CRYSTAL STRUCTURES OF ETHANOLAMINE AMMONIA-LYASE COMPLEXED WITH COENZYME B_{12} ANALOGS AND SUBSTRATES*

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Supplemental Table S1. **Summary of x-ray data collection, phasing and refinement statistics.**

	CN-Cbl/EA		AdePeCbl/EA	CN-Cbl/PA	CN-Cbl (sub.-free)
	Native	Co-SAD	Native	Native	Native
Data collection					
Beamline	BL38B1, SPring-8	BL38B1, SPring-8	BL-17A, Photon Factory	BL38B1, SPring-8	BL41XU, SPring-8
Space group	$P6_3$	$P6_3$	$P6_3$	$P6_3$	$P6_3$
Unit-cell parameters (Å)	$a = b$ = 242.76, c = 76.46	$a = b$ = 242.7, c = 76.6	$a = b$ = 242.73, c = 76.66	$a = b$ = 241.87, c = 76.29	$a = b$ = 244.12, c = 77.15
Wavelength (Å)	1.0000	1.6000	1.0000	1.0000	1.0000
Resolution range (Å)	50–2.10 (2.15–2.10)	50–2.80 (2.90–2.80)	50–2.25 (2.30–2.25)	50–2.05 (2.10–2.05)	50–2.10 (2.15–2.10)
Measured reflections	988,418	236,885	1,150,997	818,215	455,868
Unique reflections	145,836 (9,228)	98,735 (4,540)	120,002 (6,841)	158,931 (10,007)	144,730 (9,260)
Completeness (%)	97.2 (93.1)	79.6 (36.6)	98.3 (85.0)	99.5 (94.6)	94.6 (91.1)
R_{merge}	0.096 (0.413)	0.114 (0.390)	0. 101 (0.516)	0. 079 (0.463)	0.078 (0.299)
Multiplicity	6.8 (6.3)	2.6 (1.3)	9.6 (4.4)	5.2 (3.4)	3.3 (2.6)
$I/\sigma(I)$	17.9 (4.35)	6.91 (1.60)	21.9 (2.47)	18.9 (2.55)	12.7 (3.50)
SAD phasing					
Figure of merit, centric/acentric	-	0.100/0.176	-	-	-
Phasing power	-	0.373	-	-	-

Refinement					
Resolution range (Å)	35–2.10 (2.15–2.10)	-	35–2.30 (2.31–2.25)	35–2.10 (2.10–2.05)	35–2.10 (2.10–2.05)
[a] R_{work}	0.240 (0.251)	-	0.214 (0.281)	0.230 (0.282)	0.248 (0.285)
[b] R_{free}	0.266 (0.292)	-	0.244 (0.314)	0.269 (0.329)	0.285 (0.324)
R.m.s. deviations from ideal values					
Bond lengths (Å)/bond angles (°)	0.013/0.838	-	0.006/1.187	0.003/0.989	0.006/1.169
Ramachandran plot					
Favored (%)	96.8	-	97.0	97.9	97.9
Allowed (%)	99.7	-	99.8	100.0	99.9
Outliers	4	-	3	0	2

[a] $R_{work} = \Sigma_{hkl} \| \| F_{obs} \| - k \| F_{calc} \| \| (\Sigma_{hkl} \| F_{obs} \|)^{-1}$, k : scaling factor

[b] $R_{free} = \Sigma_{hkl} \| \| F_{obs} \| - k \| F_{calc} \| \| (\Sigma_{hkl} \| F_{obs} \|)^{-1}$, where all reflections belong to a test set of randomly selected data.

Values in parentheses are for the outer resolution shell.

SUPPLEMENTARY FIGURE LEGENDS

Fig. S1. Initial electron density maps around the β subunit and CN-Cbl. *A*, SAD phasing only. *B*, MR only. *C*, Combined phases, SAD+MR. A schematic model after refinement is superimposed for each panel.

Fig. S2. Overall structure of diol dehydratase and comparison with EAL.
A, Overall model of diol dehydratase. One αβγ unit is shown in a ribbon model and the other in a surface model. Color codes for each subunit: α subunit, pink/sky blue; β subunit, green/khaki; γ subunit cyan/orange. *B*, Superimposed overall models of EAL (transparent surface model) and diol dehydratase (ribbon model/Cα-trace). The $(\alpha\beta\gamma)_2$ dimer of diol dehydratase and $(\alpha\beta)_6$ hexamer of EAL were superimposed on their α subunit (A chain). The αβγ unit of diol dehydratase that was used for superimposition is shown in a ribbon model and the other in a Cα-trace model. The $(\alpha\beta)_2$ dimer of EAL that was used for superimposition is not shown to clarify the view. *C*, Ribbon presentation of the αβγ unit of diol dehydratase.

Fig. S3. A surface model viewing the solvent-exposed site of the cobalamin molecule of the EAL/AdePeCbl/EA complex. AdePeCbl is shown as a ball-and-stick model. Color codes: pink, α-subunit and cobalamin; green, β-subunit.

Fig. S4. Sigma-A weighted *F*o-*F*c electron density map at the adenine-ring binding site of the EAL/AdePeCbl/EA complex after the first refinement without the AdePe-group contoured at 3 σ level. A schematic of the final model for the AdePeCbl/EA complex is shown.

Fig. S5. Sigma-A weighted *F*o-*F*c electron density maps of EAL contoured at 3 σ level for substrates after the first refinement without substrate. *A*, The CN-Cbl/EA complex. *B*, The CN-Cbl/PA complex.

Fig. S6. The hydrogen bond network around Glnα162.

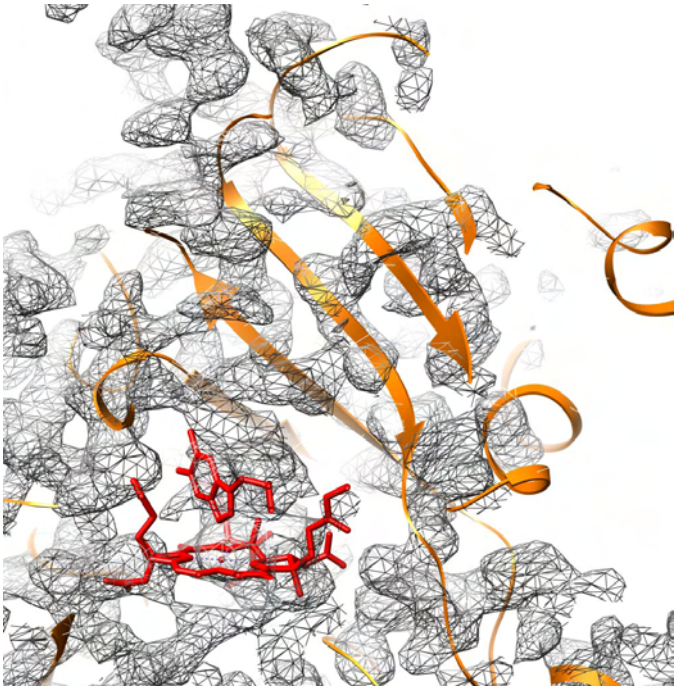


Fig. S1A

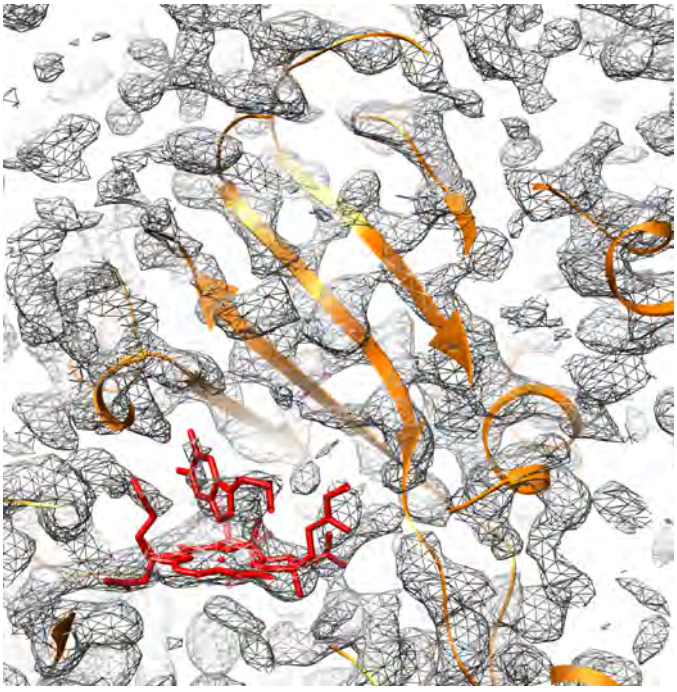


Fig. S1B

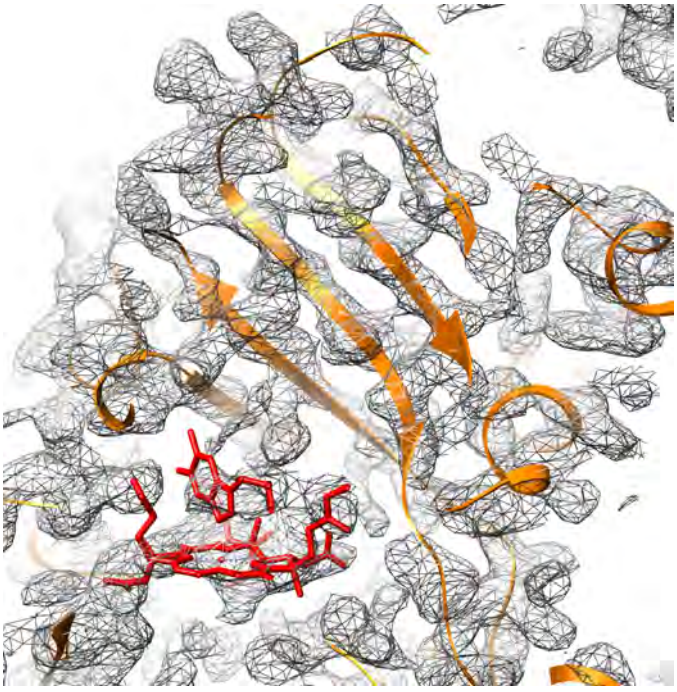


Fig. S1C

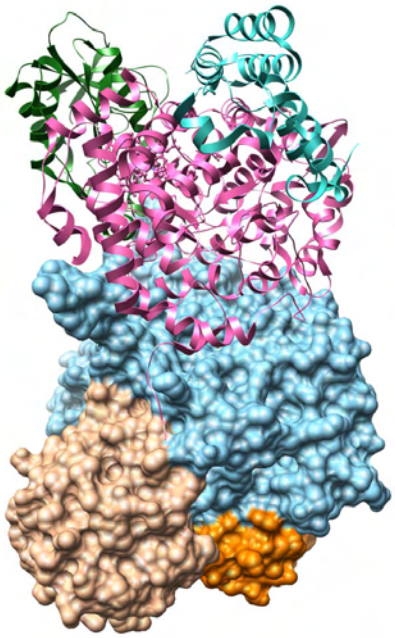


Fig. S2A

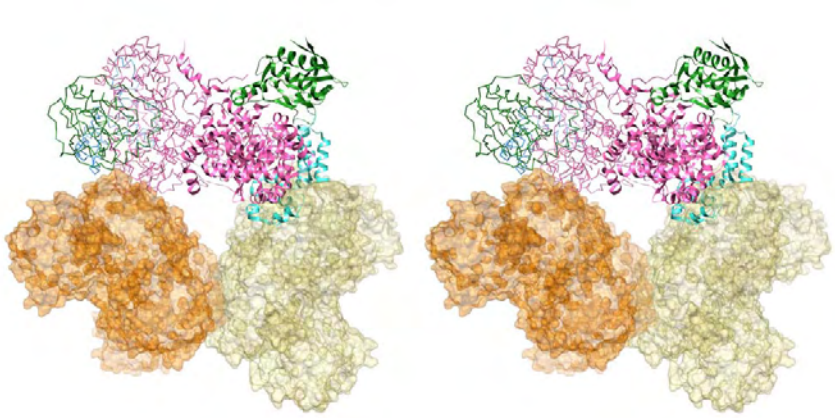


Fig. S2B

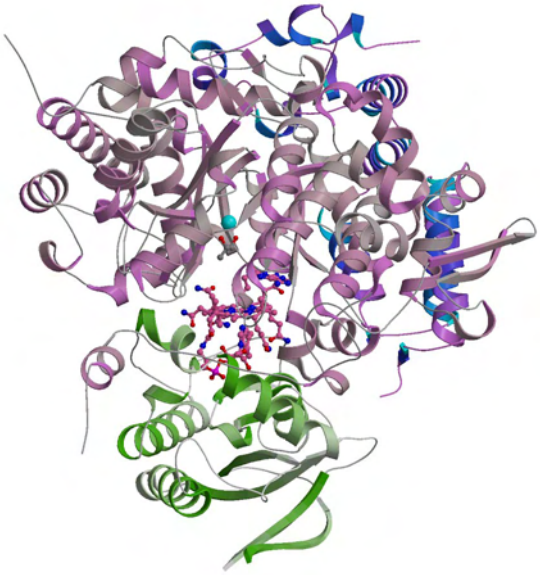


Fig. S2C

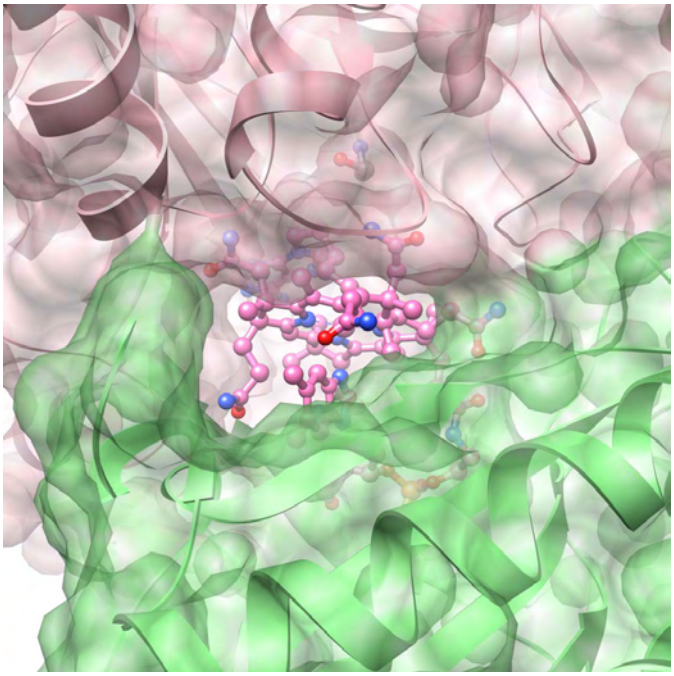


Fig. S3

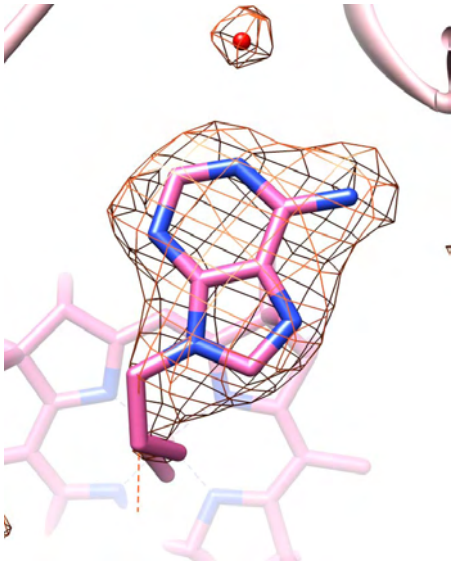
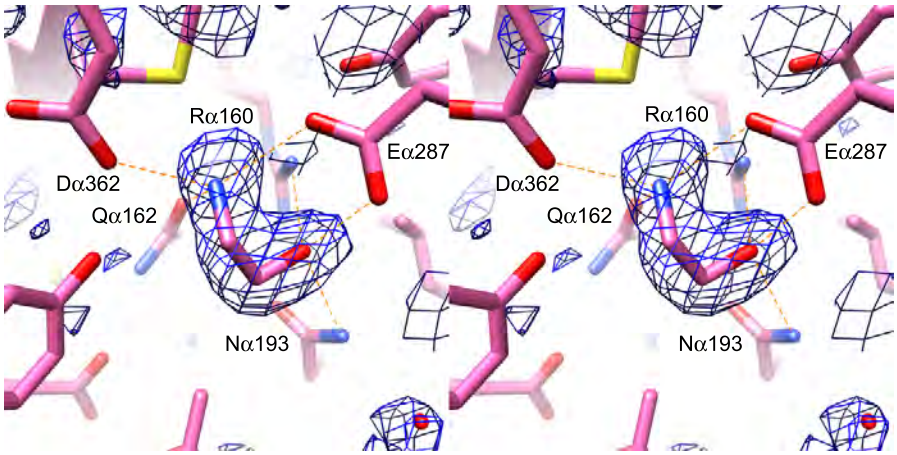


Fig. S4


Rα160
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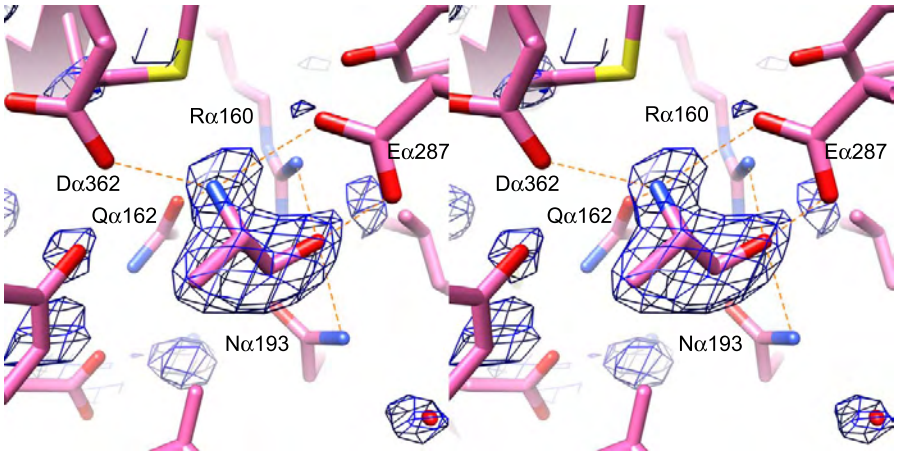
Dα362
Qα162
Nα193
Rα160
Eα287
Dα362
Qα162
Nα193

Fig. S5A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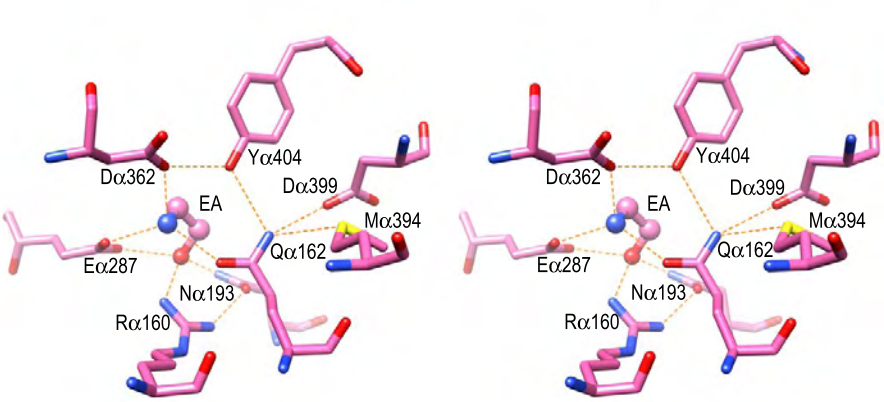
Eα287
Dα362
Qα162
Nα193
Rα160
Eα287
Dα362
Qα162
Nα193

Fig. S5B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Dα362
Dα399
EA
Mα394
Qα162
Eα287
Nα193
Rα160
Yα404
Dα362
Dα399
EA
Mα394
Qα162
Eα287
Nα193
Rα160

Fig. S6