studies of the Water Hexamer

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Prism

O	0.89740000	-1.28511100	1.37567400
H	0.93366000	-1.62024900	0.46129100
H	1.53842400	-0.56327000	1.32598100
O	-1.55921800	-0.24177800	1.42347400
H	-2.06410200	-0.50196600	2.19746400
H	-0.67765600	-0.67864600	1.52523700
O	2.09078900	0.98445200	-0.04569300
H	1.25856800	1.49842100	-0.01864600
H	2.78821600	1.64209800	-0.09388600
O	-0.44703200	2.02126000	0.01211400
H	-0.90399800	1.53998500	0.71690900
H	-0.91108100	1.70047200	-0.77105600
O	-1.77668100	-0.21141100	-1.35117600
H	-2.56069800	-0.51617900	-1.81406100
H	-1.94980100	-0.38724200	-0.40953000
O	0.92440000	-1.33940500	-1.43239500
H	0.04462600	-0.99239900	-1.63526700
H	1.46658100	-0.54508700	-1.34041000

Book

O	2.38581900	1.09081400	-0.52680600
H	3.30455500	1.31818300	-0.36917400
H	2.38351000	0.11289000	-0.61173200
O	0.18343200	1.56332400	0.96855600
H	1.03497500	1.50184000	0.48194400
H	0.32542500	2.23497000	1.64003800
O	-2.09269000	1.45268900	-0.64698300
H	-1.90616400	1.89833700	-1.47619100
H	-1.29445500	1.59785600	-0.10817600
O	2.13031200	-1.59863200	-0.47408500
H	1.99359300	-2.21133400	-1.19955200
H	1.31215100	-1.66145500	0.06658700
O	-0.09981300	-1.38285800	1.05284500
H	-0.09428600	-0.44780500	1.29637100
H	-0.96813700	-1.49288600	0.62782300
O	-2.52772600	-1.26436600	-0.34538900
H	-2.50710100	-0.31029900	-0.54335600
H	-3.41874200	-1.42805700	-0.02968300

Cage

O	-0.61663800	-1.01709300	-1.42595600
H	-0.48199700	-1.68747900	-2.10024200
H	-0.10522200	-1.33088600	-0.65758600
O	0.71421100	-1.32594900	1.02378500
H	0.17850400	-0.56002400	1.36552800
H	0.64413800	-2.00496200	1.69948000
O	2.83951700	0.01127500	-0.23955200
H	3.65774900	0.13196100	0.24666000
H	2.29497900	-0.56139100	0.32455400
O	-0.68983300	0.84373600	1.54471800
H	-0.28085500	1.37899700	0.84044400
H	-1.59264600	0.71192100	1.21534400
O	-2.88022200	-0.00526300	-0.03950300
H	-3.53060900	0.46348300	-0.56656200
H	-2.26705000	-0.39104600	-0.68464400
O	0.60542900	1.68080900	-0.81328200
H	0.19797400	1.01354700	-1.37809900
H	1.50533400	1.33575100	-0.70655300

Open bag

O	2.29483500	-1.12009300	0.07971300
H	2.76797600	-1.68826200	-0.53158200
H	1.39053600	-1.50754000	0.13778100
O	-0.25626900	-1.96303000	0.20440100
H	-0.73021100	-1.50537300	0.91558900
H	-0.72452500	-1.64425000	-0.58414800
O	1.91497400	1.53834100	-0.09048800
H	2.12916900	0.57824600	-0.08659900
H	2.46596700	1.90469900	0.60470600
O	-0.75393400	1.80334700	-0.19224700
H	-0.95678000	2.71926700	-0.39863400
H	0.23114100	1.77037000	-0.15246500
O	-1.66836700	-0.03104800	1.77122400
H	-1.41626800	0.73085900	1.22569300
H	-1.60061700	0.28233800	2.67533200
O	-1.50226000	-0.43121200	-1.82184100
H	-1.34978400	0.41876800	-1.37908300
H	-2.43843500	-0.42955200	-2.03268100

Prism/book

O	-0.02781100	0.52399700	2.05893000
H	0.51382500	1.04465100	1.44949700
H	-0.90505700	0.90020300	1.94232600
O	1.36101400	1.57004400	-0.28159400
H	1.75422200	0.71750500	-0.58466600
H	2.02907800	2.23588300	-0.46060300
O	-1.39932500	1.61321800	-0.62078500
H	-0.42896500	1.69288100	-0.65405000

H	-1.72549500	2.33507000	-1.16257900
O	2.08619300	-0.90482100	-0.97681600
H	2.90861400	-1.38199800	-0.84801700
H	1.41961700	-1.39472600	-0.43624700
O	-2.23736100	-1.07534800	-0.59133900
H	-2.66435500	-1.32906700	-1.41191900
H	-2.02717700	-0.13260000	-0.70095000
O	0.18010800	-1.92394300	0.58860600
H	0.11055600	-1.26008500	1.29363000
H	-0.68741400	-1.85289600	0.15756200

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Chair

O	-1.74825100	-2.06147400	0.16864100
H	-0.79460200	-2.23092300	0.02434900
H	-1.96461800	-2.57303200	0.95092800
O	0.91113300	-2.54430300	-0.16934100
H	1.24561000	-2.98720700	-0.95191900
H	1.53512700	-1.80356100	-0.02472800
O	-0.91116500	2.54460900	0.16816800
H	-1.24540100	2.98787100	0.95065200
H	-1.53514900	1.80369800	0.02426900
O	2.65967000	-0.48334200	0.16938800
H	3.21056800	-0.41525300	0.95190100
H	2.32991500	0.42741400	0.02515300
O	-2.65964800	0.48328400	-0.16804900
H	-2.32980200	-0.42747300	-0.02415700
H	-3.21138900	0.41525000	-0.94998300
O	1.74828700	2.06122900	-0.16882500
H	1.96500900	2.57252200	-0.95119400
H	0.79452700	2.23066300	-0.02513100

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Intermediate bag

O	-0.34984500	-1.87218000	-0.12021200
H	-0.63990300	-1.50019300	-0.95984300
H	0.62286800	-1.78173100	-0.13347400
O	-2.21263100	0.25981900	-1.31235400
H	-2.51761900	0.09074000	-0.40788400
H	-3.01336000	0.37178600	-1.82971600
O	-1.80808200	-0.24502800	1.40522100
H	-2.13769200	-0.59013600	2.23752900
H	-1.23165300	-0.95008800	1.02950700
O	2.35912200	-1.38206100	-0.06958200
H	2.47812800	-0.41171000	-0.05082200
H	3.01101100	-1.69573100	-0.69955700
O	2.38114500	1.35378100	-0.08256700
H	1.43962500	1.60664000	0.01370700
H	2.85592900	1.95827900	0.49133200
O	-0.28701900	1.87505900	0.18316400

H	-0.71729500	1.34884800	0.87293400
H	-0.81155100	1.63817100	-0.59305800

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Pentamer down + 1

O	0.98414500	2.24478800	0.23403300
H	1.09465900	2.66553300	1.08927900
H	1.68427000	1.55846600	0.20544400
O	1.51170900	-2.09979300	0.24028600
H	1.75655600	-2.97921900	-0.05338800
H	0.59861900	-1.96502800	-0.09341500
O	2.84889700	0.27276000	0.17773000
H	3.50705300	0.22789500	-0.51881800
H	2.45252400	-0.62242800	0.20324400
O	-3.05955500	-0.31169600	0.80053200
H	-2.61099100	0.45520600	0.41216600
H	-3.25000200	-0.05358600	1.70431500
O	-0.96702700	-1.54476800	-0.70770400
H	-1.70813200	-1.54783600	-0.08498000
H	-0.99451000	-0.62860700	-1.01834500
O	-1.36462900	1.34058900	-0.74950600
H	-1.62179700	1.96226500	-1.43464700
H	-0.53655800	1.71229500	-0.37382400

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Pentamer planar + 1

O	2.93396800	-0.34041200	1.03403200
H	2.55059500	0.42042600	0.57231100
H	3.08682000	-0.03308200	1.92940200
O	-0.98125800	2.27703600	-0.13302600
H	-1.22156400	3.07422600	0.34253600
H	-1.64055800	1.60552200	0.14145000
O	-1.62799000	-2.08466000	-0.11981800
H	-0.67050500	-1.96929100	-0.30197100
H	-1.93754000	-2.67446900	-0.81022700
O	0.97829100	-1.58052700	-0.66568100
H	1.64053100	-1.62574800	0.03743600
H	1.07298000	-0.65949900	-0.94987400
O	1.45050000	1.27607100	-0.76358700
H	1.78229200	1.79961100	-1.49697000
H	0.59988200	1.69934700	-0.51827800
O	-2.73168500	0.30113800	0.56275200
H	-3.04654700	0.14768600	1.45612500
H	-2.39098800	-0.57390500	0.28068300

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Twisted boat

O	1.63013500	-2.02381500	-0.56323500
H	2.03122700	-1.15443000	-0.36368400
H	1.72704500	-2.12469200	-1.51226300

O	-1.71055300	2.03494000	-0.36662700
H	-2.00456700	2.29206100	-1.24299700
H	-2.05671700	1.12676600	-0.25320600
O	0.87040100	2.48062500	0.39193900
H	-0.04960700	2.31957900	0.09749900
H	0.77164800	2.92987800	1.23402400
O	-2.61566700	-0.52918600	-0.14433800
H	-3.46347000	-0.80689300	0.20745300
H	-1.98516100	-1.21917800	0.14716000
O	-0.80632100	-2.43832000	0.59101000
H	-0.59226200	-2.67598300	1.49558900
H	0.06625400	-2.31317300	0.16423600
O	2.64561400	0.42814200	0.09898100
H	2.00995400	1.16370800	0.21390300
H	3.43678700	0.84327300	-0.24956000

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Boat

O	2.25917800	1.46890600	-0.24674500
H	2.46849800	2.02557300	-0.99985300
H	1.40411800	1.81990300	0.07506400
O	0.14312600	-2.42512200	0.66841200
H	0.26924500	-2.30108000	1.61162200
H	0.95885400	-2.05632700	0.27267200
O	-0.14895100	2.47647400	0.55056900
H	-0.97039600	2.01979900	0.27490700
H	-0.33677400	2.80337900	1.43252900
O	-2.44038200	1.20706000	-0.20878400
H	-2.85004400	1.47218300	-1.03501900
H	-2.39452200	0.23090700	-0.26522600
O	2.36865500	-1.25653400	-0.39946200
H	2.35478100	-0.27814200	-0.37406600
H	3.27534700	-1.49439900	-0.19640100
O	-2.18073600	-1.49809900	-0.42709800
H	-2.83800300	-2.17064500	-0.23861200
H	-1.34822100	-1.85263100	-0.05275500

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Double envelope

O	1.63903300	0.89778200	-1.01200900
H	2.45549300	0.62954300	-0.57184500
H	1.11798900	0.08208000	-0.95409800
O	0.14488900	-1.33358700	0.01137900
H	-0.38382100	-0.75417600	0.58236000
H	-0.54530900	-1.83560200	-0.44259400
O	-1.73219500	0.58721600	1.01465500
H	-2.03502400	0.82232800	1.89510700
H	-1.28545400	1.39388700	0.67521500
O	2.91608100	-1.20552300	0.50603100
H	2.00441800	-1.53188800	0.48552900

H	3.34409300	-1.70262700	1.20479500
O	-2.63220500	-1.56742200	-0.61967400
H	-2.60429100	-0.72578000	-0.14123800
H	-3.29554900	-1.44235300	-1.30093900
O	-0.20203100	2.58365300	0.03841600
H	0.55698900	2.09294900	-0.34514100
H	-0.39812000	3.27468700	-0.59752300

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Pentamer up + 1

O	-2.32553300	0.32936700	0.92162000
O	-0.89143600	2.32356300	-0.26429900
O	1.57236500	1.27352200	-0.71462400
O	2.43488100	-0.46204200	1.32532000
O	0.99920500	-1.61791800	-0.84494600
O	-1.66730600	-1.94133600	-0.42947700
H	-3.25938500	0.33026800	1.13998400
H	-2.16468900	-0.53576400	0.49152600
H	-1.43849400	2.63553600	-0.98863200
H	-1.45140100	1.65773100	0.18608300
H	0.69904300	1.70316800	-0.58696200
H	2.11713800	1.94417600	-1.13326000
H	2.15515800	-0.23528600	2.21464200
H	2.21508200	0.31931900	0.79303400
H	1.49932500	-1.56392700	-0.01552400
H	1.17678100	-0.74594900	-1.22127100
H	-0.70349100	-1.88621300	-0.60906900
H	-1.82246300	-2.86430600	-0.21930500

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Double tetramer

O	2.63657800	1.48487300	0.28772700
O	2.78482400	-1.29408700	-0.18462500
O	0.01202900	-1.40333700	0.40555700
O	0.00505200	1.06127300	-0.48037400
O	-2.68691400	1.50868800	0.04100000
O	-2.77539200	-1.29968400	-0.07059500
H	3.39804600	2.00317800	0.02170200
H	2.86889000	0.56333000	0.08106000
H	1.84708200	-1.53442500	-0.08980400
H	3.07908200	-1.77576200	-0.96069600
H	0.00514800	-0.45023700	0.12247200
H	0.04907500	-1.37243300	1.36616500
H	-0.78968900	1.56593900	-0.25020100
H	0.79280900	1.56381900	-0.22372300
H	-3.25046400	1.80369700	0.75878400
H	-2.85243600	0.55159200	-0.01987300
H	-1.83798600	-1.55095200	-0.00222800
H	-3.11897700	-1.82956200	-0.79318200

Tetramer trimer

O	1.35228300	-1.90104500	-0.34110100
H	1.17067500	-2.43228700	-1.11926300
H	0.60107000	-1.27755000	-0.28501800
O	-0.49100100	0.11991900	-0.02981600
H	-1.15669200	0.35767000	-0.69553200
H	0.11829900	0.88132900	0.02827400
O	1.57318300	1.92689400	0.22872900
H	1.84245500	2.67147400	-0.31293100
H	2.32888400	1.30879300	0.19508600
O	-2.98767900	0.29926400	-1.28825200
H	-3.29312200	0.05445600	-0.39970900
H	-3.61053300	0.96399400	-1.58883600
O	3.40422000	-0.11708400	0.05140000
H	2.79006000	-0.85783000	-0.11686200
H	3.97586100	-0.43152200	0.75494800
O	-2.84610600	-0.31831800	1.42012800
H	-1.89776800	-0.22032700	1.23191700
H	-2.90839700	-1.09524800	1.97922300

Tricycle + 1 (a)

O	-0.85672300	-1.44112300	1.56981600
H	-1.47900500	-2.17161800	1.55219200
H	-0.43758200	-1.45953800	0.69382500
O	1.07790100	1.60540200	0.06098000
H	0.19790900	1.62575100	0.50796900
H	1.20222000	2.48837600	-0.29536000
O	3.09876100	-0.42069500	-0.18009400
H	3.71428100	-0.64631200	0.52010200
H	2.61368000	0.34424300	0.16022400
O	-2.29833600	-0.08771500	-1.37762900
H	-2.67636800	0.09112200	-2.24112500
H	-1.45396600	-0.52545500	-1.56079100
O	0.35589900	-0.91191500	-0.97806500
H	0.61951000	0.00640900	-0.79381400
H	1.21679500	-1.33585500	-1.07947900
O	-1.40722000	1.27213200	1.00840600
H	-1.36487600	0.42937300	1.48825500
H	-1.91485300	1.02481300	0.22068800

Closed bag

O	-2.24446400	-0.35287900	1.34281300
H	-2.55670300	-1.02747000	1.94962700
H	-1.31172300	-0.21419800	1.58794100
O	2.48778200	-1.61674200	0.07370200
H	2.92723900	-2.38531100	-0.29401000
H	1.97967400	-1.24835700	-0.66367600

O	0.50571800	0.09368400	1.44070600
H	1.20869400	-0.45939100	1.79962700
H	0.57364300	-0.09962900	0.48542000
O	0.58908400	-0.05986400	-1.33681900
H	0.70017500	0.90049300	-1.37344200
H	-0.34158800	-0.22078000	-1.58067200
O	-2.12634100	-0.56280200	-1.42828500
H	-2.30104000	-0.51576800	-0.46985600
H	-2.83492500	-0.05541700	-1.82955000
O	0.77761400	2.49958700	-0.13655500
H	1.25055900	3.31295800	0.04949400
H	0.79085700	2.00499800	0.69460500

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Tricycle + 1 (b)

O	-2.51874700	0.43911100	-0.03591200
H	-2.30874400	-0.13907600	0.71296200
H	-2.25113400	-0.11167000	-0.78839300
O	3.77390100	-0.11024200	0.00681300
H	4.24011200	-0.02180400	-0.82856800
H	4.29908100	0.40105900	0.62784800
O	-1.03273900	-1.28941100	1.69828400
H	-0.22138800	-0.96093700	1.27414500
H	-0.82216500	-1.32199600	2.63355300
O	-0.95397300	-1.15640800	-1.82382300
H	-0.99250600	-2.11530500	-1.80971900
H	-0.18317500	-0.94154700	-1.27201300
O	0.91030500	-0.13131300	0.04219400
H	0.61611400	0.80076100	0.02078000
H	1.87794500	-0.10177300	0.04363000
O	-0.47302600	2.22836900	0.09566900
H	-0.58568500	2.94856100	-0.52798200
H	-1.31422800	1.72287500	0.04795600

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Pentamer + 1

O	-3.92849700	-0.05958700	0.67631100
O	-1.40651900	-0.30063700	-0.73953400
O	-0.09511500	2.14415400	-0.49638300
O	2.40979900	1.56302500	0.45785900
O	2.77070200	-1.13195700	0.26289300
O	0.36370600	-2.28067000	-0.23183800
H	-4.72368000	0.04841200	0.14827300
H	-4.00772200	0.61148600	1.35926900
H	-2.24106600	-0.20752600	-0.26197300
H	-0.98945100	0.57816600	-0.68655300
H	0.79781000	1.98769100	-0.12921200
H	0.06217700	2.70322600	-1.26019100
H	2.71163600	1.79640300	1.33806000
H	2.58760000	0.60228200	0.38606500

H	1.91525900	-1.58784500	0.11317700
H	3.35973300	-1.51356600	-0.39138900
H	-0.06438700	-2.89386500	0.36879700
H	-0.32052400	-1.59949100	-0.41878100

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Closed chair down

O	-3.17523700	0.10323700	-0.46768900
H	-4.08487400	-0.06001200	-0.21104100
H	-2.67175600	-0.63444300	-0.08369100
O	-1.06036100	-1.32331500	0.73481000
H	-0.85373000	-0.37941200	0.84458400
H	-0.39965600	-1.60507000	0.08889400
O	2.16754500	-0.07406700	1.33512800
H	1.98530900	-0.92603600	0.91890500
H	1.53534700	-0.02433400	2.05797400
O	1.61538000	1.32060900	-0.95384600
H	1.94986300	1.04500100	-0.07812700
H	2.25587400	1.95488100	-1.28461300
O	1.25559800	-1.48657600	-1.04565000
H	1.45053700	-2.04976800	-1.79818700
H	1.35675800	-0.57869900	-1.37431400
O	-0.87032500	1.47753900	0.52337700
H	-1.73462700	1.41771700	0.09209000
H	-0.24982800	1.70076000	-0.18151800

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Closed chair

O	1.22983500	-1.37193800	-0.86607900
O	1.02670900	1.47284800	-0.80413800
O	-1.36200900	1.39551000	0.86041400
O	-1.07815700	-1.41437900	0.96719000
O	3.16292300	0.07749800	0.54455700
O	-2.88727300	-0.13768600	-0.82793100
H	1.01222300	-0.46358100	-1.13277800
H	0.48998200	-1.60307300	-0.29026400
H	1.83479900	1.38162400	-0.28028400
H	0.33824200	1.66313700	-0.15429200
H	-2.02008600	1.11550400	0.19690000
H	-1.78615100	2.10097000	1.35518000
H	-1.10946300	-1.95531000	1.76027900
H	-1.02296800	-0.49965200	1.28836000
H	4.08931000	-0.10898000	0.38030700
H	2.68206800	-0.64656500	0.10614300
H	-2.45713200	-0.91506500	-0.44449600
H	-2.78705100	-0.24384700	-1.77715300

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Tetramer + 2

O	0.12346600	-1.79676300	0.08492000
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O	1.83352800	0.12732900	0.85806800
O	-0.05180800	2.03499800	0.00534800
O	-1.73025000	-0.06389600	-0.80508400
O	-4.41275700	-0.07170300	0.24050000
O	4.42319600	-0.25465800	-0.38969800
H	-0.62647500	-1.27244700	-0.27570400
H	0.33785200	-2.43206000	-0.60176700
H	1.27424400	-0.64474100	0.60918200
H	1.99717700	0.00733300	1.79767400
H	0.69622500	1.50448200	0.33121400
H	0.35140500	2.74223600	-0.50205000
H	-1.30709000	0.78565700	-0.59782600
H	-2.62608200	-0.00403100	-0.44627000
H	-5.12255500	-0.37853700	-0.32932200
H	-4.57540300	-0.51148500	1.07892100
H	3.54948800	-0.06959400	-0.01713400
H	4.56821000	0.47071500	-0.99935300

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Triple trimer

O	-3.33899100	-1.02444800	-0.01962500
H	-2.37188900	-1.10193800	0.02599700
H	-3.60773800	-1.66996500	-0.67645600
O	-0.64775200	-0.25194200	0.07855400
H	-1.07497600	0.61905400	0.11485700
H	-0.01989800	-0.26555100	0.81453700
O	3.06484800	1.30255800	-0.31338100
H	2.76726900	0.94702200	0.53484400
H	3.04529100	2.25522400	-0.20409300
O	1.77429400	-1.10862500	-1.25978800
H	2.25554700	-0.28949500	-1.43567300
H	0.85202000	-0.81842400	-1.22275200
O	-2.67471300	1.68399900	-0.04678800
H	-3.23060500	0.88853500	-0.07356400
H	-3.14364100	2.29412300	0.52588700
O	1.86388300	-0.66186700	1.42870800
H	1.98541500	-1.10906200	0.56651200
H	2.21065300	-1.26692800	2.08846600

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Trimertrimer + 1

O	-1.97135200	0.44136000	0.70984800
H	-1.09361400	0.03660900	0.65770200
H	-2.59303700	-0.26536800	0.49115100
O	2.72440900	-1.45127400	-1.12438200
H	1.88964200	-0.97175900	-0.98305700
H	2.46098400	-2.33414300	-1.39001500
O	-3.93198600	-1.59070800	0.08634400
H	-4.40992700	-1.52894900	-0.74469500
H	-4.61787700	-1.74160000	0.74175800

O	0.79643600	0.23292400	-0.02096700
H	0.52555100	1.09203300	-0.38534200
H	1.53458800	0.42650200	0.57788300
O	-0.81227600	2.39706700	-0.82813400
H	-0.91891400	3.30253000	-0.53014000
H	-1.46541600	1.88511900	-0.31744200
O	3.37156000	0.09059500	1.11912400
H	3.48514100	-0.59454300	0.44186400
H	3.78855500	-0.26614600	1.90567200

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