## **Supporting Information**

## Crowe et al. 10.1073/pnas.1717015115

## **Characterization of Metabolites**

**COCHEA-CoA.**  $C_{32}H_{49}N_7O_{20}P_3S^+$  predicted  $[M + H]^+ = 976.1960$ ; electrospray ionization (ESI)-MS:  $[M + H]^+ = 976.1974$  (1.4 ppm from prediction).

 $\lambda_{\text{max}} = 252 \text{nm} (\epsilon_{252} = 17.2 \text{ mM}^{-1} \cdot \text{cm}^{-1})$ 

**MOODA-CoA.**  $C_{30}H_{49}N_7O_{20}P_3S^+$  predicted  $[M + H]^+ = 952.1970$ ; ESI-MS:  $[M + H]^+ = 952.1989$  (2.4 ppm from prediction).

$$\begin{split} \lambda_{max} = & 258 \ nm \left( \epsilon_{258} = 11.9 \ mM^{-1} \cdot cm^{-1} \right, \\ \epsilon_{252} = & 10.4 \ mM^{-1} \cdot cm^{-1} \right) \end{split}$$

<sup>1</sup>H-NMR (600 MHz, D<sub>2</sub>O):  $\delta$ (ppm) = 8.53 (s, 1H), 8.24 (s, 1H), 6.2 (d, 1H), 4.65 (s, 1H), 4.2 (s, 2H), 4.0 (s, 2H), 3.8 (m, 1H), 3.6–3.5 (m, 2H), 3.50 (q, 2H), 3.49 (m, 3H), 3.30–3.45 (m, 4H), 2.95 (q, 2H), 2.83 (m, 1H), 2.73 (m, 1H), 2.68 (m, 1H), 2.58 (q, 2H), 2.3–2.4 (m, 4H), 1.64 (m, 1H), 1.05 (d, 3H), 0.86 (s, 3H), 0.72 (s, 3H).



**Fig. S1.** Additional bioinformatic analysis of IpdAB and CoTs. (A) Conserved ping-pong mechanism of class I CoTs. The species in red represents the glutamyl-CoA intermediate. (*B*) Bioinformatic analysis of IpdAB and homologs. Phylogenetic tree displaying IpdB and β-subunits from class I and II CoTs. Shaded regions indicate gram-positive IpdB (blue), gram-negative IpdB (green), or class I β-keto-CoA (purple), class I (yellow), and class II (gray) CoTs. Proteins displayed are IpdB from *R. jostii* RHA1 (IpdB<sub>RHA1</sub>), *R. equi* (IpdB<sub>Req</sub>; IpdB2<sub>Req</sub>), *M. smegmatis* (IpdB<sub>Msmeg</sub>), *Mtb* (IpdB<sub>Mtbb</sub>), *S. denitrificans* (IpdB<sub>ACG33</sub>), and *C. testosteroni* CN*B*-2 (IpdB<sub>CNB-2</sub>); β-ketoadipyl-CoT from *P. putida* (Pcal); glutaconate CoT from *A. fermentans* (GCT), citrate lyases from *E. aerogenes* (CitC), and *C. argentinense* (CitF); butyrate-acetoacetate CoT from *C. acetobutylicum* (CtfB); acetate CoTs from *E. coli* (ACT and YdiF); succinyl-CoTs from *B. subtillus* (ScoB<sub>Bsub</sub>), *H. pylori* (ScoB<sub>Hpy</sub>), pig heart (SCT); and propionyl-CoT from 100 maximum-likelihood calculations. (*B*) Amino acid alignment of IpdB (C) and IpdA (*D*) from CNB-2, *Mtb*, and RHA1 with well-characterized class I CoTs, YdiF, SCT, GCT, and PcaIJ. Red box indicates location of highly conserved catalytic glutamic acid in class I CoTs (C) or IpdA orthologs (*D*). Blue and green boxes indicate confirmed catalytic residues and CoA binding residues, respectively. Numbering corresponds to residue number in IpdAB<sub>RHA1</sub>.



**Fig. S2.** Characterization of IpdAB. (A) SDS/PAGE showing  $\sim 1 \ \mu g$  of indicated protein. (*B*) SEC-MALS analysis of IpdAB and variants. Shown is the absorbance at 280 nm and the calculated molecular weight by the ASTRA6 software of proteins eluting from a Superdex 200 5/150 column. (*C*) CD spectra of 3  $\mu$ M IpdAB (blue) or variants E105<sup>A</sup>A (green), E105<sup>A</sup>D (black), E58<sup>B</sup>A (red), R126<sup>B</sup>M (purple), and R92<sup>B</sup>M (light blue) in 10 mM sodium phosphate, pH 8.0.

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**Fig. S3.** FadA6 is a  $\beta$ -keto-CoA thiolase. (A) Steady-state kinetic analysis of FadA6 with acetoacetyl-CoA (*Inset*). Initial velocities were determined by monitoring the loss of absorbance at 310 nm due to thiolytic activity of the acetoacetyl-CoA-Mg<sup>2+</sup> enolate in Hepes, pH 7.5, and 10 mM MgCl<sub>2</sub> (I = 0.05 M). (B) Effect on the mole ratio between IpdAB and FadA6 on in vitro turnover of COCHEA-CoA to MOODA-CoA. Curves for A and B indicate best squares least fit of the Michaelis–Menten equation to the data as calculated by Origin. (C) The <sup>1</sup>H-<sup>13</sup>C HMBC NMR spectra of MOODA-CoA (blue) and MOODA (red). Data were collected on a Bruker 600-MHz spectrophotometer using 1 mM MOODA-CoA dissolved in 400  $\mu$ L D<sub>2</sub>O. Shown is the 180–230 ppm region containing the carbonyl carbons identified in the *Inset*.



Fig. 54. Overlay of IpdAB<sub>Mtb</sub> and IpdAB<sub>RHA1</sub>·COCHEA-CoA structures. (A) Superposition of the heterotetramers. (B) Overlay of the respective active sites and orientation of catalytic residues. (C) Conformational differences of the 10-residue loop between  $\beta$ -sheets 6 and 7. Distance measurement is from C<sub>a</sub> of IpdA<sub>Mtb</sub>. Coloring represents IpdA<sub>Mtb</sub> (blues shades), IpdB<sub>Mtb</sub> (orange shades), and IpdAB<sub>RHA1</sub> (gray).



**Fig. S5.** Additional NaBH<sub>4</sub> and <sup>18</sup>O experimental data. (*A*) Intact protein LC-MS of IpdAB<sub>RHA1</sub> treated with sodium borohydride in the presence and absence of COCHEA-CoA. Shown are reconstructed masses. Red boxes indicate the species corresponding to IpdA<sub>RHA1</sub> where an acyl-enzyme intermediate is predicted to be identified as a mass adduct of 760–980 Da. Instrument is accurate to  $\pm 1$  Da. (*B*) Treatment with sodium borohydride did not trap an intermediate. Fifty-microliter samples of IpdAB were incubated for 20 min in the presence of the indicated compounds (10 mM sodium phosphate, pH 8.0) then desalted. The specific activity of each sample was determined in the presence of 50  $\mu$ M COCHEA-CoA, 150  $\mu$ M CoASH, and 4  $\mu$ M FadA6 in 200  $\mu$ L Hepes, 1 mM MgCl<sub>2</sub>, pH 7.5 (*l* = 0.01 M) at 25 °C. Activities are reported relative to the no-treatment control. Bars indicate SD (*n* = 3).

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**Fig. S6.** Isotopic labeling data. LC-MS/MS spectra of MOODA-CoA (*A*) and acetyl-CoA (*B*) produced from 100  $\mu$ M COCHEA-CoA in the presence of 10  $\mu$ M FadA6, 2  $\mu$ M IpdAB, and 125  $\mu$ M CoASH incubated in 10 mM sodium phosphate, pH 8.0, prepared in water (blue) or D<sub>2</sub>O (red). Relative mass intensities are displayed. (*C*) Incubation of 100  $\mu$ M COCHEA-CoA with IpdAB<sub>RHA1</sub> WT (red) or E105A<sup>A</sup> (blue) in the presence of D<sub>2</sub>O as described above. (*D*) Alternate mechanisms of hydrolysis of COCHEA-CoA that are not supported by experimental evidence. (*E*) The <sup>18</sup>O incorporation into COCHEA-CoA. LC- MS mass spectra of 100  $\mu$ M COCHEA-CoA following incubation with 5  $\mu$ M IpdAB (*E*) or (*F*) 2  $\mu$ M IpdAB, 20  $\mu$ M FadA6, and 125  $\mu$ M CoASH in 10 mM sodium phosphate, pH 8.0, prepared in H<sub>2</sub>O or 97% (<sup>18</sup>O abundance) H<sub>2</sub><sup>18</sup>O. Red box indicates mass spectra of MOODA-CoA.

Table S1.	Enzymes	used in	bioint	formatic	analyses
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Enzyme name	Organism	Accession no.	Oligomer	Amino acid length	Refs.
IpdA	RHA1	WP_011597005	α2β2	296	1
IpdB		WP_011597004		253	
IpdA	Mtb	WP_003900094	$\alpha_2\beta_2$	292	1
IpdB		NP 218069		250	
IpdA	MC <sup>2</sup> 155	WP_011730966	$\alpha_2\beta_2$	295	1
IpdB		WP_011730967		249	
IpdA	R. equi	WP_005515561	$\alpha_2\beta_2$	296	2
IpdB		WP_005515563		249	
IpdA	ACG33	WP_066922609	$\alpha_2\beta_2$	291	3
IpdB		WP_066917840		255	
IpdA	CNB2	WP_012837471	$\alpha_2\beta_2$	292	1
IpdB		WP_012837472		256	
IpdA2	R. equi	CBH46238	$\alpha_2\beta_2$	291	2
IpdB2		WP_013414424		252	
GCT <sub>α</sub>	A. fermentans	1POI_A*	$\alpha_2\beta_2$	317	4
GCT <sub>β</sub>		1POI_B*		260	
Pcal	P. putida	AEJ14813	$\alpha_2\beta_2$	276	5
PcaJ		WP_063422683		213	
YdiF	E. coli	2AHV*	α4	531	6
РСТ	C. propionicum	WP_066048121	α4	524	
CitF	C. argentinense	WP_039636687	*	517	
CitC	E. aerogenes	WP_015368306	†	508	7
ACT <sub>α</sub>	E. coli	5DBN_A*	$\alpha_2\beta_2$	221	
ΑCT <sub>β</sub>		5DBN_B*		223	
ScoA	H. pylori	WP_001045174	$\alpha_2\beta_2$	232	
ScoB		WP_015427828		207	
ScoA	B. subtilis	3CDK_A*	$\alpha_2\beta_2$	232	
ScoB		3CDK_B*		207	
CtfA	C. acetobutylicum	WP_010890847	$\alpha_2\beta_2$	218	
CtfB		WP_010890848		221	
SCT	Porcine	30X0*	$\alpha_4$	488	8

\*PDB ID code provided.

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<sup>†</sup>Biological assembly unknown.

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Monetania         09777         09777         09784         154           Workengin         68771         09777         09784         420-160         420-160           Workengin         68721         27752-21         8373         473-440         420-160         420-160           Stee outinum more         68.21         2775-21         833         413-3         410-160         420-160           Stee outinum more         68.871         35.851         55.830         55.91         55.813         57.812         52.93         51.21         52.93         51.21         52.91         55.21         52.91         52.91         52.91         52.91         52.91         55.91<	Data collection and efinement	IpdAB <sub>Mtb</sub> WT (twinned)	IpdAB <sub>Mtb</sub> WT (no twin)	IpdAB <sub>RHA1</sub> WT	IpdAB <sub>RHA1</sub> E105 <sup>A</sup> A·COCHEA-CoA	lpdAB <sub>RHA1</sub> WT-COCHEA-CoA
Control         <	Data collection Wavelength		77770.0	0.97948	0.97874	1.54
Unit caref. A. A. A. A. C. A. S. A. S	Resolution range Spare proup	66.88–2.1 (2.17–2.1) P 2.1	88.86–2.1 (2.17–2.1) P 2.1	48./3-1./0 (1./6-1./0) P 4.2.2	4/.94-1.40 (1.45-1.40) P 4.2.2	48.02-1.60 (1.66-1.60) P 4.2.2
Total reflection: $36,34,37,39$ $37,346,39$ $39,342,930$ $39,342,930$ Total reflection: $38,53,87,570$ $58,54,17,570$ $58,54,17,530$ $38,434,17,530$ $38,44,17,530$ $38,44,17,530$ $38,44,17,530$ $38,44,17,530$ $38,44,17,530$ $38,44,17,530$ $38,44,17,530$ $38,44,17,530$ $38,34,17,530$	Unit cell, Å, Å, Å, °, °, °	66.8779 133.823 118.845	66.8779 133.823 118.845 90	68.91 68.91 241.37	69.17 69.17 241.87	69.29 69.29 241.86
			90.2304 90		90 90 90 210 171 171 210	06 06 06
Molection         38 (15)         38 (15)         38 (15)         10 (10)         17 (16)	l otal reflections I Iniciua raflactions	456,039 (37,871) 119 966 (10 849)	456,641 (37,87) 119 967 (10 850)	(2013) 222,304 65 036 (6 374)	819,431 (75,359) 116 083 (11 331)	831,439 (27,240) 77 704 (6 844)
Memory (s)         98.0 (83.1)         98.0 (83.1)         1.0 (100)         1.0 (100)         1.0 (100)         0.0 (0.8)	Multiplicity	3.8 (3.5)	3.8 (3.5)	8.0 (8.0)	7.1 (6.7)	10.8 (4.0)
Mean biggina ()         11.65 (3.3)         11.65 (3.3)         11.65 (3.3)         11.65 (3.3)         11.65 (3.3)         11.61 (3.3)         20.61 (1.6)         20.61 (1.6)	Completeness, %	98.60 (89.74)	98.60 (89.74)	1.00 (1.00)	1.00 (0.99)	0.99 (0.89)
Wittener         13.30         23.31         23.31         21.51         21.51           Wittener         0.07115 (0.1349)         0.0305 (0.6473)         0.0305 (0.4443)         0.0353 (0.4612)         0.0365 (0.2625)         0.036 (0.273)         1.00 (0.373)         1.00 (0.373)         1.00 (0.373)         1.00 (0.363)           References         5.383 (431)         5.383 (431)         3.311 (3.71)         5.304 (657)         77;596 (623)         0.01610 (0.403)         0.00 (633)         0.00 (6	Mean l/sigma (l)	11.66 (5.33)	11.66 (5.33)	16.54 (2.31)	20.62 (1.53)	31.31 (2.13)
Remere         003/115 (0.1843)         003075 (0.2773)         00363 (0.460)         00363 (0.460)           Remere         00371 (0.1843)         00371 (0.1843)         00371 (0.1736)         00363 (0.461)           CC12         0.995 (0.847)         0.999 (0.861)         0.995 (0.847)         0.0936 (0.847)         1.00 (0.837)           CC13         0.995 (0.847)         0.995 (0.847)         0.995 (0.847)         0.0936 (0.847)         1.00 (0.837)           Referenct         0.995 (0.849)         119 566 (0.830)         119 566 (0.830)         1.10 (0.837)         1.00 (0.837)           Referencts         0.995 (0.849)         1.9366 (0.935)         0.991 (0.937)         3.311 (3.47)         5.504 (567)         3.338 (37)           Referencts         0.472 (0.289)         0.231 (0.2350)         0.116 (0.2766)         0.1856 (0.380)           References         0.472 (0.2891)         0.231 (0.2361)         0.116 (0.2766)         0.1856 (0.350)           References         0.472 (0.2891)         0.231 (0.2362)         0.116 (0.2766)         0.1856 (0.395)           References         0.472 (0.2891)         0.231 (0.2821)         0.116 (0.2766)         0.1856 (0.395)           References         0.471 (0.2357)         0.156 (0.2366)         0.1510 (0.2366)         0.1510 (0.236)	Wilson B-factor	23.30	23.29	18.06	16.09	21.51
Reflections used in 2177)         0.06621 (0.2177)         0.06631 (0.2177)         0.06631 (0.2177)         0.06631 (0.2177)         0.06631 (0.2177)         0.06631 (0.2177)         0.06631 (0.2177)         0.06631 (0.2177)         0.06633 (0.2483)         0.06633 (0.2483)         0.06633 (0.2433)         0.06633 (0.2433)         0.006 (0.2433)         0.00633 (0.2433)         0.006 (0.2433)         0.00633 (0.2433)         0.00633 (0.2433)         0.00633 (0.2433)         0.00633 (0.2433)         0.00633 (0.2433)         0.00633 (0.2433)         0.00633 (0.2433)         0.00633 (0.2433)         0.00633 (0.2433)         0.00633 (0.2433)         0.00633 (0.2433)         0.00633 (0.2433)         0.00160 (0.	R-merge	0.07415 (0.1848)	0.07415 (0.1849)	0.09076 (0.9778)	0.0541 (1.336)	0.0436 (0.4061)
C12         0.995 (0.34)         0.995 (0.34)         0.00 (0.34)         1.00 (0.53.)	R-meas	0.08621 (0.2177)	0.08621 (0.2177)	0.09699 (1.044)	0.05838 (1.448)	0.04563 (0.4612)
Cr         0.999 (0.966)         0.999 (0.966)         0.999 (0.966)         1.00 (0.37)         1.00 (0.37)         1.00 (0.37)           Reflections used in         119.965 (10.849)         119.965 (10.849)         119.965 (10.849)         1.00 (0.37)         1.00 (0.37)         1.00 (0.37)           Reflections used in         119.965 (10.849)         119.965 (10.849)         1.919.66 (10.849)         3.311 (1.917)         7.799 (6.823)           Reflections used for         5.983 (493)         5.983 (493)         0.371 (0.235)         0.156 (0.256)         0.151 (0.235)         0.150 (0.405)           Reflection used for         0.985 (0.807)         0.271 (0.2351)         0.161 (0.2257)         0.156 (0.266)         0.150 (0.405)           Row         0.0172         0.271 (0.2351)         0.1916 (0.2266)         0.156 (0.260)         0.501 (0.310)         0.371 (0.311)         0.371 (0.310)           Row         0.0172         0.833 (0.822)         0.271 (0.2311)         0.971 (0.310)         0.936 (0.80)           Row         0.017         0.0173         0.383 (0.822)         0.931 (0.911)         0.971 (0.716)         0.946 (0.800)           Row         0.017         0.0173         0.383 (0.822)         0.931 (0.911)         0.971 (0.911)         0.971 (0.910)           Row         0	CC1/2	0.995 (0.944)	0.995 (0.945)	0.999 (0.818)	1.00 (0.624)	1.00 (0.934)
entiment         inspect (0.840)         inspect (0.840)         inspect (0.340)         inspect (0.340) <thinspect (0.340)<="" th="">         inspect (0.340)         <thinspect (0.340)<="" th="">         inspect (0.340)<td>* CC*</td><td>0.999 (0.986)</td><td>0.999 (0.986)</td><td>1.00 (0.949)</td><td>1.00 (0.877)</td><td>1.00 (0.983)</td></thinspect></thinspect>	* CC*	0.999 (0.986)	0.999 (0.986)	1.00 (0.949)	1.00 (0.877)	1.00 (0.983)
Reflections used in refinement         119-965 (0.849)         116-97 (11-321)         117-90 (0.4059)         116-97 (0.4059)         0.1510 (0.4059)         0.1510 (0.4059)         0.1510 (0.4059)         0.1510 (0.4059)         0.1561 (0.4059)         0.1561 (0.2568)         0.1561 (0.4059)         0.1561 (0.4059)         0.1561 (0.4059)         0.1561 (0.4059)         0.1561 (0.4059)         0.1561 (0.4059)         0.1561 (0.4059)         0.1561 (0.4059)         0.1561 (0.4059)         0.1561 (0.4059)         0.1561 (0.4059)         0.1561 (0.4059)         0.1561 (0.4059)         0.1560 (0.4059)         0.1560 (0.4059)         0.1560 (0.4059)         0.1560 (0.4059)         0.1560 (0.4059)         0.1560 (0.4059)         0.1560 (0.4059)         0.1560 (0.4059)         0.1560 (0.4059)         0.1560 (0.4059)         0.1560 (0.4059)	Ketinement					
Reflections used for Reflections for Reflections used for Reflections	Reflections used in refinement	119,965 (10,849)	119,966 (10,850)	65,021 (6,374)	116,047 (11,327)	77,599 (6,823)
Reference of the formation of the	Reflections used for	5 983 (493)	5 983 (203)	3 311 (347)	5 804 (567)	3 838 (357)
Rvork         0.1462 (0.2567)         0.2411 (0.2351)         0.1611 (0.2257)         0.1504 (0.2756)         0.1610 (0.4059)           Rviree         0.172 (0.2801)         0.2741 (0.2802)         0.2711 (0.2166)         0.1586 (0.3093)         0.37186 (0.3395)           Rviree         0.172 (0.2801)         0.857 (0.709)         0.853 (0.802)         0.971 (0.776)         0.1616 (0.4059)           CC(revic)         0.857 (0.709)         0.853 (0.802)         0.871 (0.776)         0.973 (0.903)           CC(revic)         0.857 (0.709)         0.853 (0.802)         0.971 (0.776)         0.974 (0.800)           No <of nonhydrogen<="" td="">         17,607         17,607         0.714 (0.2766)         0.1610 (0.4059)           No<of nonhydrogen<="" td="">         17,607         0.853 (0.822)         0.951 (0.776)         0.954 (0.800)           No<of nonhydrogen<="" td="">         17,607         1,7607         1,4148         4,714           Macronolecules         16612         1,6612         1,4148         4,714           No<of nonhydrogen<="" td="">         2,164         2,164         2,164         2,164           Romachadian         1,677         1,493         78         78         78           Romachadian         3,77         3,82         57         97         97</of></of></of></of>	R-free					
Rfree         0.1772 (0.2891)         0.2741 (0.2867)         0.196 (0.2566)         0.1866 (0.3955)           C(work)         0.855 (0.807)         0.861 (0.822)         0.971 (0.911)         0.971 (0.766)         0.1886 (0.3955)           C(twork)         0.855 (0.807)         0.853 (0.822)         0.957 (0.911)         0.971 (0.776)         0.997 (0.780)           C(twork)         0.855 (0.807)         0.853 (0.822)         0.957 (0.913)         0.971 (0.776)         0.954 (0.80)           No of nonhydrogen         17,607         17,607         17,607         4,700         5.014         4,874           Natomolecules         16/1         16/12         16,612         16,612         0.4138         0.971 (0.716)         0.954 (0.800)           Natomolecules         16/1         0.013         0.006         0.006         0.006         0.006           Natomolecules         16/7         1.49         7.8         7.8         7.8         7.8           Protein residues         1.67         1.49         0.13         0.035         9.7         8.7           Ranchandran         0.71         0.71         0.71         0.71         9.7         9.7           Ranchandran         0.28         0.78         0.78         0.8<	R-work	0.1462 (0.2567)	0.2411 (0.2351)	0.1611 (0.2257)	0.1504 (0.2756)	0.1610 (0.4059)
CC(work)         0.855 (0.807)         0.861 (0.822)         0.971 (0.911)         0.973 (0.830)         0.973 (0.933)	R-free	0.1772 (0.2891)	0.2741 (0.2867)	0.1916 (0.2508)	0.1716 (0.2766)	0.1886 (0.3955)
Cc(free)         0.857 (0.709)         0.853 (0.682)         0.962 (0.893)         0.971 (0.776)         0.964 (0.800)           No. of nonlydrogen         17,607         17,607         4,700         5,014         4,814           No. of nonlydrogen         17,607         17,607         4,700         5,014         4,814           No. of nonlydrogen         17,607         17,607         17,607         4,700         5,014         4,814           Nacromolecules         16,612         16,612         16,612         4,148         4,215         4,814           Nacromolecules         2,164         2,164         5,51         5,43         5,43         5,43           RNS bords, C         0.0017         0.0114         0.013         0.022         0.93         5,93           RNS bords, C         0.0017         0.013         0.0164         5,93         5,13         5,	CC(work)	0.856 (0.807)	0.861 (0.822)	0.971 (0.911)	0.978 (0.830)	0.973 (0.903)
No. of nonlydrogen         17,607         17,607         17,607         4,700         5,014         4,874           atoms         16,612         16,612         16,612         4,148         4,215         4,183           atoms         16,612         16,612         16,612         4,148         4,215         4,183           Ligands         955         955         957         79         78         78         78           Protein residues         0.017         0.013         0.006         0.006         0.006         0.006         0.006           RMS shords, A         0.017         0.013         0.006         0.017         0.017	CC(free)	0.857 (0.709)	0.853 (0.682)	0.962 (0.893)	0.971 (0.776)	0.964 (0.880)
atomsatomatomsatomMaconolecules16,61216,6124,1484,2154,183Naconolecules9599579787878Ugands95595599579787878Rotein residues2,1642,1645,115,43543542RNS bonds, Å0.0170.0130.0060.0060.0060.006RNS angles1.671.490.830,979798Ranachandran95.9595.959797989798Ranachandran0.280.2300000Ranachandran0.280.23000000Ranachandran0.280.230000000Ranachandran0.281.2300.2300000Ranachandran0.281.2300.2300000Ranachandran0.281.2300.230.230.450.230.450.23Ranachandran0.191.230.230.230.230.230.230.450.23Ranachandran0.282.5022.5332.352.42.42.70Macroneleules81.991.232.352.42.42.13Rotener82.532.42.132.62	No. of nonhydrogen	17,607	17,607	4,700	5,014	4,874
Macromolecules         16,612         16,612         16,612         4,148         4,215         4,183           Ligands         995         995         79         78         78         78           Ligands         2,164         5,51         5,31         5,33         5,43         5,43           RNS bonds, A         0,017         0,013         0,066         0,006         0,006         0,005           RNS bonds, A         0,017         1,49         0,013         0,73         5,4         95           Rns bonds, A         0,017         1,49         0,83         0,92         0,93         5,4           Rnanchandran         3,77         3,82         3         2,5         2,4         95           Ranchandran         0,28         0,23         0,23         0,7         9         2,4           Ranchandran         0,28         0,23         0,0         0         0         0         0           Ranchandran         0,28         0,23         0,23         0,23         0,23         0,23           Ranchandran         0,28         0,23         0,23         0,23         0,23         0,23           Ranchandran         0,28	atoms					
Ligands         995         79         78         78           Protein residues         2.164         2.164         5.3         5.3         5.3         5.4           RNS bonds, Å         0.017         0.013         0.006         0.00         0.00         0.00         0.00         0.00         0.00         0.00         0.00         0.00         0.00         0.00	Macromolecules	16,612	16,612	4,148	4,215	4,183
Protein residues         2,164         2,164         551         543         542           RNS bonds, Å         0.017         0.013         0.006         0.006         0.006         0.006         0.006         0.006         0.006         0.006         0.006         0.006         0.006         0.005         0.005         0.005         0.005         0.005         0.005         0.005         0.006         0.00         0         0	Ligands	995	995	79	78	78
RMS bonds, Å         0.017         0.013         0.006	Protein residues	2,164	2,164	551	543	542
RMS angles,*         1.67         1.49         0.83         0.92         0.93         0.93           Ramachandran         95.95         95.95         97         97         98         97         98           Ramachandran         3.77         3.82         3.82         3         2.5         2.4           Ramachandran         3.77         3.82         3.82         3         2.5         2.4           Ramachandran         0.28         0.23         0 <td>RMS bonds, Å</td> <td>0.017</td> <td>0.013</td> <td>0.006</td> <td>0.006</td> <td>0.006</td>	RMS bonds, Å	0.017	0.013	0.006	0.006	0.006
Ramachandran         95.95         97         97         97         98           favored, %         3.77         3.82         3         2.5         2.4           favored, %         3.77         3.82         3         2.5         2.4           Ranachandran         3.77         3.82         3         2.5         2.4           allowed, %         0.28         0.23         0         0         0         0           outliers, %         1.99         1.23         0.23         0.45         0.23         0.23           Rotamer outliers, %         1.99         1.23         0.23         0.45         0.23         0.23           Average B-factor, Å <sup>2</sup> 2.13         2.35         1.56         2.13         3.23           Average B-factor, Å <sup>2</sup> 25.82         25.02         21.3         27.0           Macromolecules         25.82         25.02         21.3         22.0         24.3           Ligands         1.56         30.35         31.7         40.4         39.6           Solvent         30.76         0         N         N         19         18	RMS angles, °	1.67	1.49	0.83	0.92	0.93
Tavored, % and the data $3.71$ $3.82$ $3.2$ $3.2$ $2.4$ Ramachandran $3.71$ $3.82$ $3.82$ $3.25$ $2.4$ allowed, % and the dran $0.28$ $0.23$ $0$ $0$ $0$ Ramachandran $0.28$ $0.23$ $0.23$ $0$ $0$ Ramachandran $0.28$ $0.23$ $0.23$ $0.23$ $0.23$ Routilers, % outilers, % $1.99$ $1.23$ $0.23$ $0.45$ $0.23$ Rotante values $2.13$ $2.35$ $2.13$ $2.01$ $3.23$ Average B-factor, Å <sup>2</sup> $2.532$ $25.02$ $21.3$ $22.0$ $24.3$ Macromolecules $2.532$ $21.3$ $25.4$ $27.0$ Macromolecules $30.76$ $30.35$ $71.7$ $66.3$ $71.9$ Solvent $30.76$ $N$ $N$ $19$ $18$ $18$	Ramachandran	95.95	95.95	97	97	98
Ramachandran $3.77$ $3.82$ $3$ $2.5$ $2.4$ allowed, % $3.77$ $0.28$ $0.23$ $0$ $0$ $0$ Ramachandran $0.28$ $0.23$ $0.23$ $0$ $0$ $0$ Ramachandran $0.28$ $0.23$ $0.23$ $0.45$ $0.23$ $0.23$ Rotamer outliers, % $1.99$ $1.23$ $0.23$ $0.45$ $0.23$ $0.23$ Rotamer outliers, % $1.99$ $1.23$ $0.23$ $0.45$ $0.23$ $0.23$ Rotamer outliers, % $2.13$ $2.35$ $2.35$ $2.01$ $3.23$ Average B-factor, Å <sup>2</sup> $2.13$ $2.35$ $2.13$ $2.01$ $3.23$ Average B-factor, Å <sup>2</sup> $2.5.82$ $2.5.02$ $2.13$ $2.01$ $3.23$ Average B-factor, Å <sup>2</sup> $2.5.82$ $2.5.02$ $2.13$ $2.01$ $3.23$ Average B-factor, Å <sup>2</sup> $2.5.82$ $2.5.02$ $2.13$ $2.13$ $2.01$ $3.23$ Igends $0.76$ $30.35$ $3.5.7$ $40.4$ $39.6$ No. of TLS groupsNANANANA1918	tavored, %					
	Ramachandran allowed %	3.77	3.82	£	2.5	2.4
Outliers, $\%$ 0.230.450.23Notame outliers, $\%$ 1.991.230.230.450.23Rotame outliers, $\%$ 2.132.351.562.013.23Rotame outliers, $\%$ 2.132.351.562.013.23Average B-factor, $\AA^2$ 26.1025.3323.62.7024.3Average B-factor, $\AA^2$ 25.8225.0221.322.024.3Macromolecules2.58225.0271.766.371.9Solvent30.7630.3535.740.439.6No. of TLS groupsNA191818	Ramachandran	0.28	0.23	c	c	c
Rotamer outliers, %         1.99         1.23         0.23         0.45         0.23           Clash score         2.13         2.35         1.56         2.01         3.23           Clash score         2.13         2.35         1.56         2.01         3.23           Average B-factor, Å <sup>2</sup> 26.10         25.33         23.6         25.4         27.0           Average B-factor, Å <sup>2</sup> 25.82         25.02         21.3         22.0         24.3         27.0           Macromolecules         25.82         25.02         21.3         22.0         24.3         27.0         24.3         27.0         24.3         27.0         24.3         27.0         24.3         27.0         24.3         27.0         24.3         27.0         24.3         27.0         24.3         27.0         24.3         27.0         24.3         27.0         24.3         27.0         24.3         27.0         27.0         24.3         27.0 <td< td=""><td>outliers. %</td><td>0</td><td></td><td>,</td><td>)</td><td>•</td></td<>	outliers. %	0		,	)	•
Clash score       2.13       2.35       1.56       2.01       3.23         Average B-factor, Å <sup>2</sup> 26.10       25.33       23.6       25.4       27.0         Average B-factor, Å <sup>2</sup> 25.82       25.33       23.6       25.4       27.0         Macromolecules       25.82       25.02       71.7       66.3       71.9         Ligands       30.76       30.35       35.7       40.4       39.6         No. of TLS groups       NA       NA       19       18       18	Rotamer outliers. %	1.99	1.23	0.23	0.45	0.23
Clash sole     2.13     2.33     2.33     2.31     2.01     3.23       Average B-factor, Å <sup>2</sup> 26.10     25.33     23.6     25.4     27.0       Average B-factor, Å <sup>2</sup> 26.10     25.33     23.6     25.4     27.0       Macromolecules     25.82     25.02     21.3     22.0     24.3       Igands     71.7     66.3     71.9       Solvent     30.76     30.35     35.7     40.4     39.6       No. of TLS groups     NA     19     18     18		67 C	3 25	2.EC		5715 CC C
Macromolecules         25.82         25.02         21.3         22.0         24.3           Macromolecules         25.82         25.02         21.3         22.0         24.3           Ligands         71.7         66.3         71.9         56.3         71.9           Solvent         30.76         30.35         35.7         40.4         39.6           No. of TLS groups         NA         19         18         18	Averade R-factor Å <sup>2</sup>	26.10	25.33	23.6	25.4	0.75
Ligands 24.0 2.00 2.00 2.00 2.00 2.00 2.00 2.00	Marromoloculor	75.87		c f c	0 0 0	
Desired         30.76         30.35         35.7         40.4         39.6           Solvent         No. of TLS groups         NA         19         18         18	ligands	20.02	20.02	C.12 7 1 7	5.2.2 66.3	2.4.2 71 0
Solvent 30.7b 30.55 33.7 40.4 39.6 No. of TLS groups NA 19 18 18	rigando C-linet					
No. of ILS groups NA NA 19 18 18	Solvent	30.76	c5.05	7.65	40.4	39.6
	No. of TLS groups	NA	NA	19	18	18
		-		-		

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Translation/Libration/Screw.