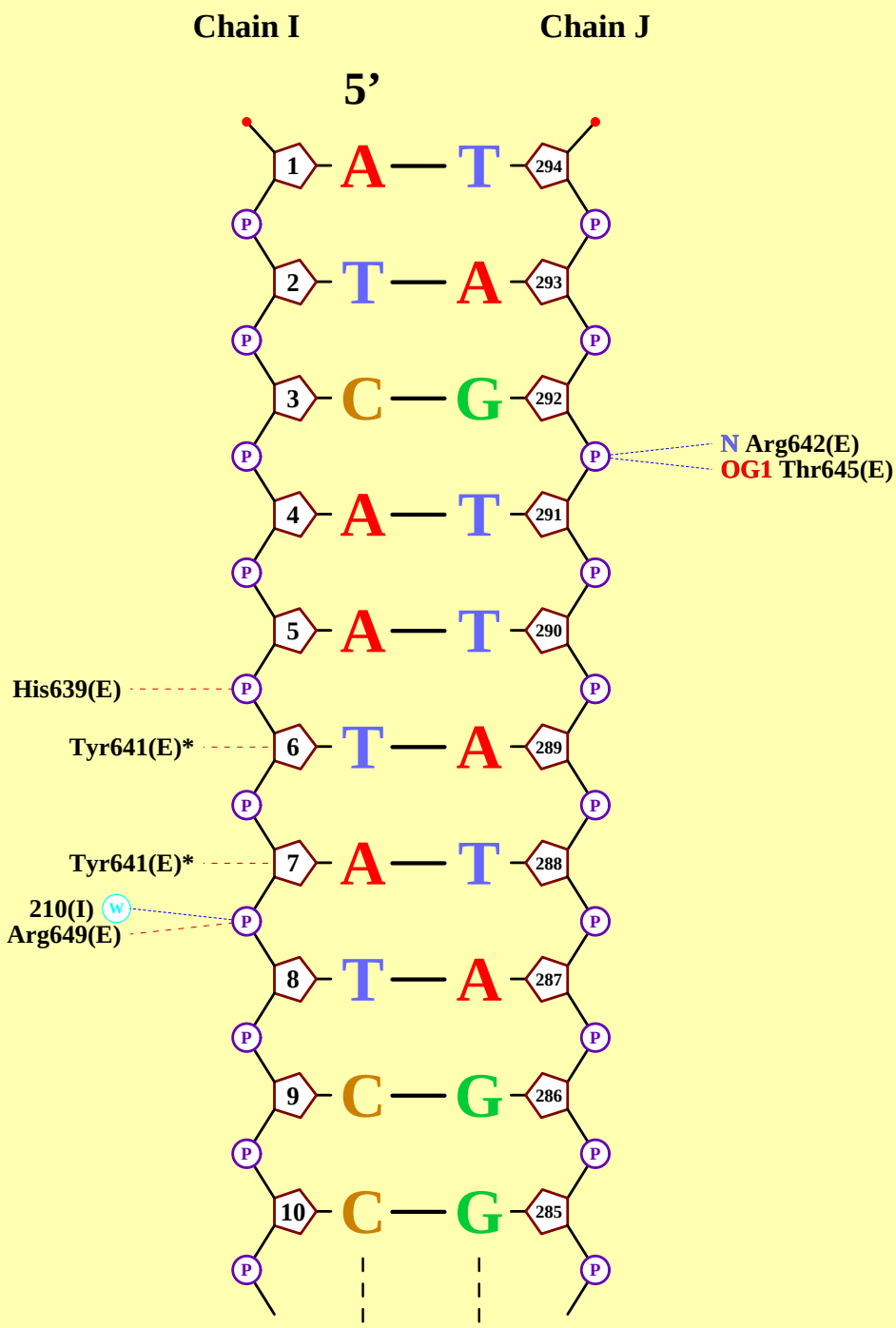


## Key

- 3 — Backbone sugar and base-number
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- Hydrogen bond to DNA
- Nonbonded contact to DNA (< 3.35A)
- 88 W — Water molecule and number

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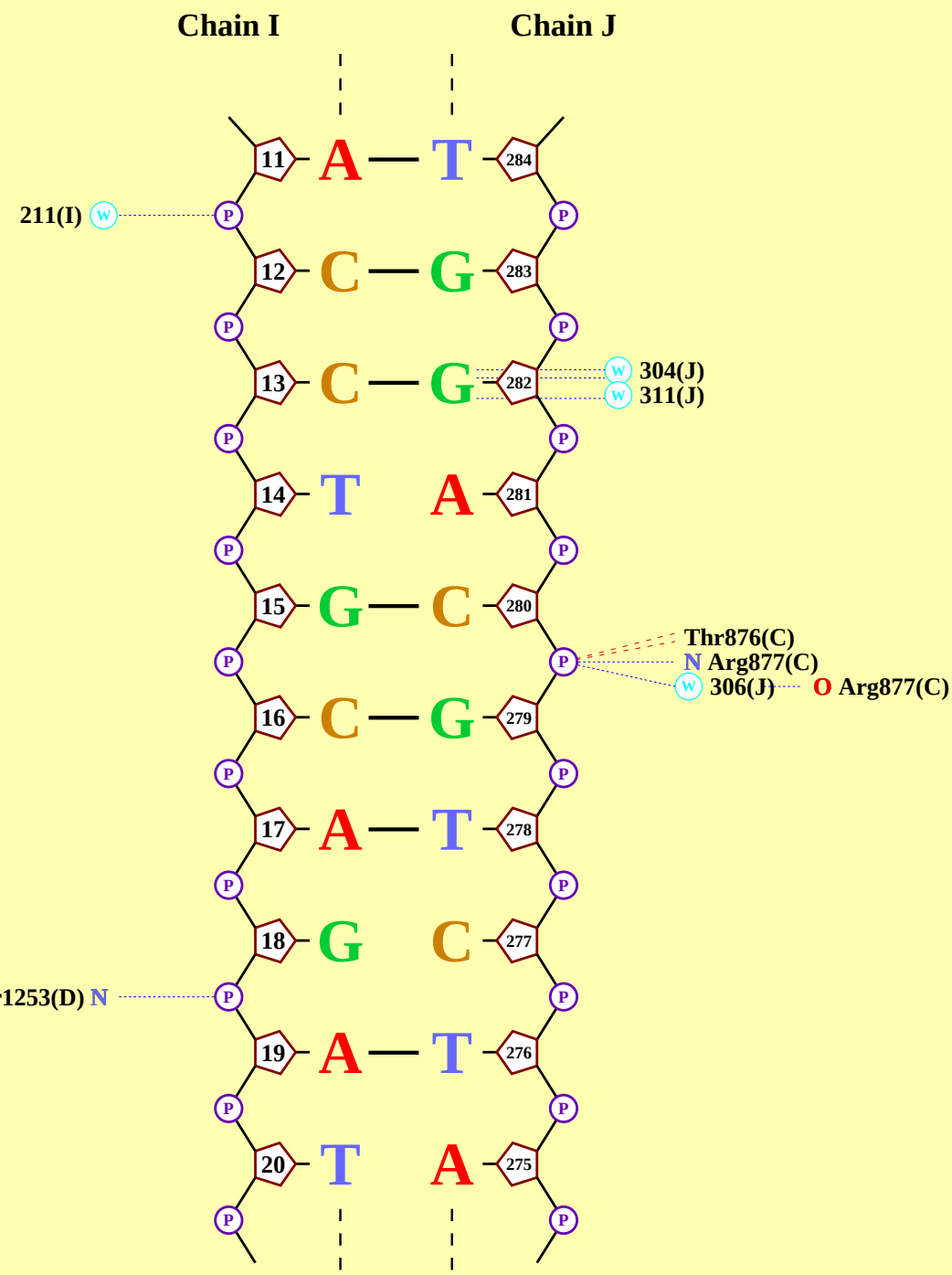


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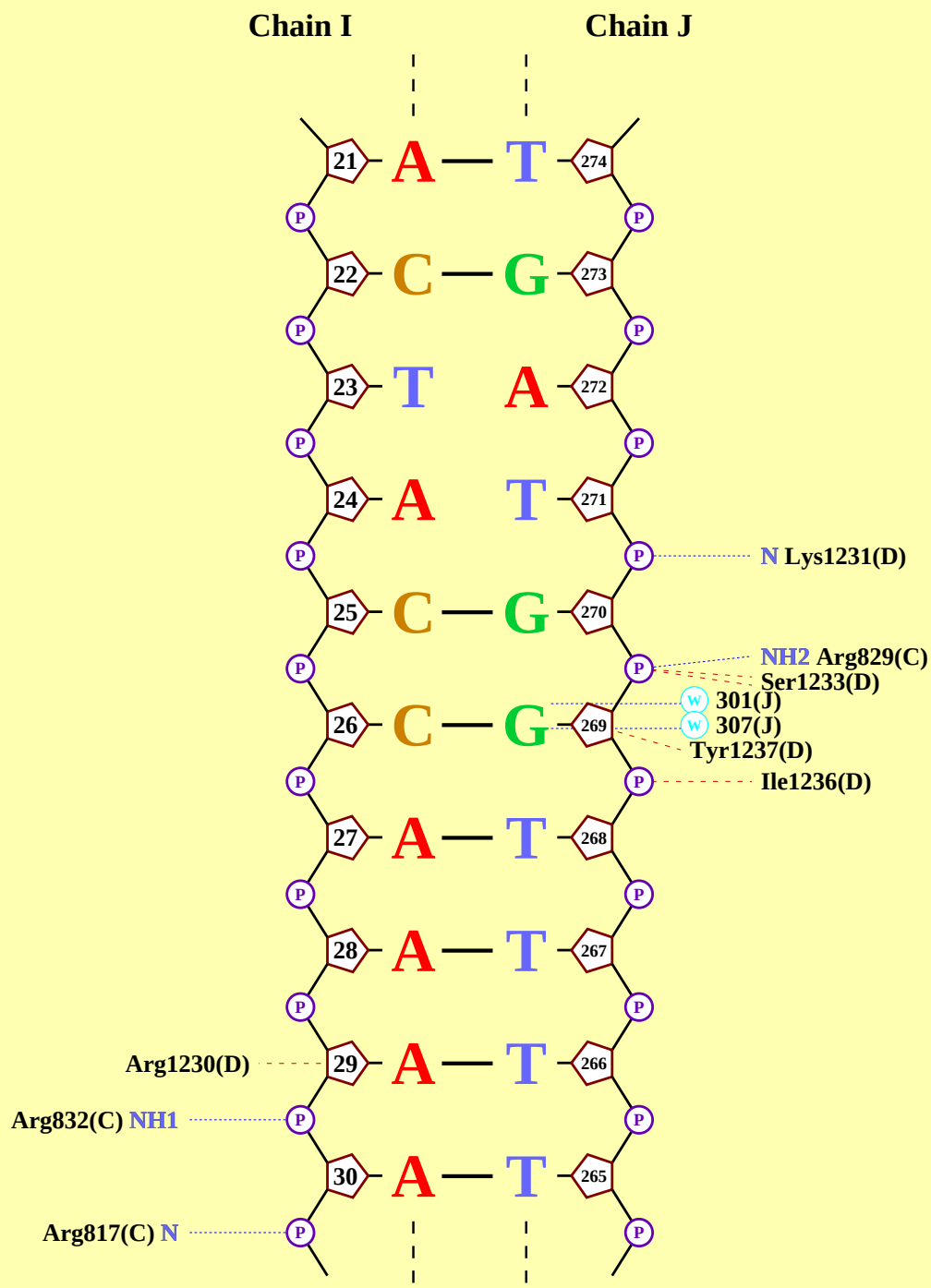


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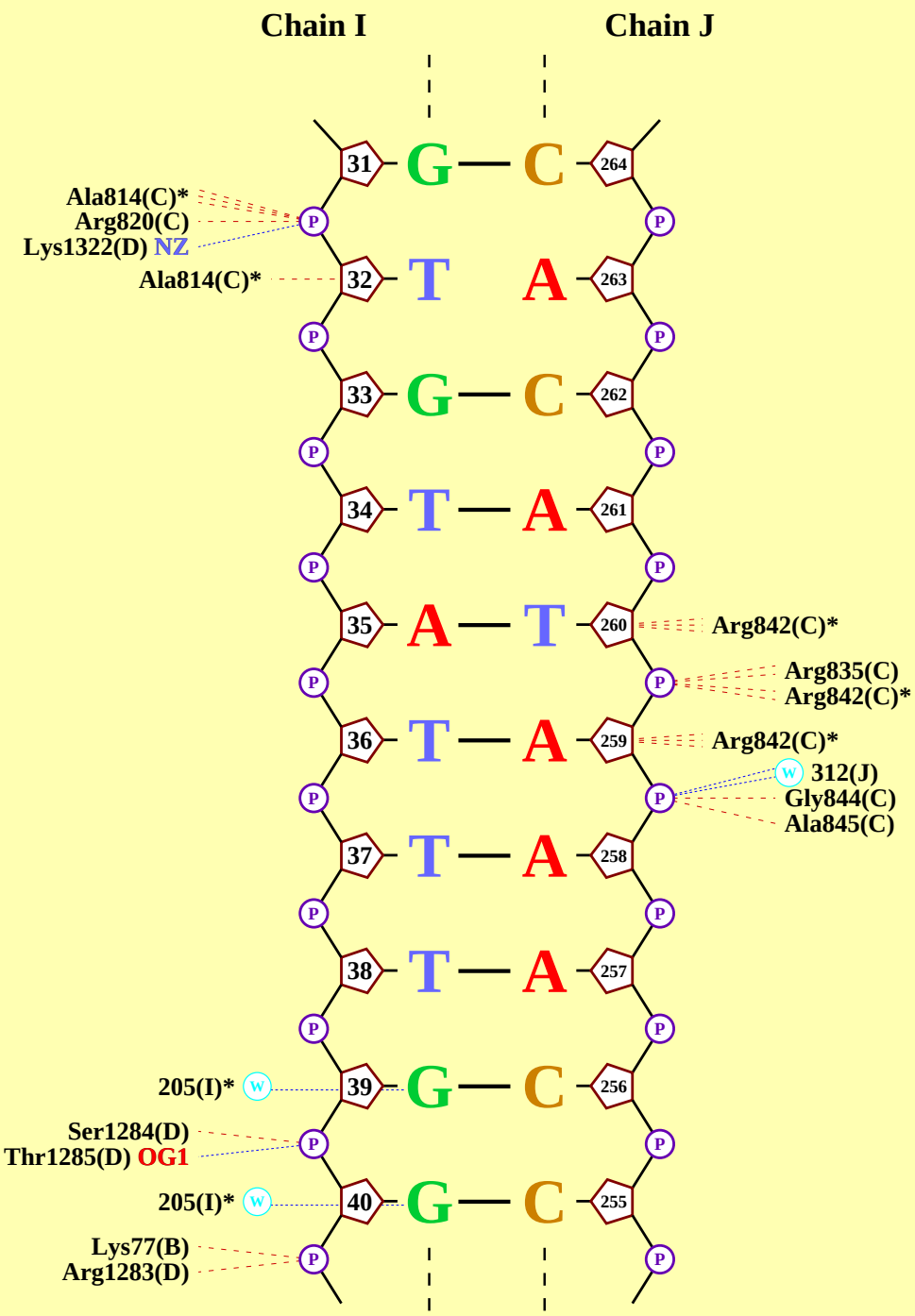


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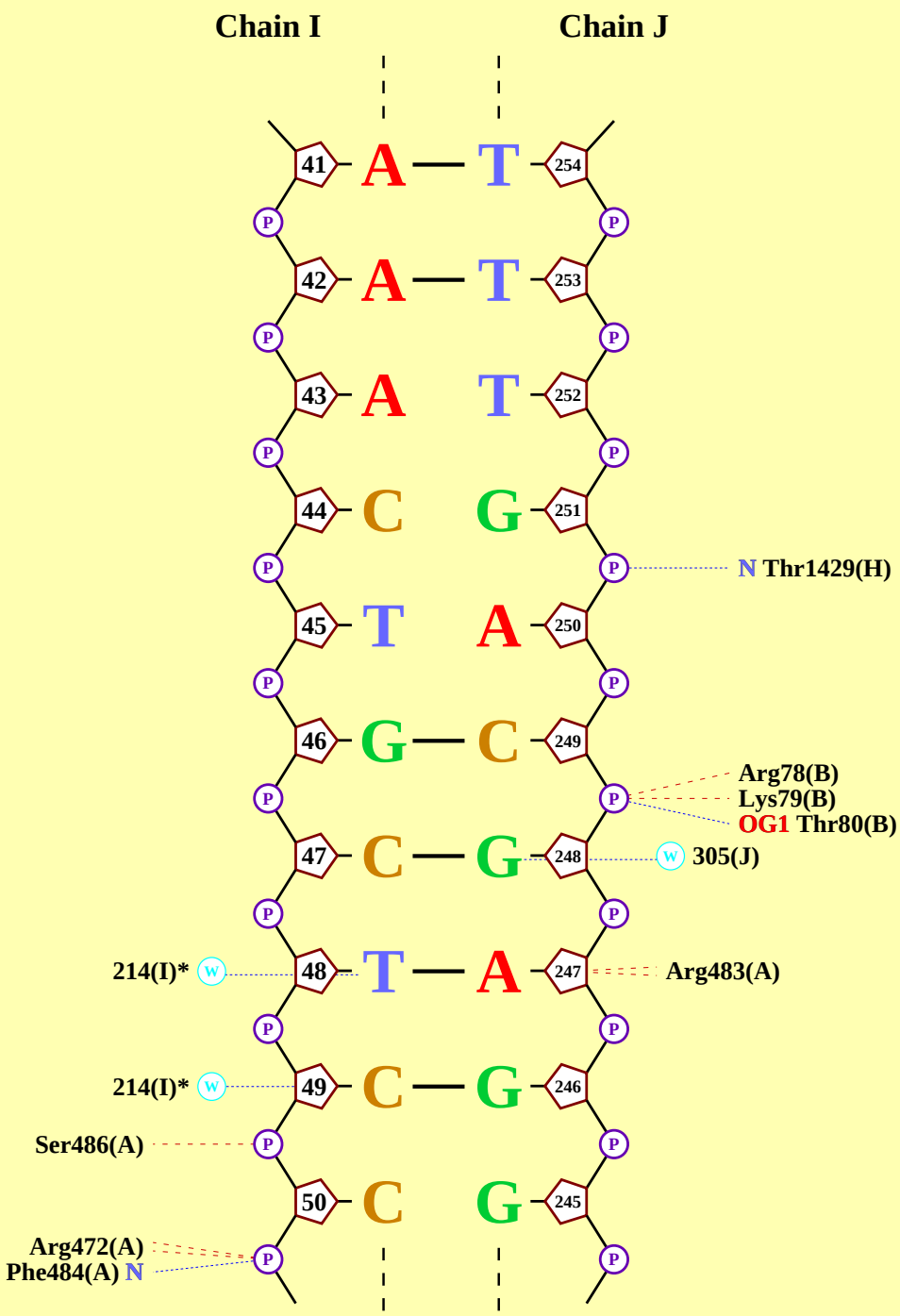


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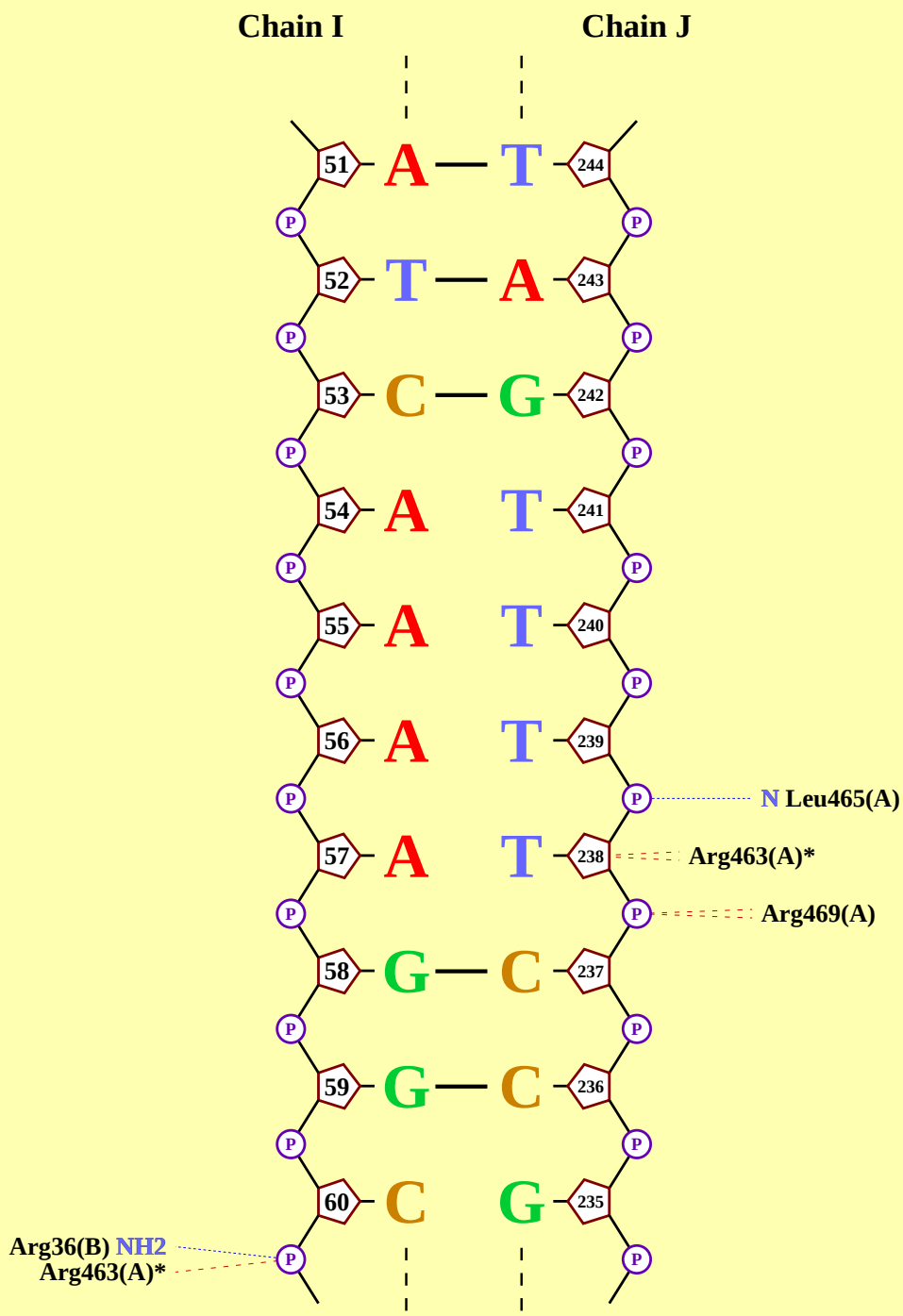


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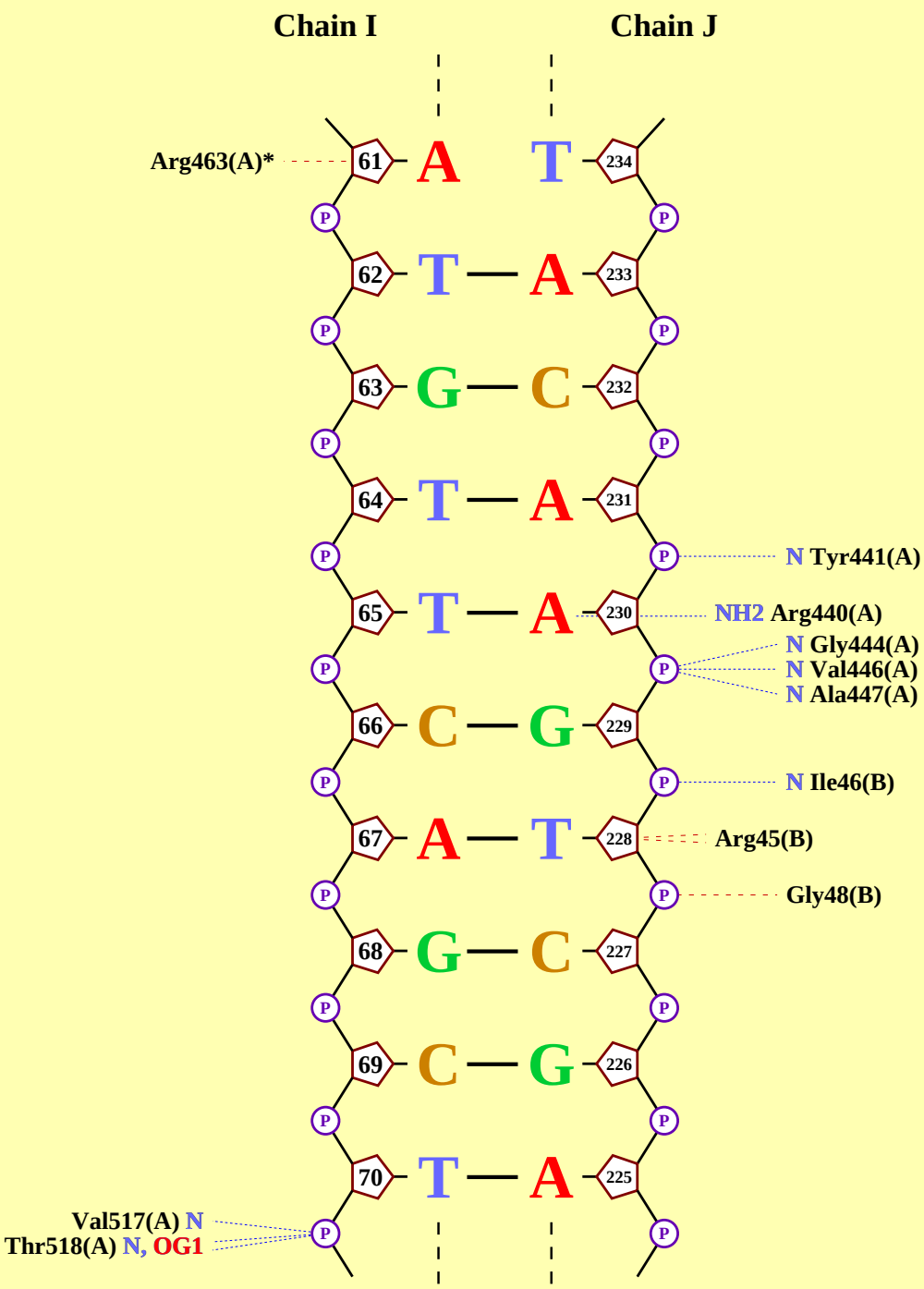


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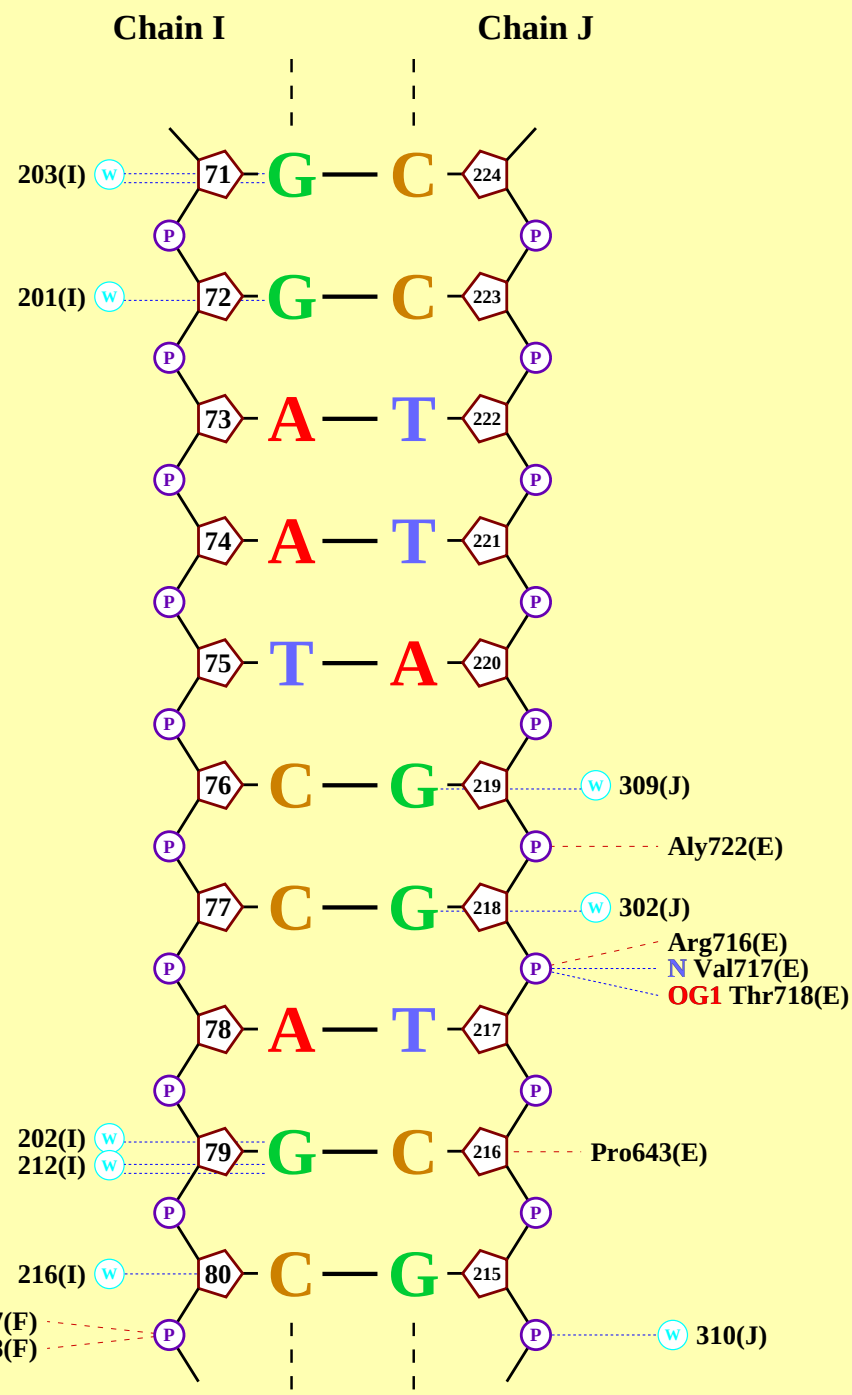


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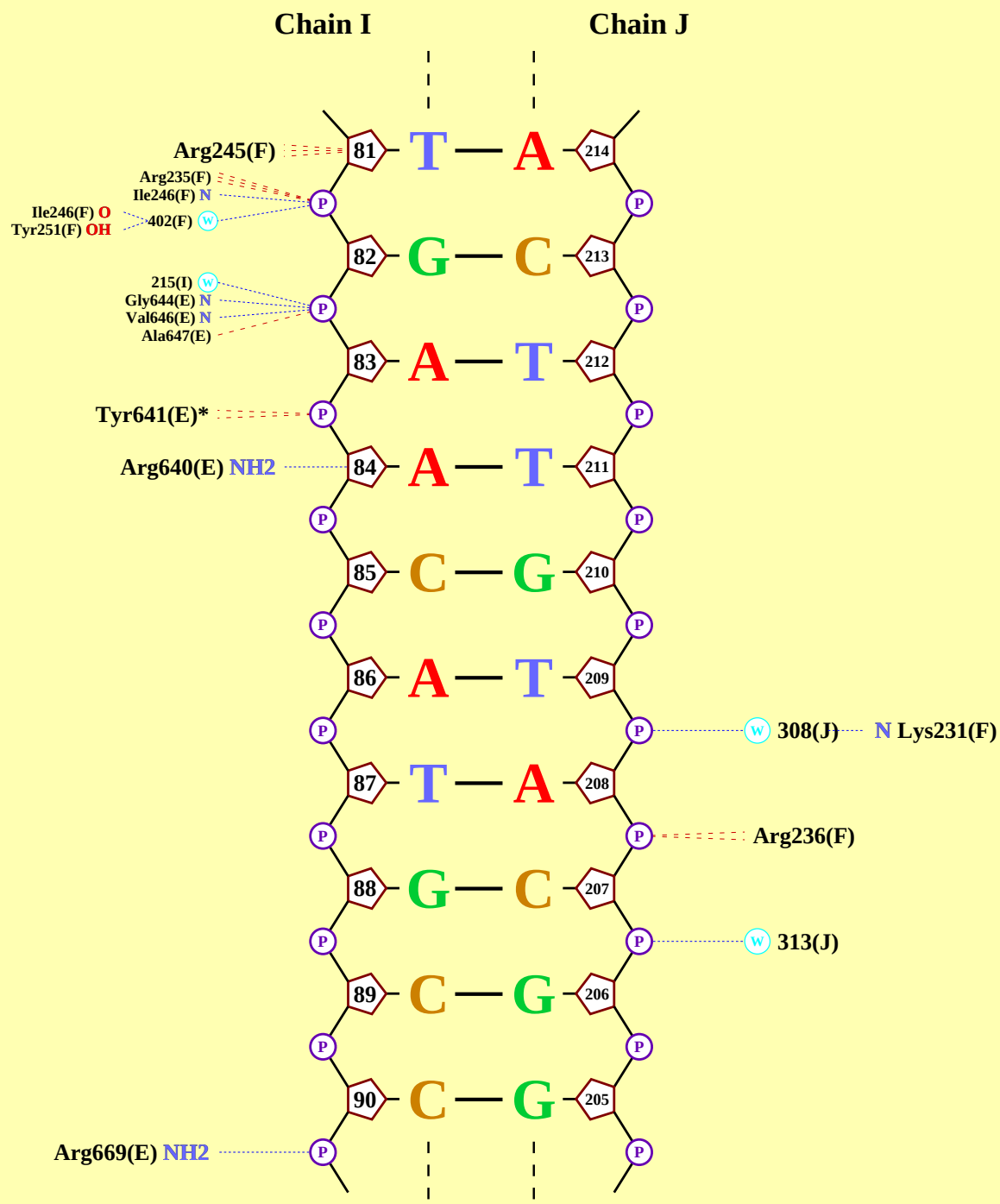


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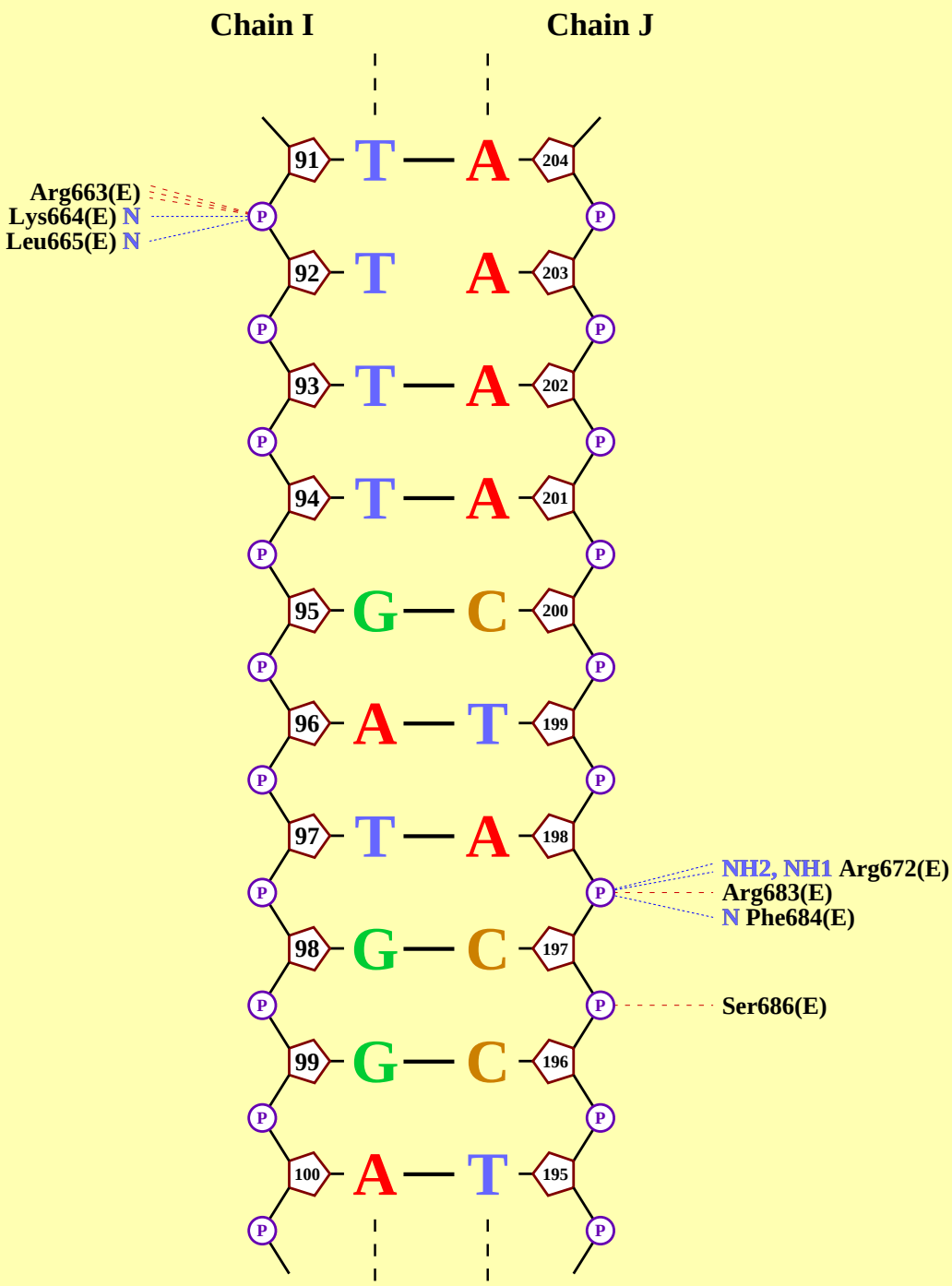


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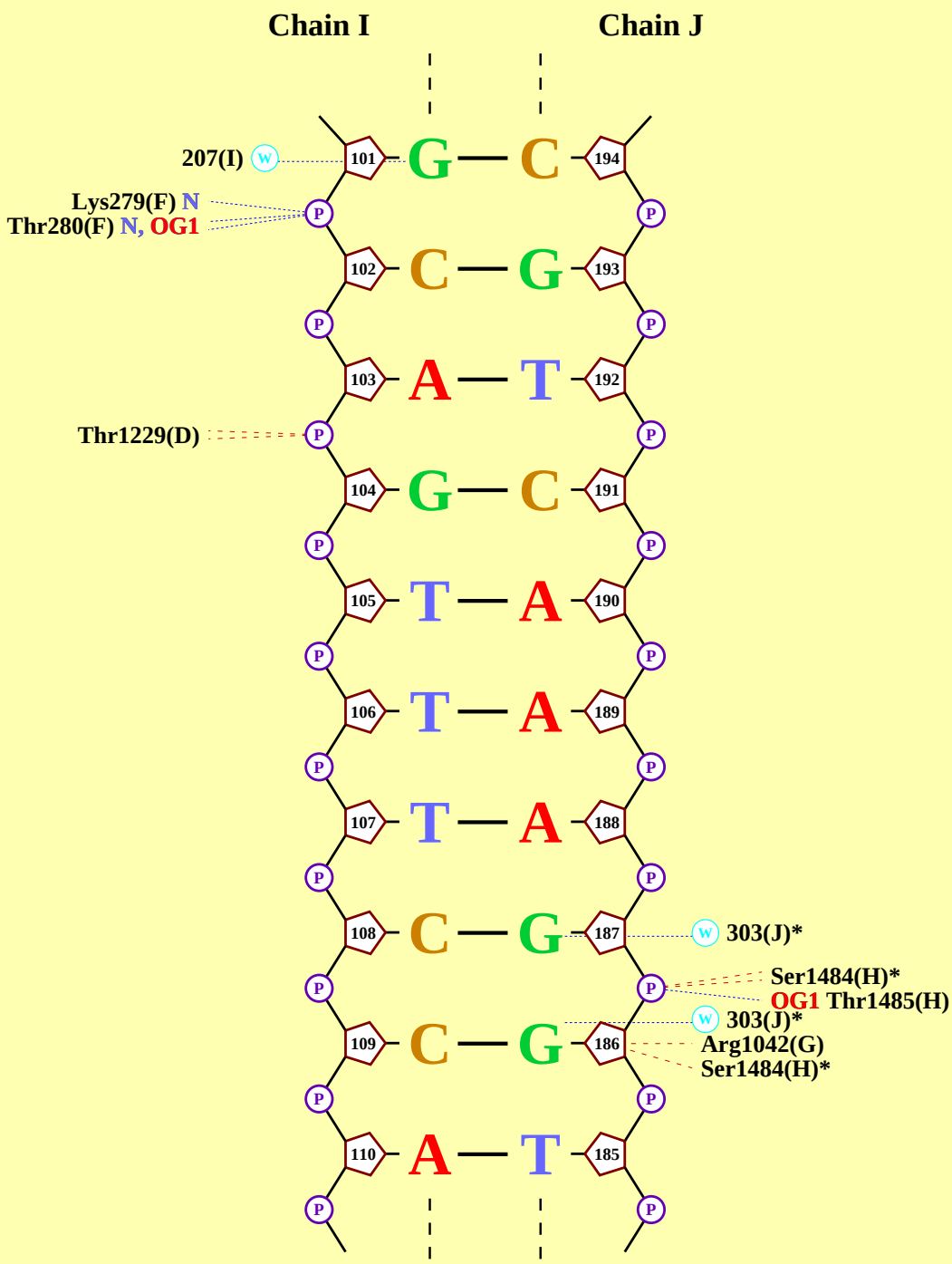


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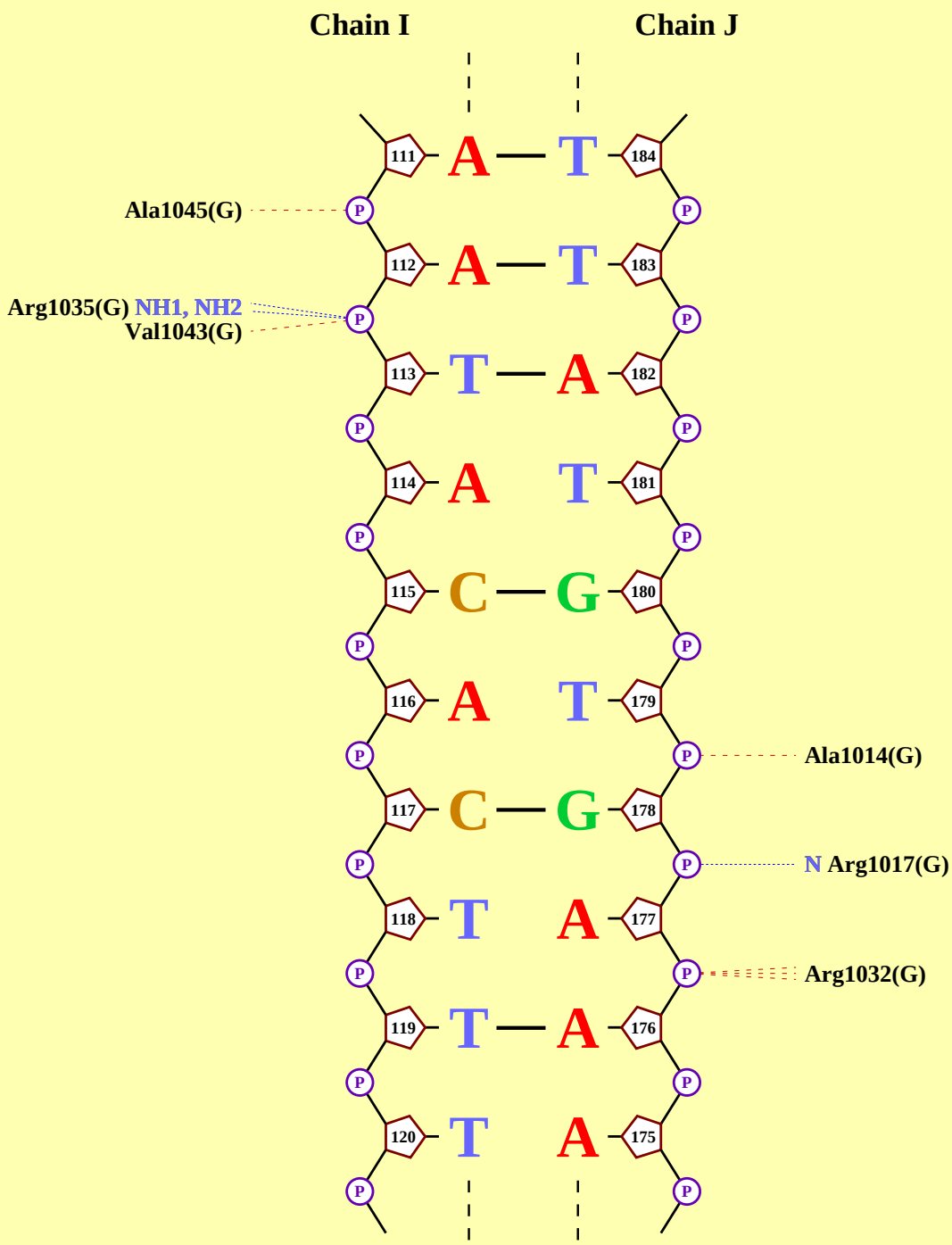


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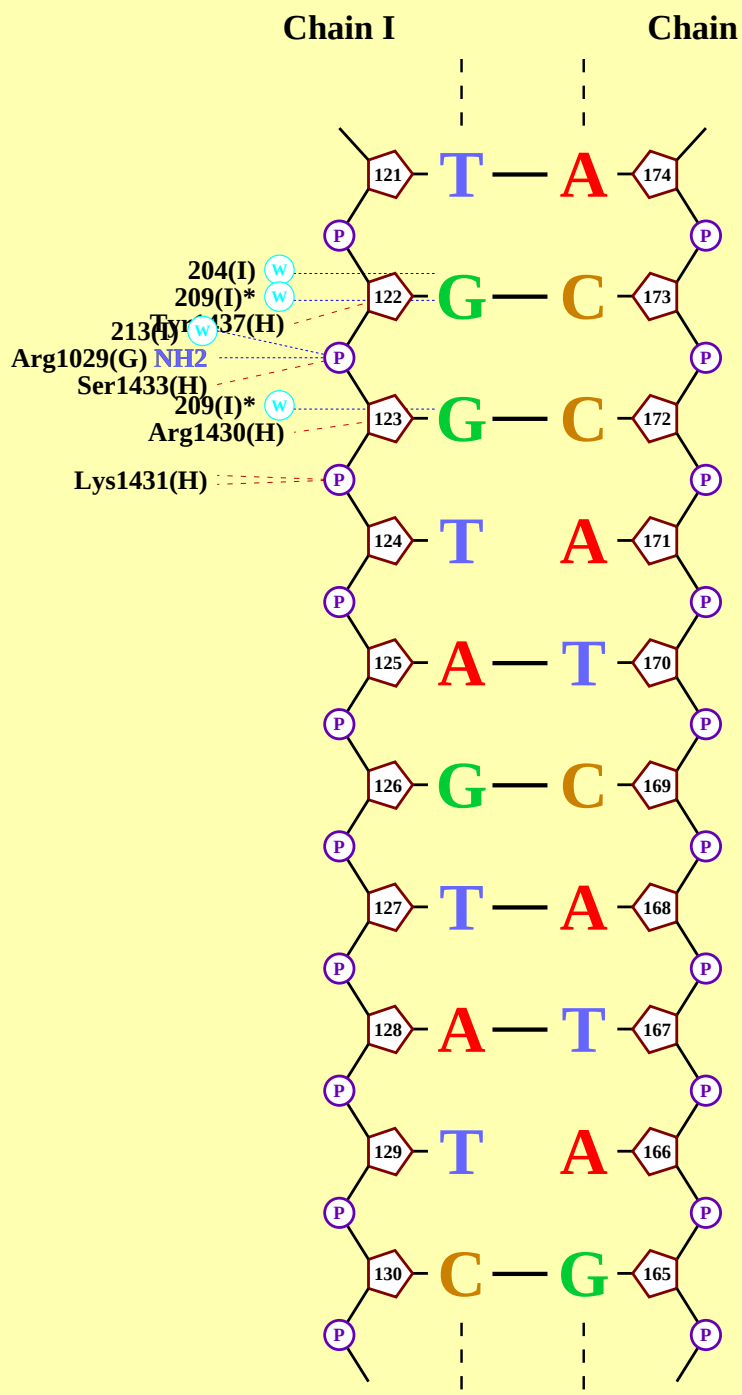


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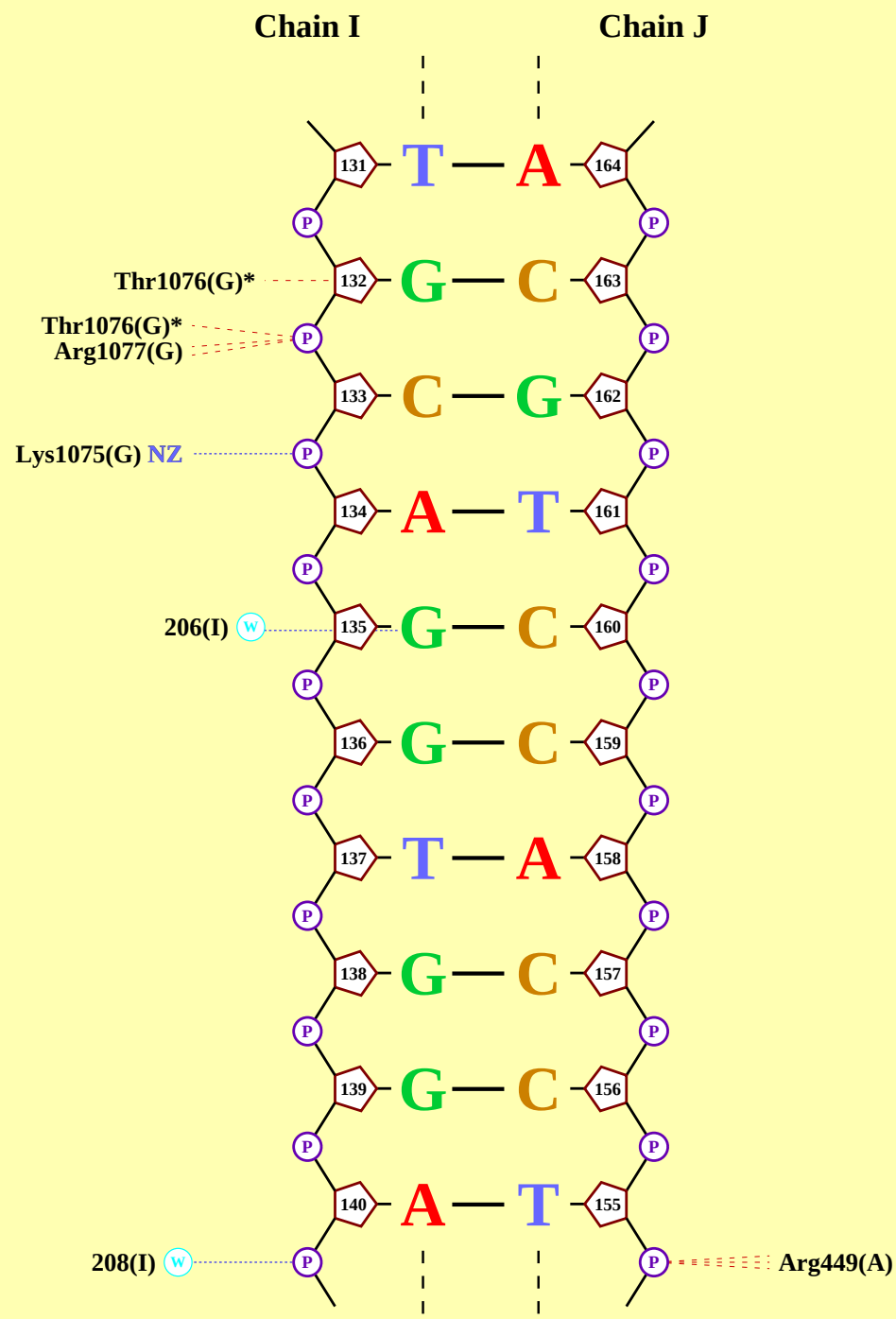


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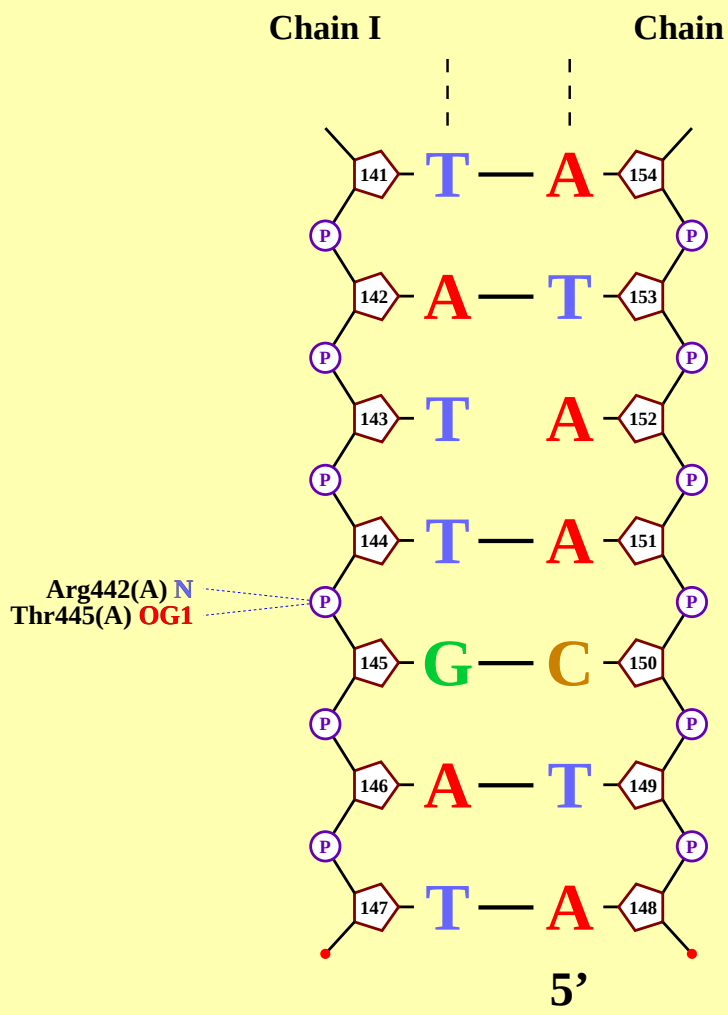


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