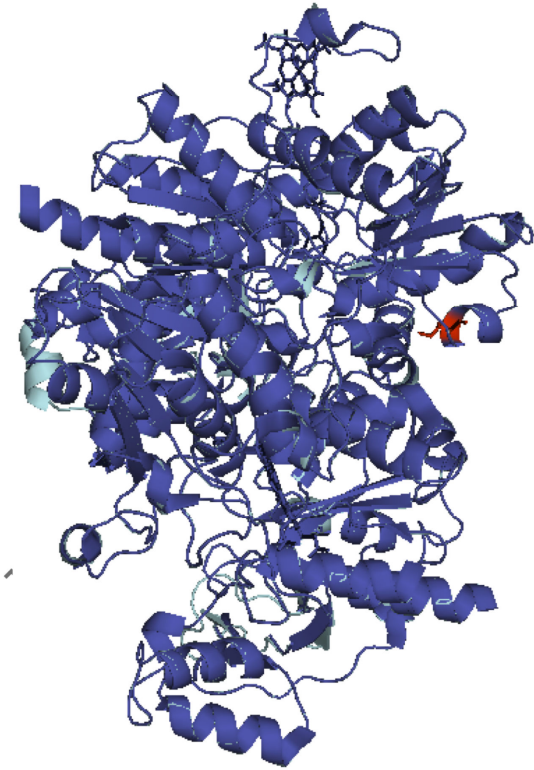
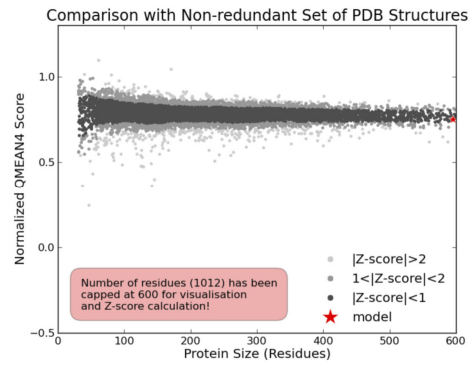
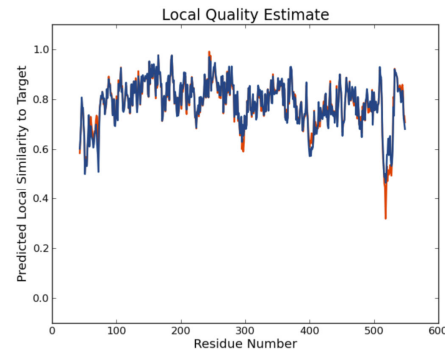


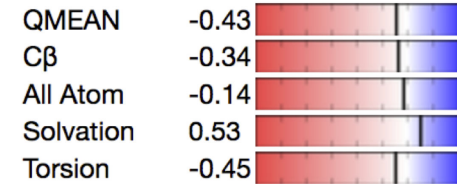
S2 A) Figure



Model-Template Alignment

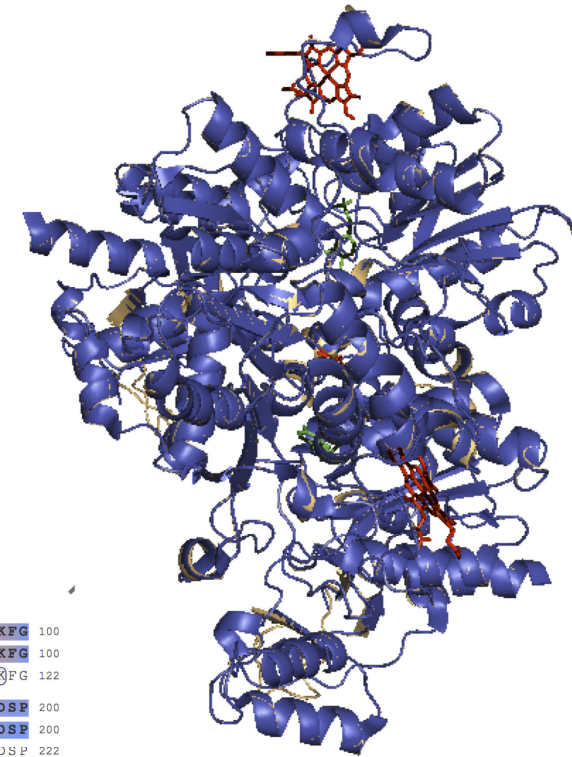
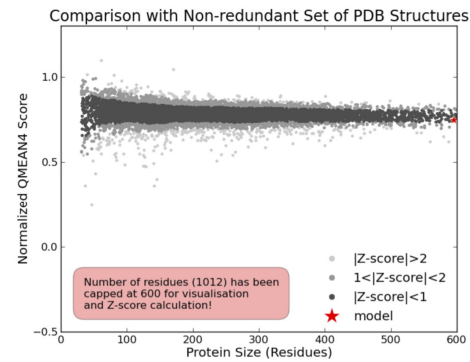
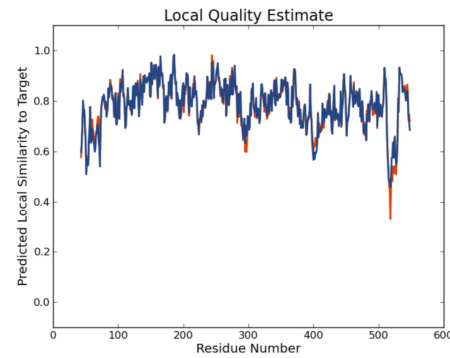
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Model_02:A MPSETPQAEVGTGCPHRSRSGPHSAKGSLEKSPEDKEAKEPLWIRFPDAPSRCTWQLGRPAESP...
Model_02:B MPSETPQAEVGTGCPHRSRSGPHSAKGSLEKSPEDKEAKEPLWIRFPDAPSRCTWQLGRPAESP...
4coo.1.A MPSETPQAEVGTGCPHRSRSGPHSAKGSLEKSPEDKEAKEPLWIRFPDAPSRCTWQLGRPAESP...
Model_02:A LKCELLAKCEFFNAGGSVKDRISLRMIEDAERDGTLLKPGDITIEPTSGNTGIGLALAAAVRGYRCI...
Model_02:B LKCELLAKCEFFNAGGSVKDRISLRMIEDAERDGTLLKPGDITIEPTSGNTGIGLALAAAVRGYRCI...
4coo.1.A LKCELLAKCEFFNAGGSVKDRISLRMIEDAERDGTLLKPGDITIEPTSGNTGIGLALAAAVRGY...
Model_02:A ESHVGVAVRLKNEIPNSHILDQYRNASNPLAHYDTTAADEILQQCDGKLDMLVASVGTGGTITGIARKL...
Model_02:B ESHVGVAVRLKNEIPNSHILDQYRNASNPLAHYDTTAADEILQQCDGKLDMLVASVGTGGTITGIARKL...
4coo.1.A ESHVGVAVRLKNEIPNSHILDQYRNASNPLAHYDTTAADEILQQCDGKLDMLVASVGTGGTITGI...
Model_02:A YEVEGIGYDFIPTVLDRTVVVDKWFKSNDEEAFTFARMLIAQEGLLCGGSAGSTVAVAVKAAQELQEG...
Model_02:B YEVEGIGYDFIPTVLDRTVVVDKWFKSNDEEAFTFARMLIAQEGLLCGGSAGSTVAVAVKAAQELQEG...
4coo.1.A YEVEGIGYDFIPTVLDRTVVVDKWFKSNDEEAFTFARMLIAQEGLLCGGSAGSTVAVAVKAAQEL...
Model_02:A DLTEKKPWWWHLRVQELGLSAPLTVLPTITCGHTIEILREKGFDAQPVVDEAGVILGMVTLGNMLSS...
Model_02:B DLTEKKPWWWHLRVQELGLSAPLTVLPTITCGHTIEILREKGFDAQPVVDEAGVILGMVTLGNMLSS...
4coo.1.A DLTEKKPWWWHLRVQELGLSAPLTVLPTITCGHTIEILREKGFDAQPVVDEAGVILGMVTLGNM...
Model_02:A HILEMDHFALVVHEQIQYHSTGKSSQRQMVFGVVTAIDLNFVAAQERDQK
Model_02:B HILEMDHFALVVHEQIQYHSTGKSSQRQMVFGVVTAIDLNFVAAQERDQK
4coo.1.A HILEMDHFALVVHEQIQYHSTGKSSQRQMVFGVVTAIDLNFVAAQERDQK
    
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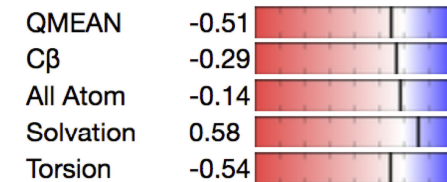
| Template | Seq Identity | Oligo-state | Found by | Method | Resolution | Seq Similarity | Range | Coverage | Description |
|----------|--------------|-------------|----------|--------|------------|----------------|----------|----------|-----------------------------|
| 4coo.1.A | 99.82 | homo-dimer | BLAST | X-ray | 2.00Å | 0.61 | 43 - 548 | 0.98 | CYSTATHIONINE BETA-SYNTHASE |

S2 B) Figure



Model-Template Alignment

| | | | | | | |
|------------|--|--|----------|---------------|--|-----|
| Model_03:A | MPSETPQAEVGP | TCGPHRSGPHSAKGSLEKGSPEDEKAKEPL | WIRPDAPS | RCTWQLGR | PASESPHHHTAPAKSPKILPDILKKIGDTPMVRINKIGKFFG | 100 |
| Model_03:B | MPSETPQAEVGP | TCGPHRSGPHSAKGSLEKGSPEDEKAKEPL | WIRPDAPS | RCTWQLGR | PASESPHHHTAPAKSPKILPDILKKIGDTPMVRINKIGKFFG | 100 |
| 4coo.1.A | MPSETPQAEVGP | TCGPHRSGPHSAKGSLEKGSPEDEKAKEPL | WIRPDAPS | RCTWQLGR | PASESPHHHTAPAKSPKILPDILKKIGDTPMVRINKIGKFFG | 122 |
| Model_03:A | LKCELLAKCVFFNAGGSVKDRISLRMIEDAERDGLKPGD | TIIIEPTSGNTGIGLALAAAVRGYRCIIIVMPEKMSSEKVDVLRALGAEIVRTPTNARFDSF | | | | 200 |
| Model_03:B | LKCELLAKCVFFNAGGSVKDRISLRMIEDAERDGLKPGD | TIIIEPTSGNTGIGLALAAAVRGYRCIIIVMPEKMSSEKVDVLRALGAEIVRTPTNARFDSF | | | | 200 |
| 4coo.1.A | LKCELLAKCVFFNAGGSVKDRISLRMIEDAERDGLKPGD | TIIIEPTSGNTGIGLALAAAVRGYRCIIIVMPEKMSSEKVDVLRALGAEIVRTPTNARFDSF | | | | 222 |
| Model_03:A | ESHVGVAVRLKNEIPNSHILDQYRNASNPLAHYD | TDAEILQQCDGKLDMLVASVGTGGTITGIARKLKEKCPGCR | RIIGVD | PEGSILAEPEELN | QTEQTT | 300 |
| Model_03:B | ESHVGVAVRLKNEIPNSHILDQYRNASNPLAHYD | TDAEILQQCDGKLDMLVASVGTGGTITGIARKLKEKCPGCR | RIIGVD | PEGSILAEPEELN | QTEQTT | 300 |
| 4coo.1.A | ESHVGVAVRLKNEIPNSHILDQYRNASNPLAHYD | TDAEILQQCDGKLDMLVASVGTGGTITGIARKLKEKCPGCR | RIIGVD | PEGSILAEPEELN | QTEQTT | 322 |
| Model_03:A | YEVEGIGYDFIPTVLDRTVVVDKWFKSNDEEAFTFARMLIAQEG | LLCGGSAGSTVAVAVKAAQELQEGQRCVVILPDSVRNYMTKFLSDRWMLQKGFLEE | | | | 400 |
| Model_03:B | YEVEGIGYDFIPTVLDRTVVVDKWFKSNDEEAFTFARMLIAQEG | LLCGGSAGSTVAVAVKAAQELQEGQRCVVILPDSVRNYMTKFLSDRWMLQKGFLEE | | | | 400 |
| 4coo.1.A | YEVEGIGYDFIPTVLDRTVVVDKWFKSNDEEAFTFARMLIAQEG | LLCGGSAGSTVAVAVKAAQELQEGQRCVVILPDSVRNYMTKFLSDRWMLQKGFLEE | | | | 422 |
| Model_03:A | DLTEKKPWWHHLRVQELGLSAPLTVLPTITCGHTIEILREKGF | QAPVVD EAGVILGMVTLGNMSSL LAGKVQPSDQVGVVIYKQFKQIRLTDTLGRLS | | | | 500 |
| Model_03:B | DLTEKKPWWHHLRVQELGLSAPLTVLPTITCGHTIEILREKGF | QAPVVD EAGVILGMVTLGNMSSL LAGKVQPSDQVGVVIYKQFKQIRLTDTLGRLS | | | | 500 |
| 4coo.1.A | DLTEKKPWWHHLRVQELGLSAPLTVLPTITCGHTIEILREKGF | QAPVVD EAGVILGMVTLGNMSSL LAGKVQPSDQVGVVIYKQFKQIRLTDTLGRLS | | | | 522 |
| Model_03:A | HILEMDHFALVVHEQIQYHSTGKSSQRQMVFGVVT | AIDL NLFVAAQERDQK | | | | 551 |
| Model_03:B | HILEMDHFALVVHEQIQYHSTGKSSQRQMVFGVVT | AIDL NLFVAAQERDQK | | | | 551 |
| 4coo.1.A | HILEMDHFALVVHEQIQYHSTGKSSQRQMVFGVVT | AIDL NLFVAAQERDQK | | | | 563 |



| Template | Seq Identity | Oligo-state | Found by | Method | Resolution | Seq Similarity | Range | Coverage | Description |
|----------|--------------|-------------|----------|--------|------------|----------------|----------|----------|-----------------------------|
| 4coo.1.A | 99.82 | homo-dimer | BLAST | X-ray | 2.00Å | 0.61 | 43 - 548 | 0.98 | CYSTATHIONINE BETA-SYNTHASE |