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RELEASE DATE

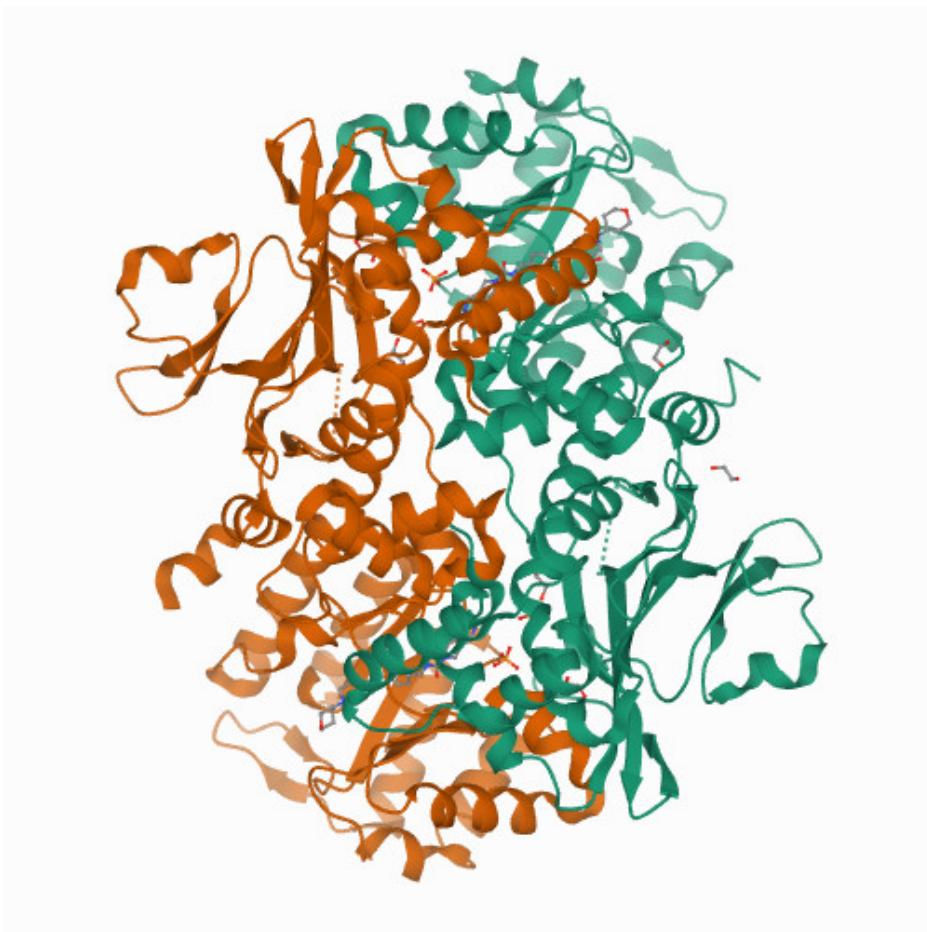
- 2005 - 2009 (17)
- 2010 - 2014 (36)
- 2015 - 2019 (17)
- 2020 - 2024 (3)

ENZYME CLASSIFICATION
NAME

- Transferases (73)

SYMMETRY TYPE

- Cyclic (73)
- Asymmetric (2)



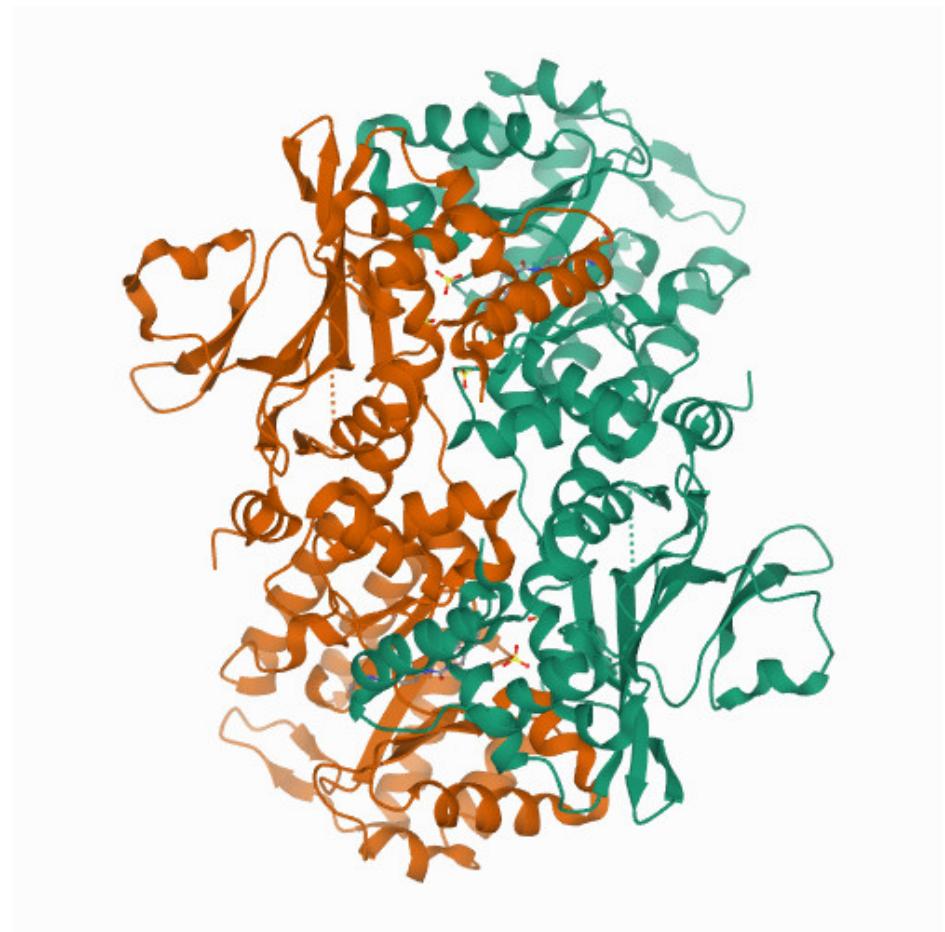
4KFP

Identification of 2,3-dihydro-1H-pyrrolo[3,4-c]pyridine-derived Ureas as Potent Inhibitors of Human Nicotinamide Phosphoribosyltransferase (NAMPT)

Dragovich, P.S., Bair, K.W., Baumeister, T., Ho, Y., Liederer, B.M., Liu, X., O'Brien, T., Oeh, J., Sampath, D., Skelton, N., Wang, L., Wang, W., Wu, H., Xiao, Y., Yuen, P., Zak, M., Zhang, L., Zheng, X.

(2013) Bioorg Med Chem Lett **23**: 4875-4885

Released	2013-08-14
Method	X-RAY DIFFRACTION 1.84 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	1R7, EDO, PO4

[3D View](#)[Download File](#) [View File](#)

5U2M

Crystal structure of human NAMPT with A-1293201

Longenecker, K.L., Raich, D., Korepanova, A.V.

(2017) Mol Cancer Ther **16**: 1236-1245

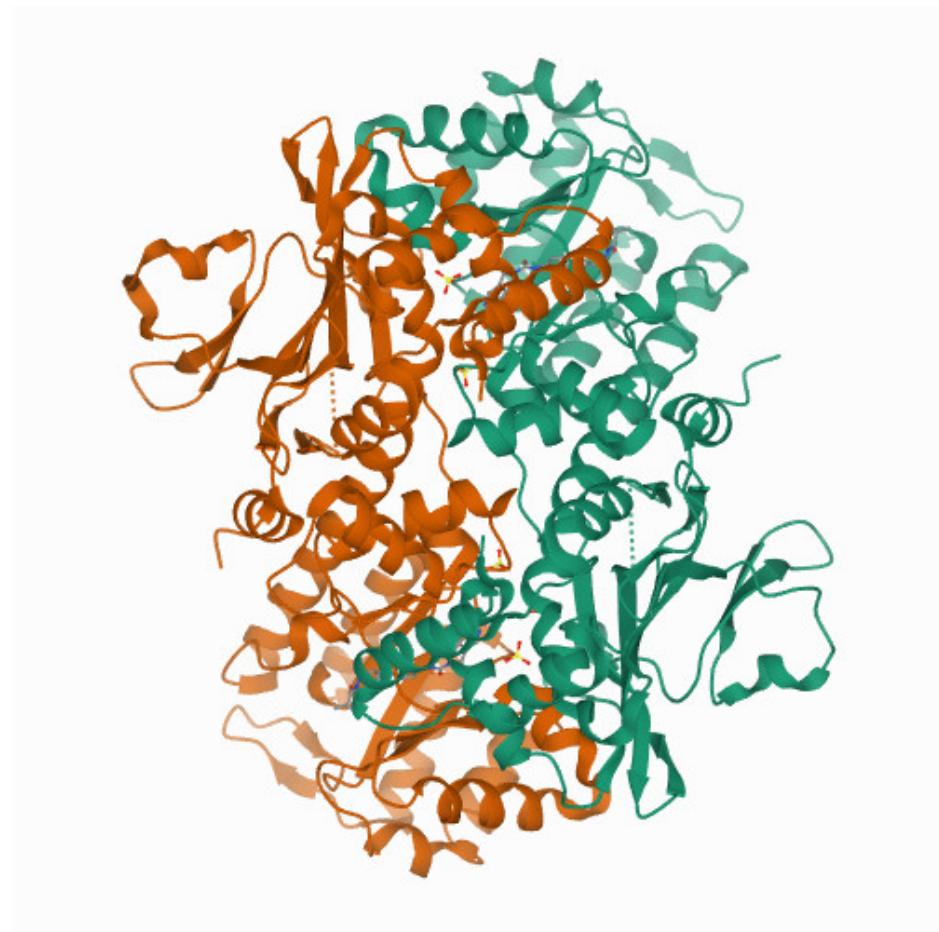
Released 2017-06-28

Method X-RAY DIFFRACTION 1.89 Å

Organisms Homo sapiens

Macromolecule Nicotinamide phosphoribosyltransferase (protein)

Unique Ligands 7T7, SO4

[3D View](#)[Download File](#) [View File](#)

5U2N

Crystal structure of human NAMPT with A-1326133

Longenecker, K.L., Raich, D., Korepanova, A.V.

(2017) Mol Cancer Ther **16**: 1236-1245

Released

2017-06-28

Method

X-RAY DIFFRACTION 1.73 Å

Organisms

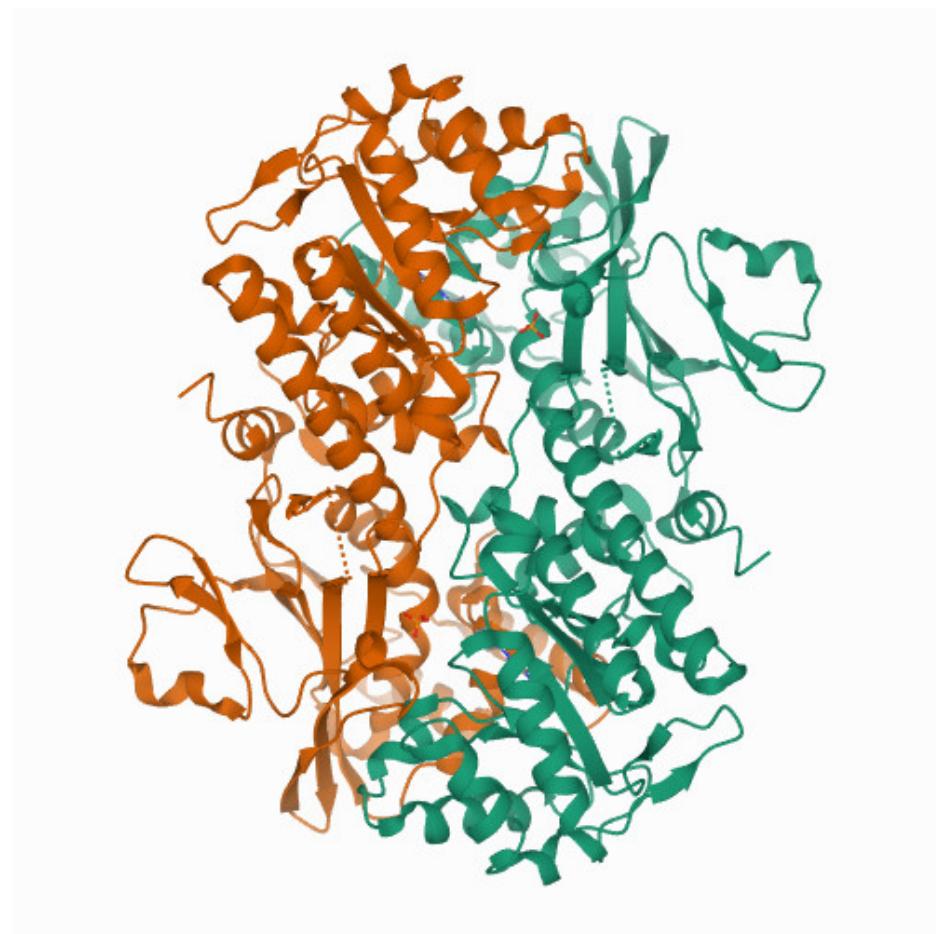
Homo sapiens

Macromolecule

Nicotinamide phosphoribosyltransferase (protein)

Unique Ligands

7TA, SO4

[3D View](#)

4N9B

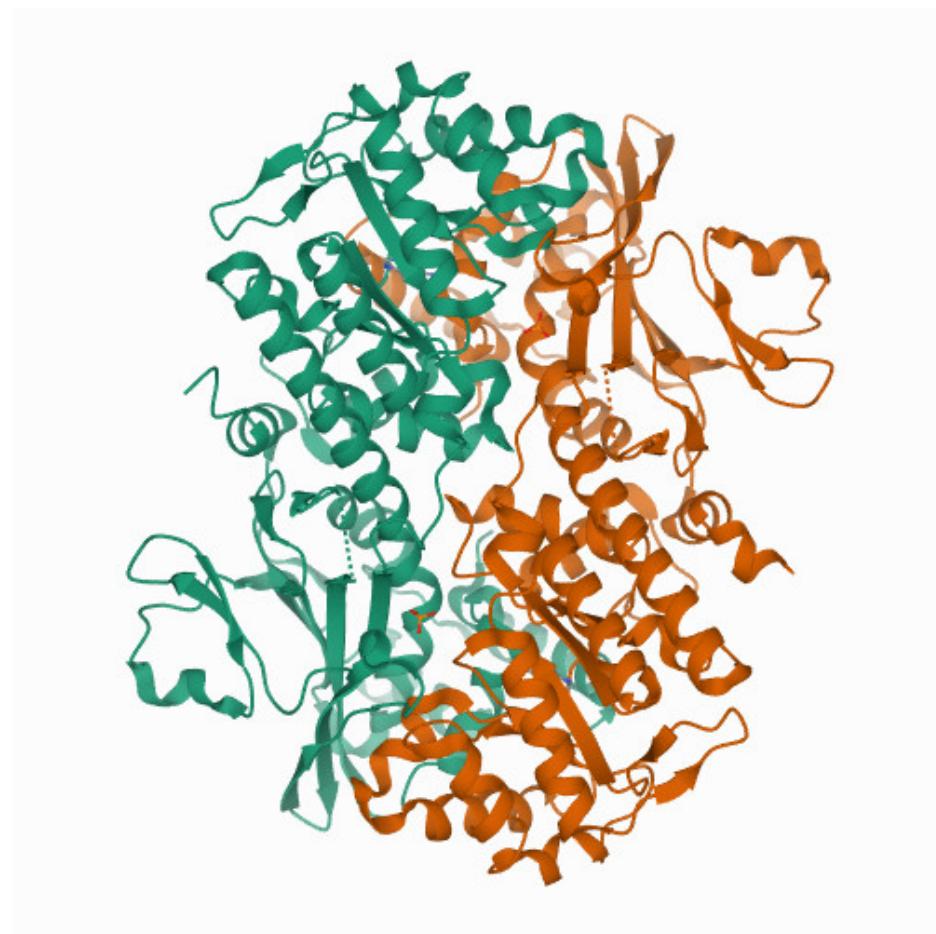
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Fragment-based Design of 3-Aminopyridine-derived Amides as Potent Inhibitors of Human Nicotinamide Phosphoribosyltransferase (NAMPT)

Dragovich, P.S., Zhao, G., Baumeister, T., Bravo, B., Giannetti, A.M., Ho, Y., Hua, R., Li, G., Liang, X., O'Brien, T., Skelton, N.J., Wang, C., Zhai, Q., Oh, A., Wang, W., Wang, Y., Xiao, Y., Yuen, P., Zak, M., Zheng, X.

(2014) Bioorg Med Chem Lett **24**: 954-962

Released	2014-02-19
Method	X-RAY DIFFRACTION 2.859 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	2HH, PO4

[3D View](#)

4N9C

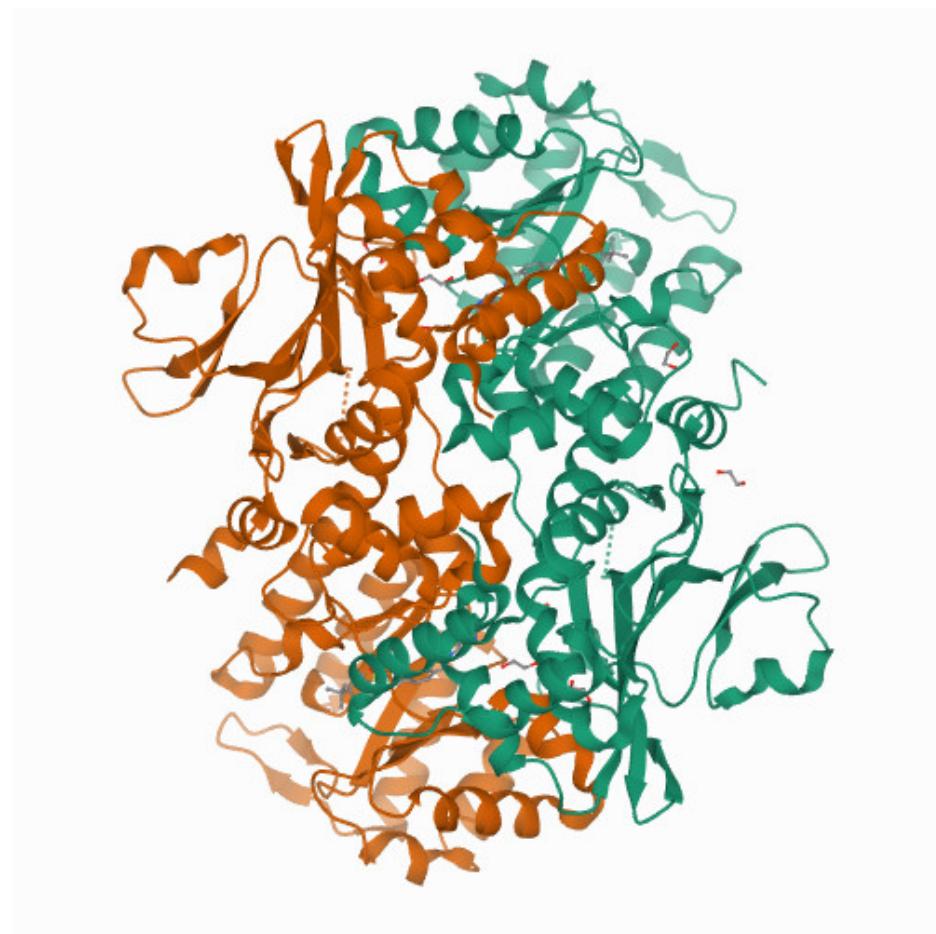
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Fragment-based Design of 3-Aminopyridine-derived Amides as Potent Inhibitors of Human Nicotinamide Phosphoribosyltransferase (NAMPT)

Dragovich, P.S., Zhao, G., Baumeister, T., Bravo, B., Giannetti, A.M., Ho, Y., Hua, R., Li, G., Liang, X., O'Brien, T., Skelton, N.J., Wang, C., Zhao, Q., Oh, A., Wang, W., Wang, Y., Xiao, Y., Yuen, P., Zak, M., Zheng, X.

(2014) Bioorg Med Chem Lett **24**: 954-962

Released	2014-02-19
Method	X-RAY DIFFRACTION 1.751 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	2ZM, PO4

[3D View](#)**4N9D**[Download File](#) [View File](#)

Fragment-based Design of 3-Aminopyridine-derived Amides as Potent Inhibitors of Human Nicotinamide Phosphoribosyltransferase (NAMPT)

Dragovich, P.S., Zhao, G., Baumeister, T., Bravo, B., Giannetti, A.M., Ho, Y., Hua, R., Li, G., Liang, X., O'Brien, T., Skelton, N.J., Wang, C., Zhao, Q., Oh, A., Wang, W., Wang, Y., Xiao, Y., Yuen, P., Zak, M., Zheng, X.

(2014) *Bioorg Med Chem Lett* **24**: 954-962

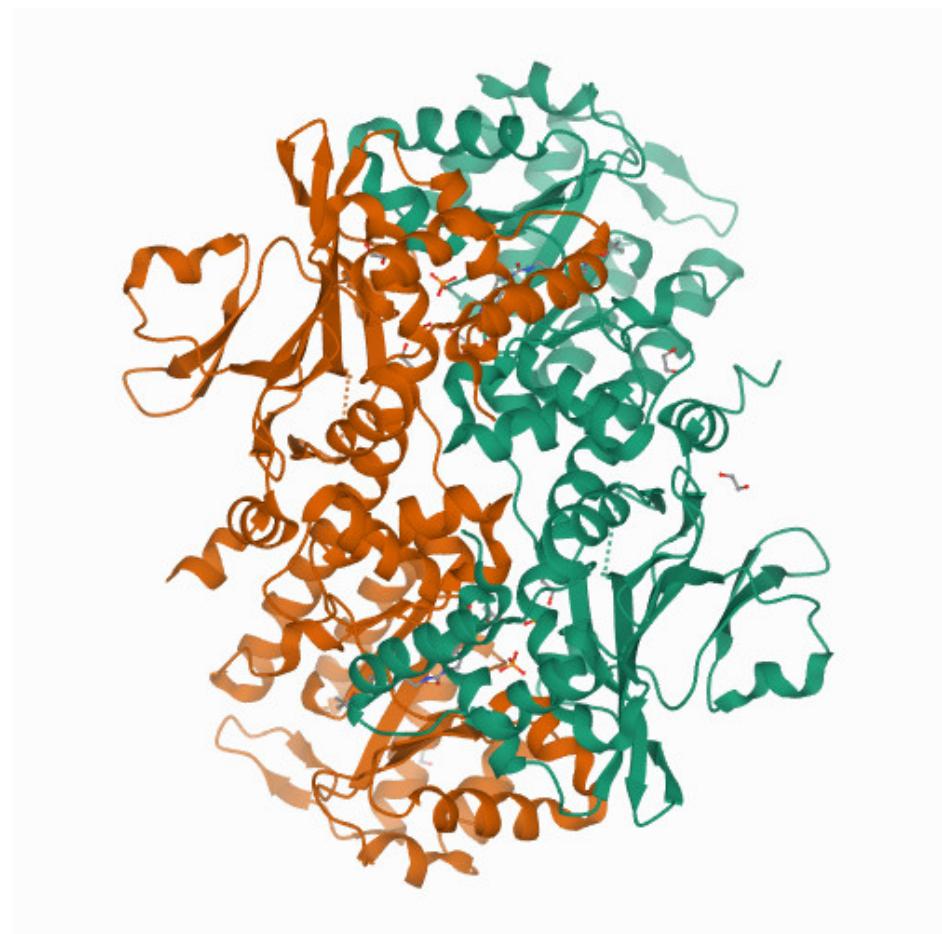
Released 2014-02-19

Method X-RAY DIFFRACTION 1.701 Å

Organisms Homo sapiens

Macromolecule Nicotinamide phosphoribosyltransferase (protein)

Unique Ligands 2HJ, EDO, PO4

[3D View](#)

5KIT

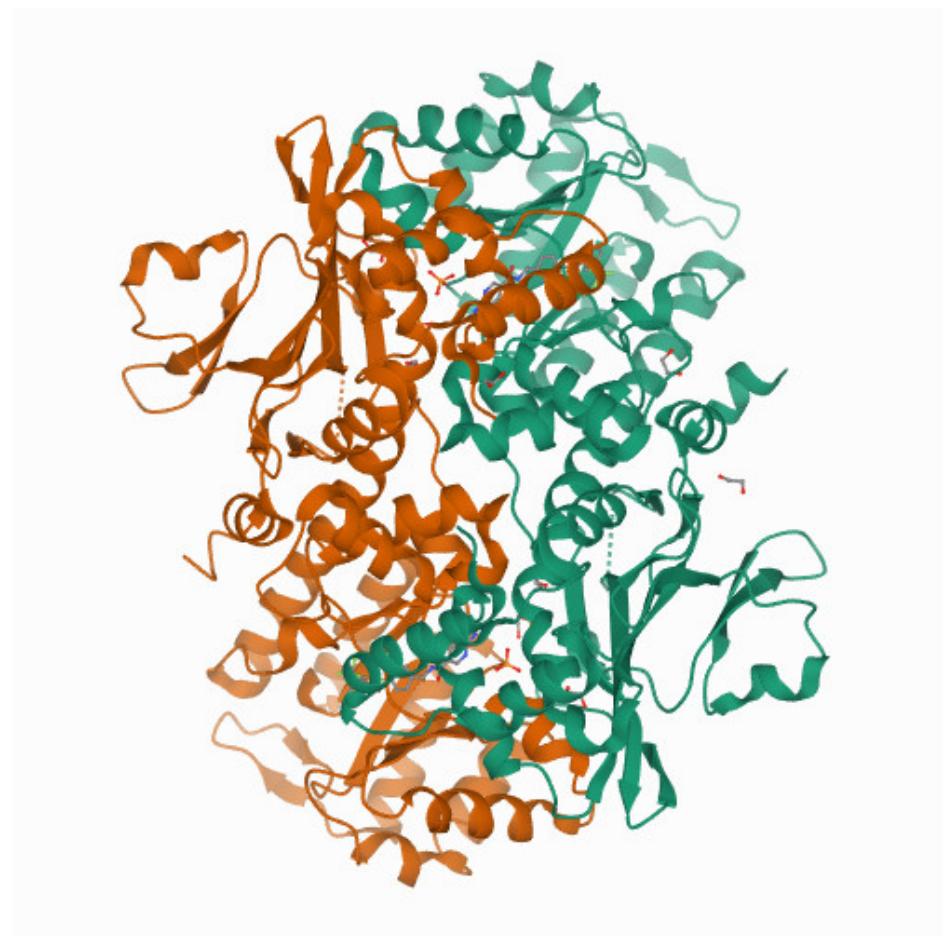
[Download File](#) [View File](#)

Crystal Structure of Nicotinamide Phosphoribosyltransferase (Nampt) in Complex with Inhibitors 37

Li, D., Wang, W.

(2016) J Med Chem **59**: 8345-8368

Released	2016-08-31
Method	X-RAY DIFFRACTION 1.6 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	6TA, EDO, PO4

[3D View](#)

4O13

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The crystal structure of NAMPT in complex with GNE-618

Oh, A., Coons, M., Brillantes, B., Wang, W.

(2014) PLoS One **9**: e109366-e109366

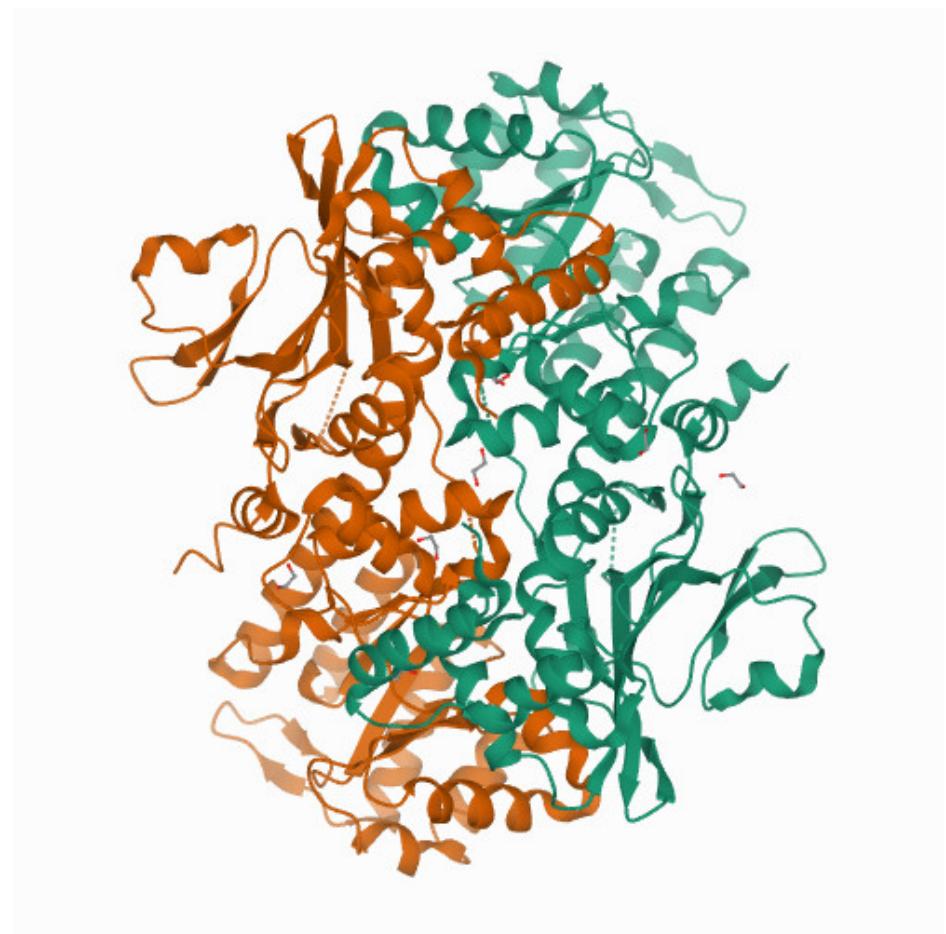
Released 2014-10-22

Method X-RAY DIFFRACTION 1.75 Å

Organisms Homo sapiens

Macromolecule Nicotinamide phosphoribosyltransferase (protein)

Unique Ligands 2P1, EDO, PO4

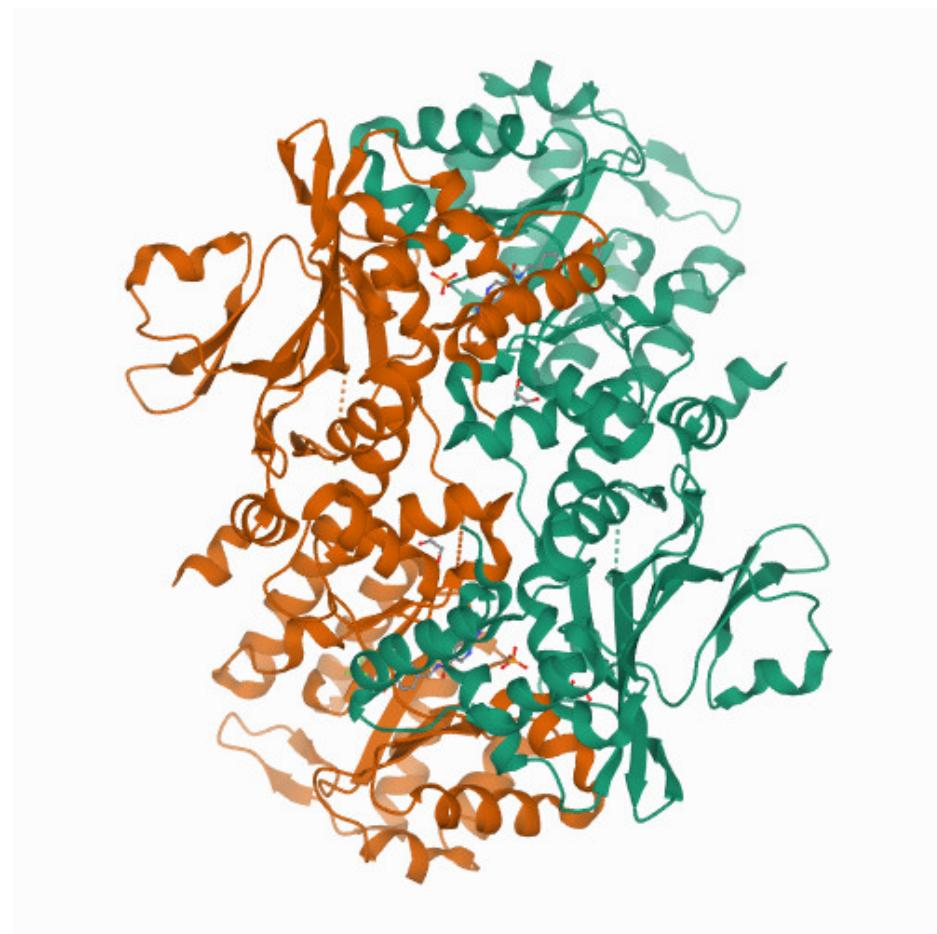
[3D View](#)**4O14**[Download File](#) [View File](#)

Structural Basis for Resistance to Diverse Classes of NAMPT Inhibitors

Oh, A., Coons, M., Brillantes, B., Wang, W.

(2014) PLoS One **9**: e109366-e109366

Released	2014-10-22
Method	X-RAY DIFFRACTION 1.871 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	EDO, PO4

[3D View](#)

4O15

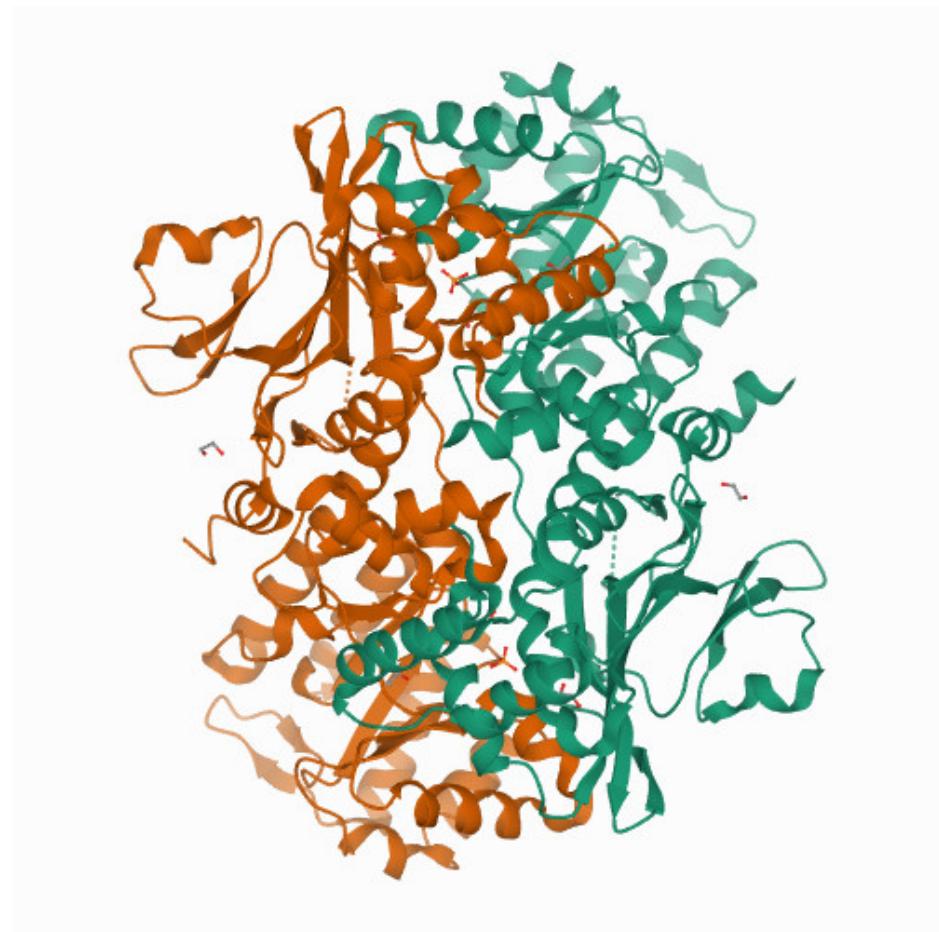
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The crystal structure of a mutant NAMPT (S165F) in complex with GNE-618

Oh, A., Coons, M., Brillantes, B., Wang, W.

(2014) PLoS One **9**: e109366-e109366

Released	2014-10-22
Method	X-RAY DIFFRACTION 1.8 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	2P1, EDO, PO4

[3D View](#)

4O1A

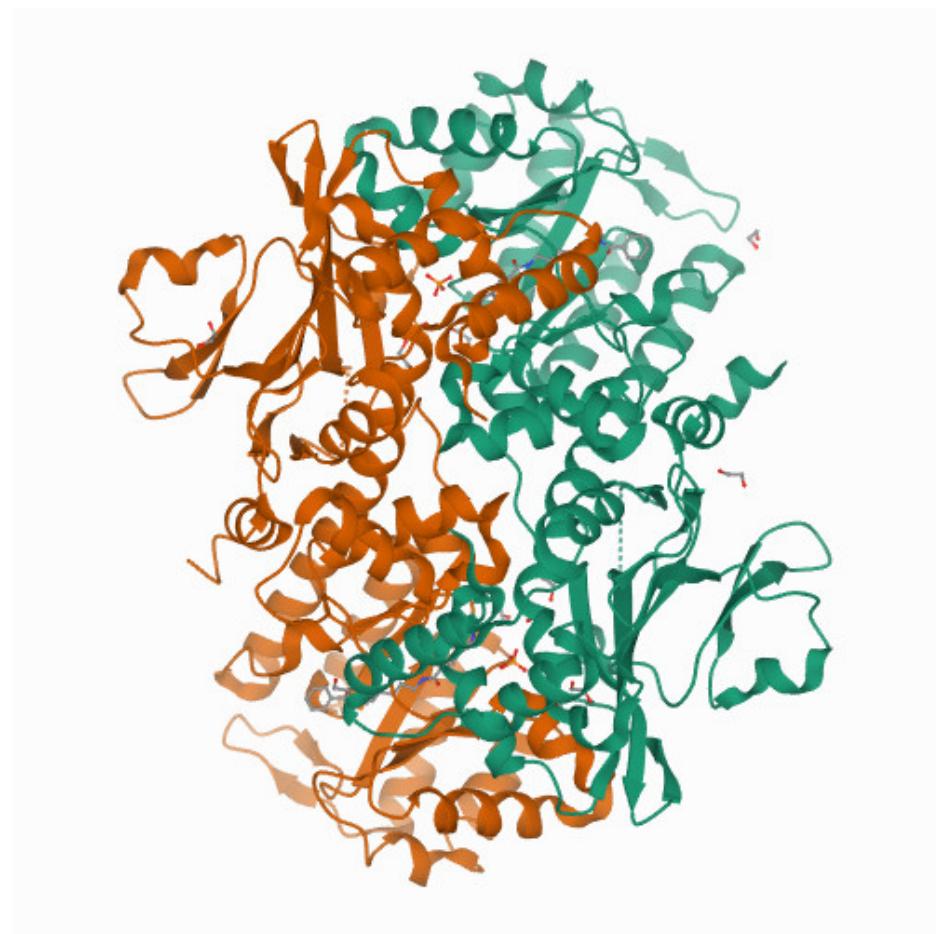
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The crystal structure of the mutant NAMPT G217R

Oh, A., Coons, M., Brillantes, B., Wang, W.

(2014) PLoS One **9**: e109366-e109366

Released	2014-10-22
Method	X-RAY DIFFRACTION 1.87 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	EDO, PO4

[3D View](#)

4O1B

[Download File](#) [View File](#)

The crystal structure of a mutant NAMPT (G217R) in complex with an inhibitor APO866

Oh, A., Coons, M., Brillantes, B., Wang, W.

(2014) PLoS One 9: e109366-e109366

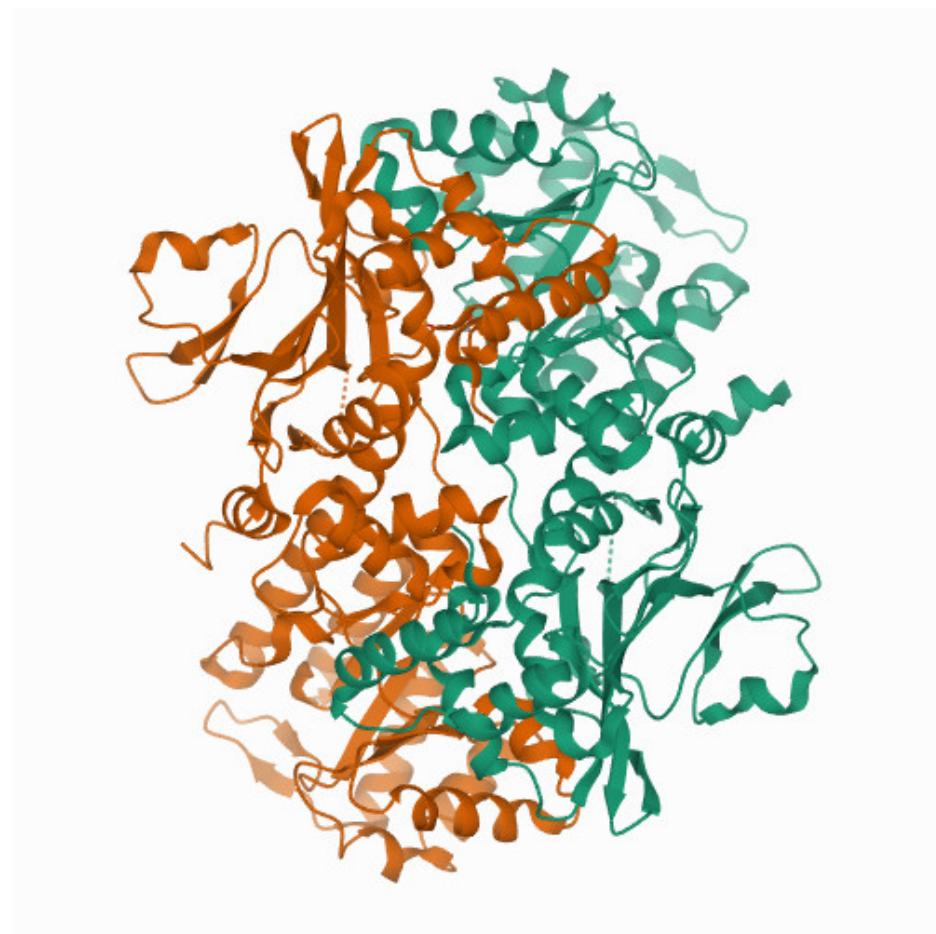
Released 2014-10-22

Method X-RAY DIFFRACTION 1.65 Å

Organisms Homo sapiens

Macromolecule Nicotinamide phosphoribosyltransferase (protein)

Unique Ligands DGB, EDO, PO4

[3D View](#)

4O1C

[Download File](#) [View File](#)

The crystal structures of a mutant NAMPT H191R

Oh, A., Coons, M., Brillantes, B., Wang, W.

(2014) PLoS One **9**: e109366-e109366

Released

2014-10-22

Method

X-RAY DIFFRACTION 2.092 Å

Organisms

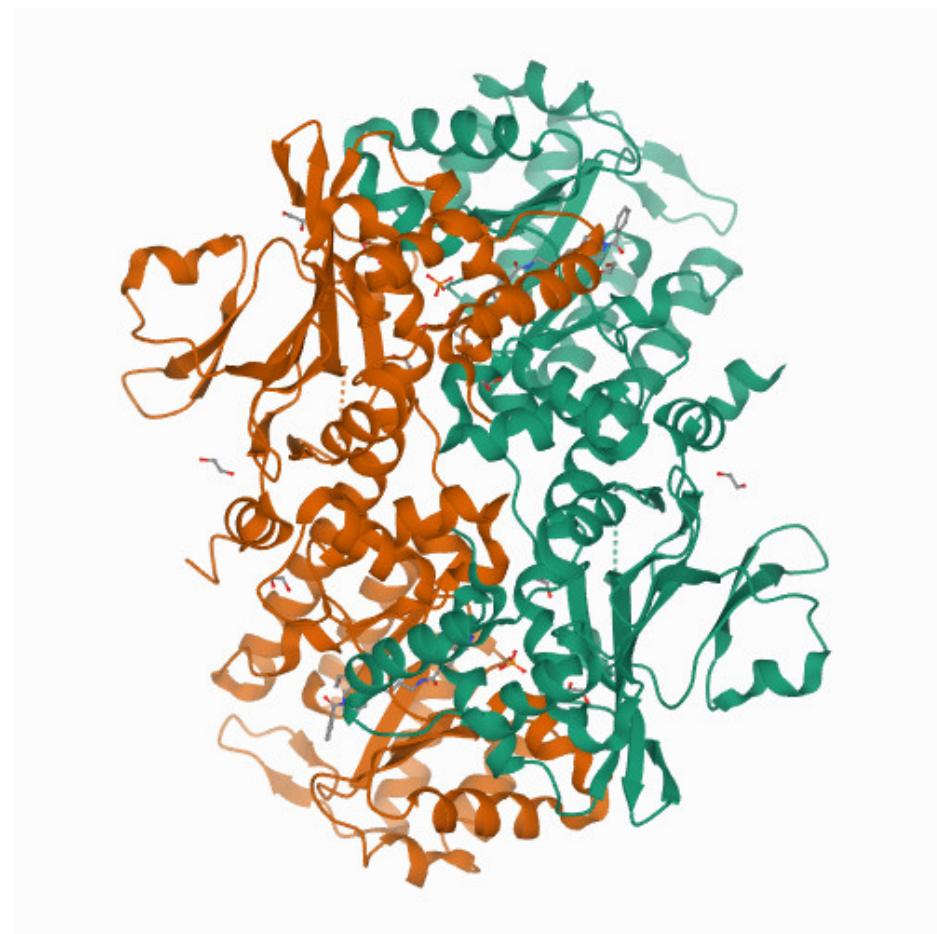
Homo sapiens

Macromolecule

Nicotinamide phosphoribosyltransferase (protein)

Unique Ligands

EDO, PO4

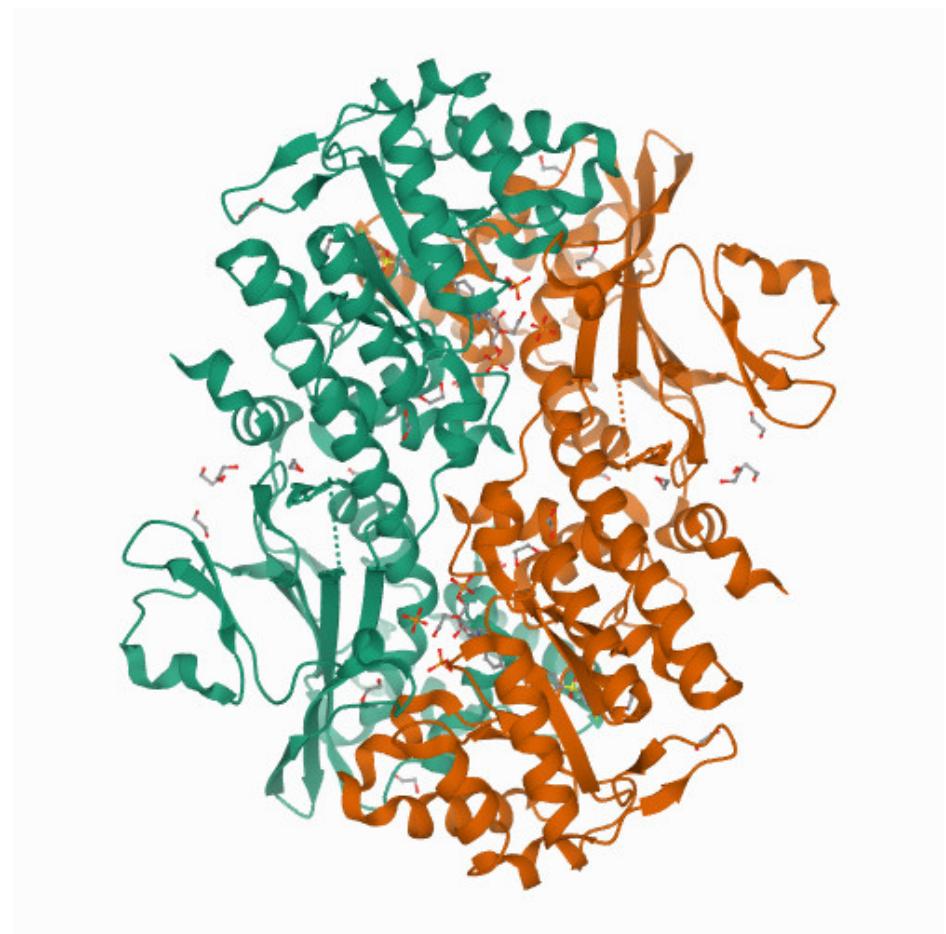
[3D View](#)**4O1D**[Download File](#) [View File](#)

Structural Basis for Resistance to Diverse Classes of NAMPT Inhibitors

Oh, A., Coons, M., Brillantes, B., Wang, W.

(2014) PLoS One **9**: e109366-e109366

Released	2014-10-22
Method	X-RAY DIFFRACTION 1.705 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	DGB, EDO, PO4

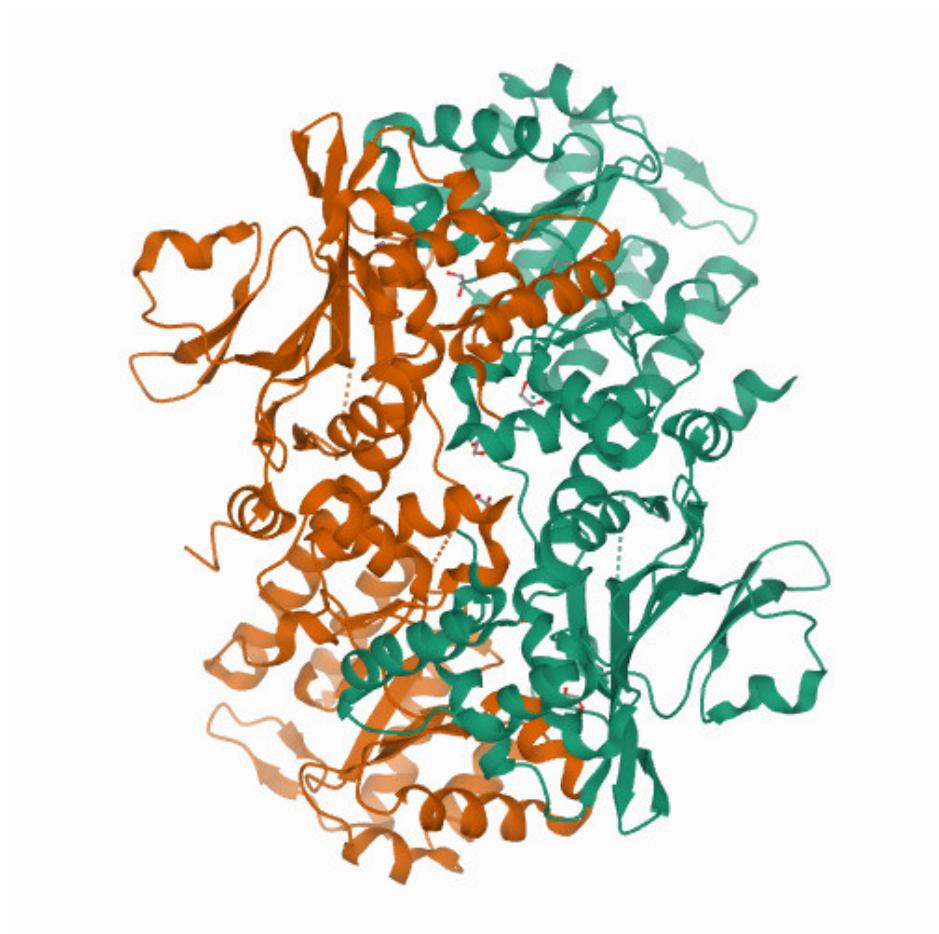
[3D View](#)**4O16**[Download File](#) [View File](#)

Structural Basis for Resistance to Diverse Classes of NAMPT Inhibitors

Oh, A., Coons, M., Brillantes, B., Wang, W.

(2014) PLoS One **9**: e109366-e109366

Released	2014-10-22
Method	X-RAY DIFFRACTION 1.783 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	1XC, EDO, PO4

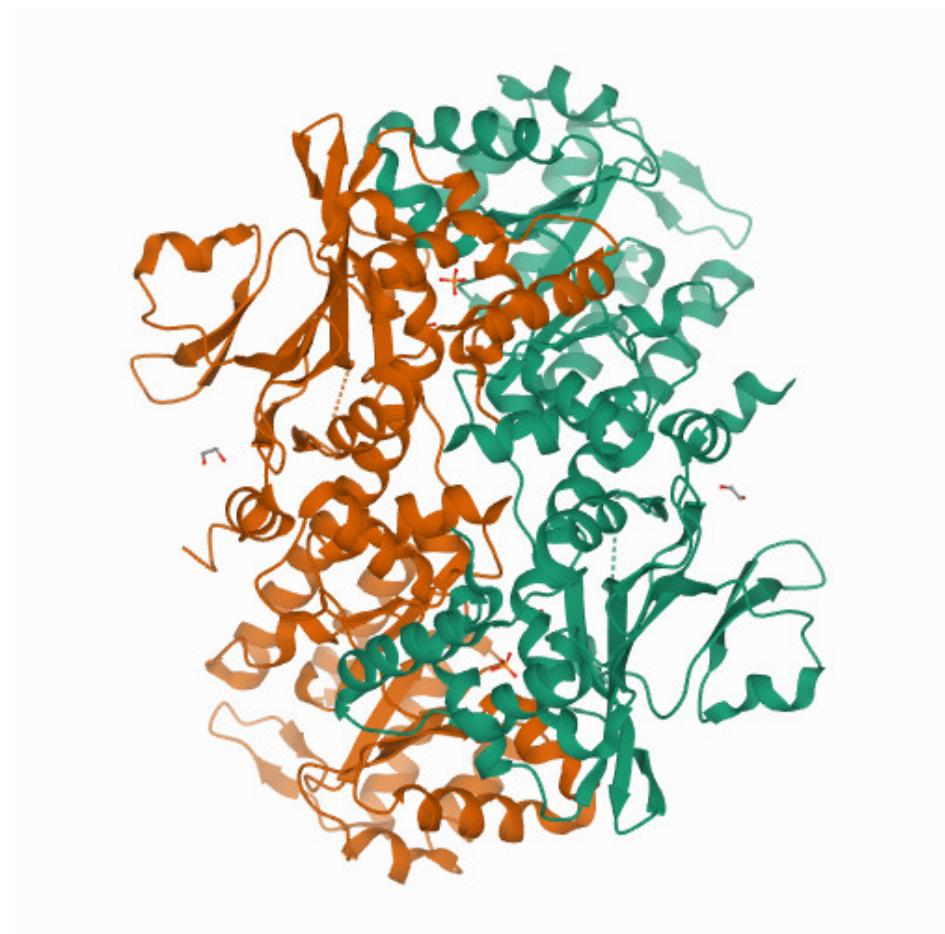
[3D View](#)**4O17**[Download File](#) [View File](#)

Structural Basis for Resistance to Diverse Classes of NAMPT Inhibitors

Oh, A., Coons, M., Brillantes, B., Wang, W.

(2014) PLoS One **9**: e109366-e109366

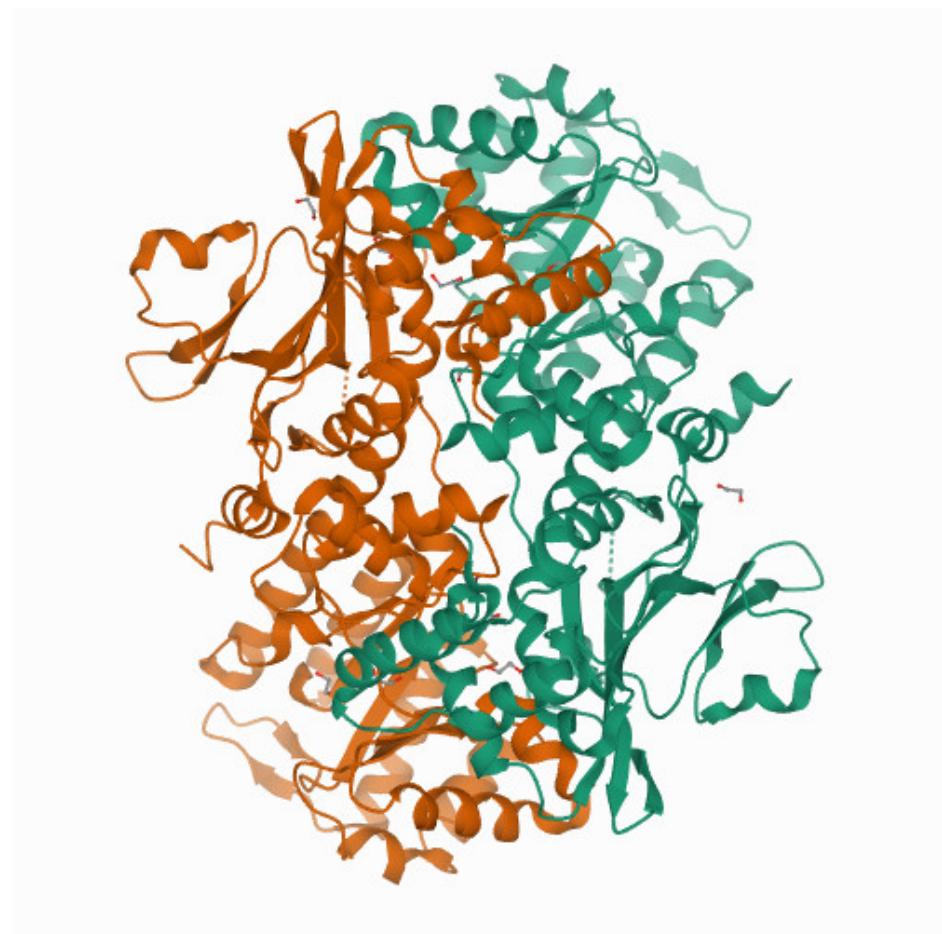
Released	2014-10-22
Method	X-RAY DIFFRACTION 1.82 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	EDO, PO4

[3D View](#)**4O18**[Download File](#) [View File](#) **Structural Basis for Resistance to Diverse Classes of NAMPT Inhibitors**

Oh, A., Coons, M., Brillantes, B., Wang, W.

(2014) PLoS One **9**: e109366-e109366

Released	2014-10-22
Method	X-RAY DIFFRACTION 1.92 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	EDO, PO4

[3D View](#)**4O19**[Download File](#) [View File](#) **The crystal structure of a mutant NAMPT (G217V)**

Oh, A., Coons, M., Brillantes, B., Wang, W.

(2014) PLoS One **9**: e109366-e109366**Released**

2014-10-22

Method

X-RAY DIFFRACTION 1.75 Å

Organisms

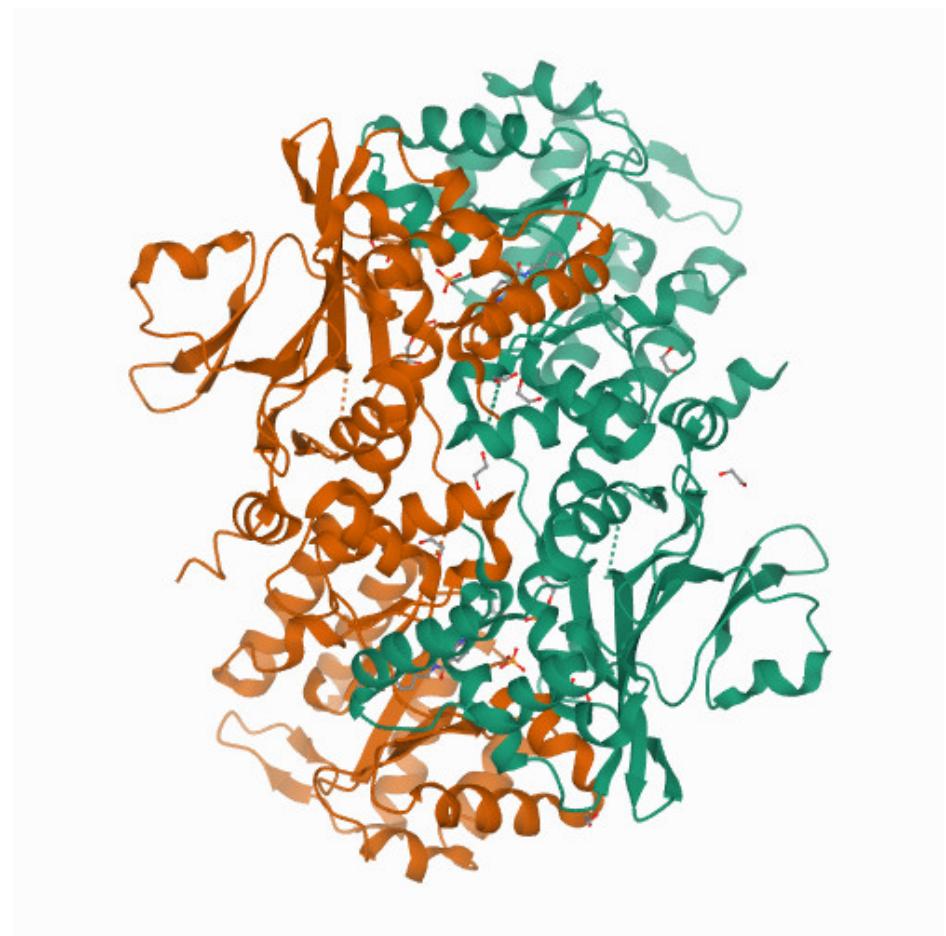
Homo sapiens

Macromolecule

Nicotinamide phosphoribosyltransferase (protein)

Unique Ligands

EDO, PO4

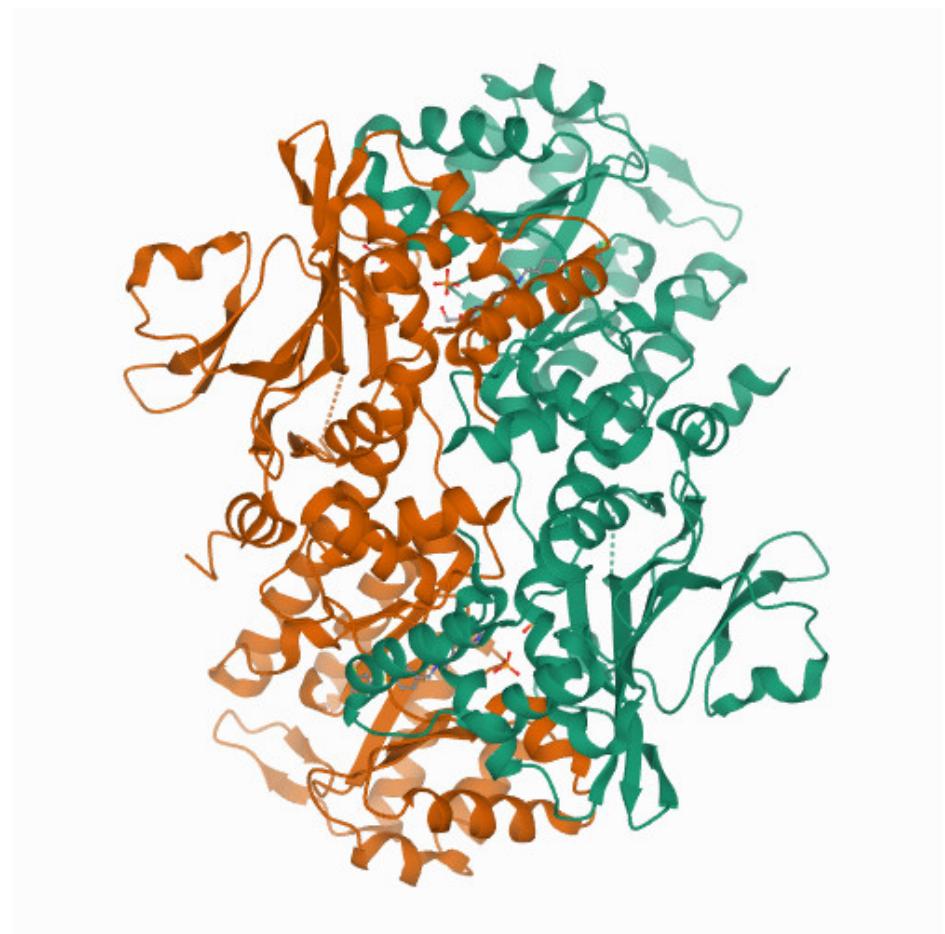
[3D View](#)**4O28**[Download File](#) [View File](#)

Structural Basis for Resistance to Diverse Classes of NAMPT Inhibitors

Oh, A., Coons, M., Brillantes, B., Wang, W.

(2014) PLoS One **9**: e109366-e109366

Released	2014-10-22
Method	X-RAY DIFFRACTION 2 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	1QS, EDO, PO4

[3D View](#)**4L4M**[Download File](#)[View File](#)

Structural Analysis of a Phosphoribosylated Inhibitor in Complex with Human Nicotinamide Phosphoribosyltransferase

Oh, A., Ho, Y., Zak, M., Liu, Y., Yuen, P., Zheng, X., Dragovich, S.P., Wang, W.

(2014) Chembiochem **15**: 1121-1130

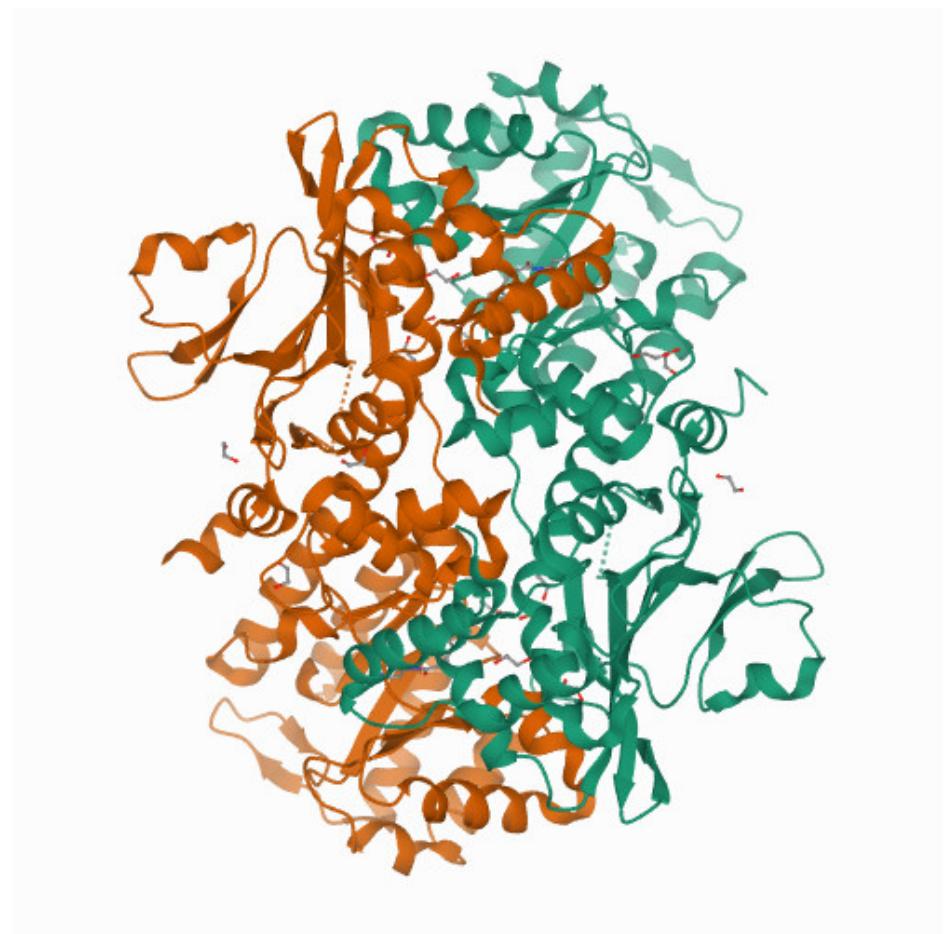
Released 2014-06-11

Method X-RAY DIFFRACTION 2.445 Å

Organisms Homo sapiens

Macromolecule Nicotinamide phosphoribosyltransferase (protein)

Unique Ligands 1XD, EDO, PO4

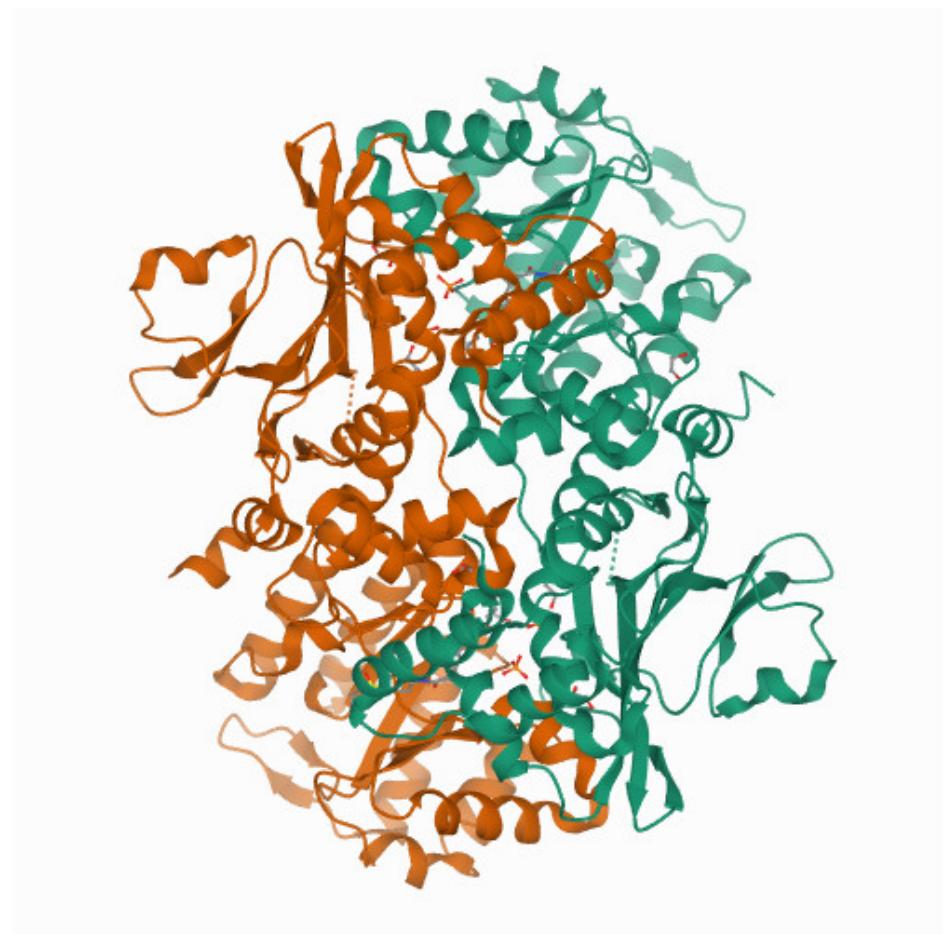
[3D View](#)**4LVF**[Download File](#) [View File](#)

Fragment-based Identification of Amides Derived From
trans-2-(Pyridin-3-yl)cyclopropanecarboxylic Acid as Potent
Inhibitors of Human Nicotinamide
Phosphoribosyltransferase (NAMPT)

Giannetti, A.M., Zheng, X., Skelton, N., Wang, W., Bravo, B., Feng, Y.,
Gunzner-Toste, J., Ho, Y., Hua, R., Wang, C., Zhao, Q., Liederer, B.M., Liu,
Y., O'Brien, T., Oeh, J., Sampath, D., Shen, Y., Wang, L., Wu, H., Xiao, Y.,
Yuen, P., Zak, M., Zhao, G., Dragovich, P.S.

(2013) Bioorg Med Chem Lett **23**: 5488-5497

Released	2013-09-25
Method	X-RAY DIFFRACTION 1.5 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	20P, EDO, PO4

 3D View

4LVG

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Fragment-based Identification of Amides Derived From trans-2-(Pyridin-3-yl)cyclopropanecarboxylic Acid as Potent Inhibitors of Human Nicotinamide Phosphoribosyltransferase (NAMPT)

Giannetti, A.M., Zheng, X., Skelton, N., Wang, W., Bravo, B., Feng, Y., Gunzner-Toste, J., Ho, Y., Hua, R., Wang, C., Zhao, Q., Liederer, B.M., Liu, Y., O'Brien, T., Oeh, J., Sampath, D., Shen, Y., Wang, L., Wu, H., Xiao, Y., Yuen, P., Zak, M., Zhao, G., Dragovich, P.S.

(2013) Bioorg Med Chem Lett **23**: 5488-5497

Released

2013-09-25

Method

X-RAY DIFFRACTION 1.702 Å

Organisms

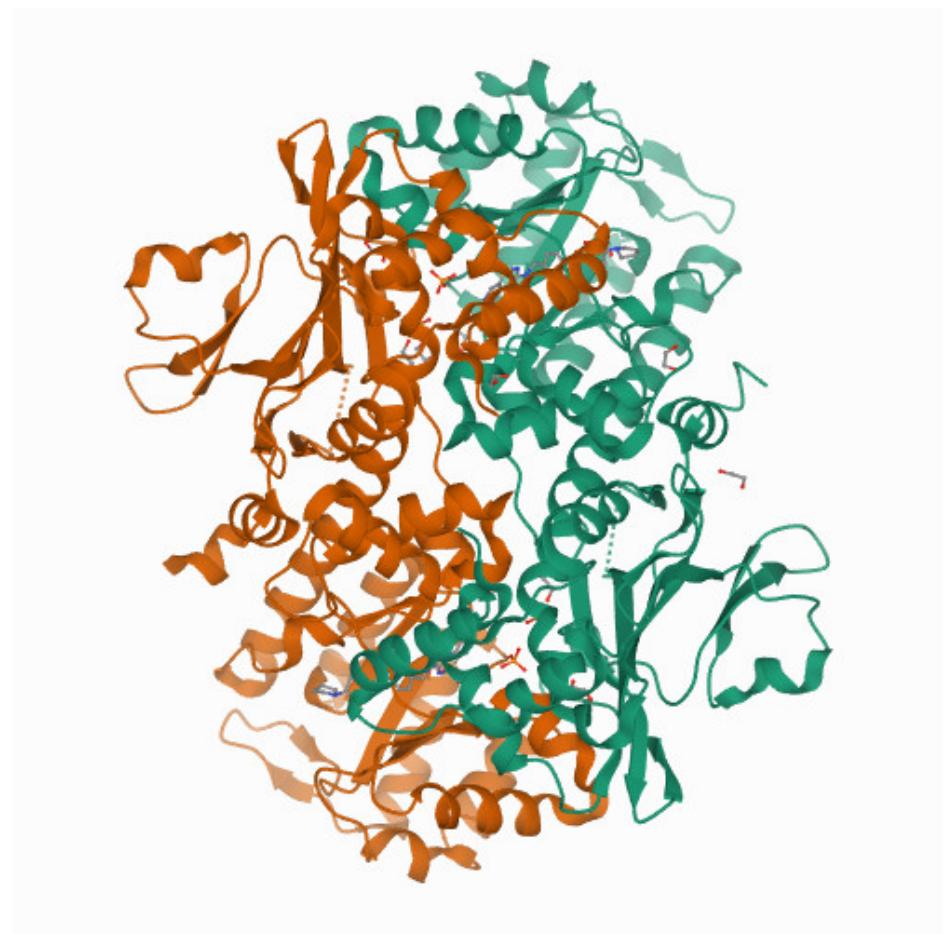
Homo sapiens

Macromolecule

Nicotinamide phosphoribosyltransferase (protein)

Unique Ligands

20O, EDO, PO4

[3D View](#)**4LVA**[Download File](#) [View File](#)

Fragment-based Identification of Amides Derived From
trans-2-(Pyridin-3-yl)cyclopropanecarboxylic Acid as Potent
Inhibitors of Human Nicotinamide
Phosphoribosyltransferase (NAMPT)

Giannetti, A.M., Zheng, X., Skelton, N., Wang, W., Bravo, B., Feng, Y.,
Gunzner-Toste, J., Ho, Y., Hua, R., Wang, C., Zhao, Q., Liederer, B.M., Liu,
Y., O'Brien, T., Oeh, J., Sampath, D., Shen, Y., Wang, L., Wu, H., Xiao, Y.,
Yuen, P., Zak, M., Zhao, G., Dragovich, P.S.

(2013) Bioorg Med Chem Lett **23**: 5488-5497

Released

2013-09-25

Method

X-RAY DIFFRACTION 1.55 Å

Organisms

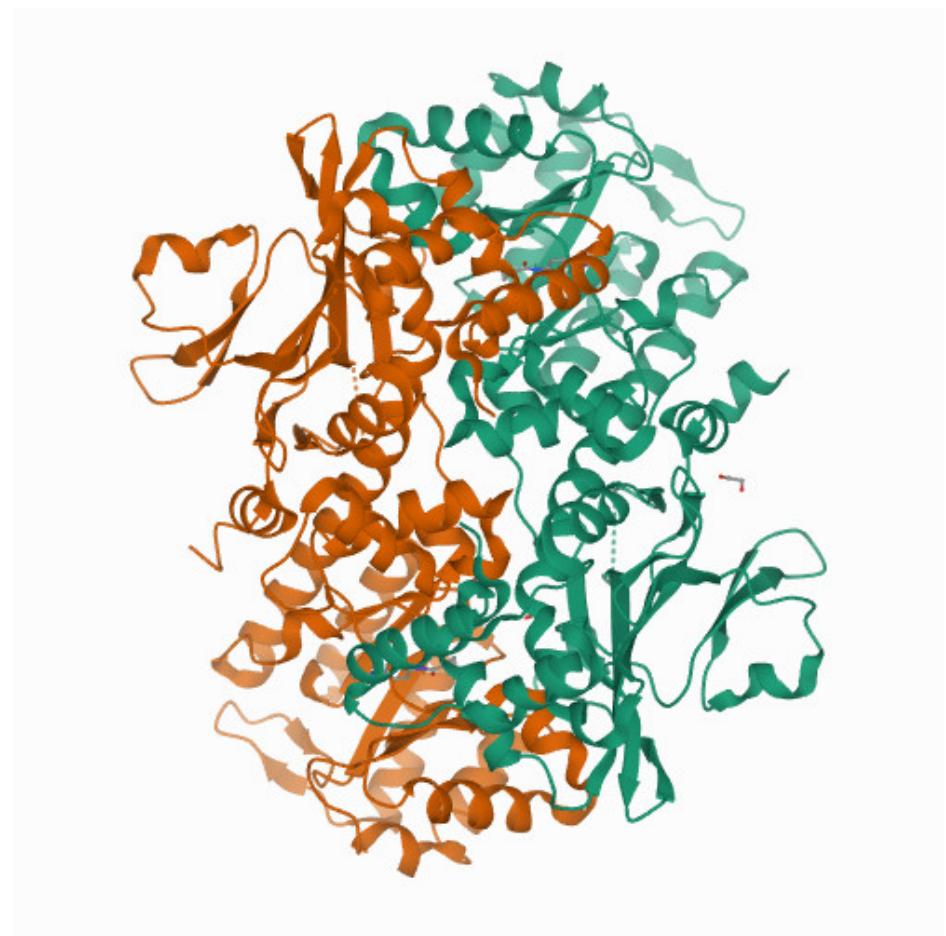
Homo sapiens

Macromolecule

Nicotinamide phosphoribosyltransferase (protein)

Unique Ligands

20M, EDO, PO4

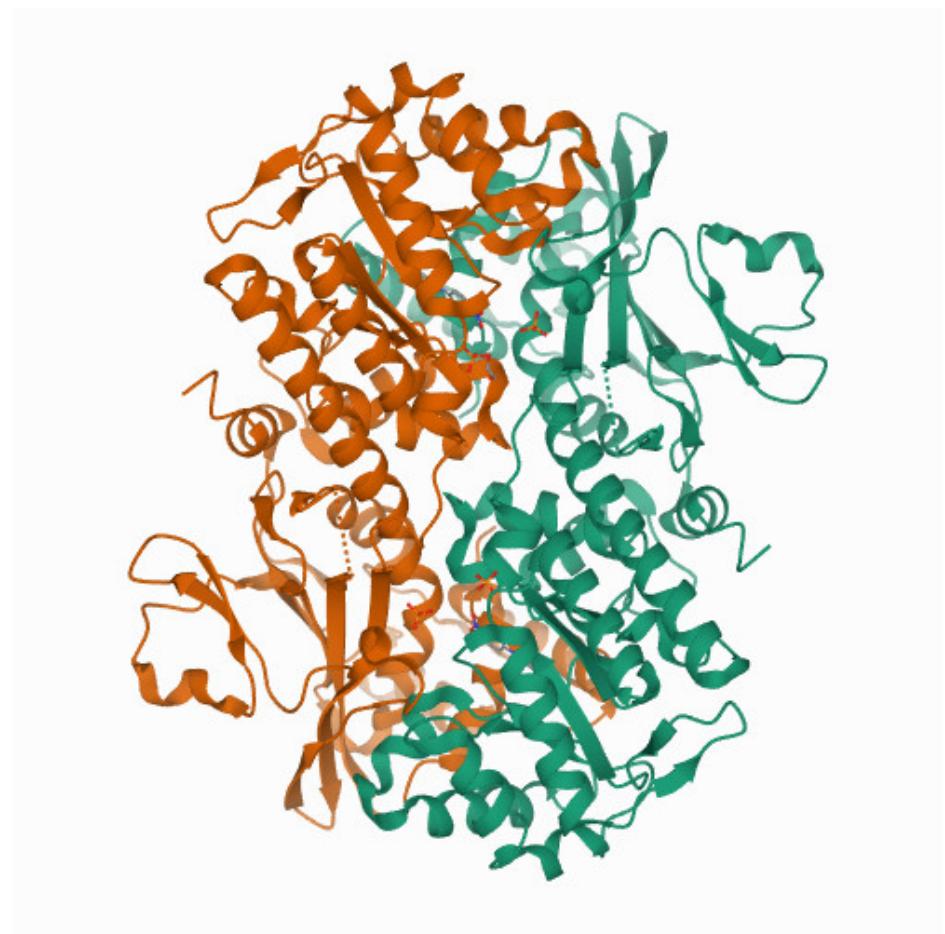
 3D View**4LVB** Download File View File

Fragment-based Identification of Amides Derived From trans-2-(Pyridin-3-yl)cyclopropanecarboxylic Acid as Potent Inhibitors of Human Nicotinamide Phosphoribosyltransferase (NAMPT)

Giannetti, A.M., Zheng, X., Skelton, N., Wang, W., Bravo, B., Feng, Y., Gunzner-Toste, J., Ho, Y., Hua, R., Wang, C., Zhao, Q., Liederer, B.M., Liu, Y., O'Brien, T., Oeh, J., Sampath, D., Shen, Y., Wang, L., Wu, H., Xiao, Y., Yuen, P., Zak, M., Zhao, G., Dragovich, P.S.

(2013) Bioorg Med Chem Lett **23**: 5488-5497

Released	2013-09-25
Method	X-RAY DIFFRACTION 1.836 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	20N, EDO, PO4

[3D View](#)**4LVD**[Download File](#) [View File](#)

Fragment-based Identification of Amides Derived From
trans-2-(Pyridin-3-yl)cyclopropanecarboxylic Acid as Potent
Inhibitors of Human Nicotinamide
Phosphoribosyltransferase (NAMPT)

Giannetti, A.M., Zheng, X., Skelton, N., Wang, W., Bravo, B., Feng, Y.,
Gunzner-Toste, J., Ho, Y., Hua, R., Wang, C., Zhao, Q., Liederer, B.M., Liu,
Y., O'Brien, T., Oeh, J., Sampath, D., Shen, Y., Wang, L., Wu, H., Xiao, Y.,
Yuen, P., Zak, M., Zhao, G., Dragovich, P.S.

(2013) Bioorg Med Chem Lett **23**: 5488-5497

Released

2013-09-25

Method

X-RAY DIFFRACTION 1.75 Å

Organisms

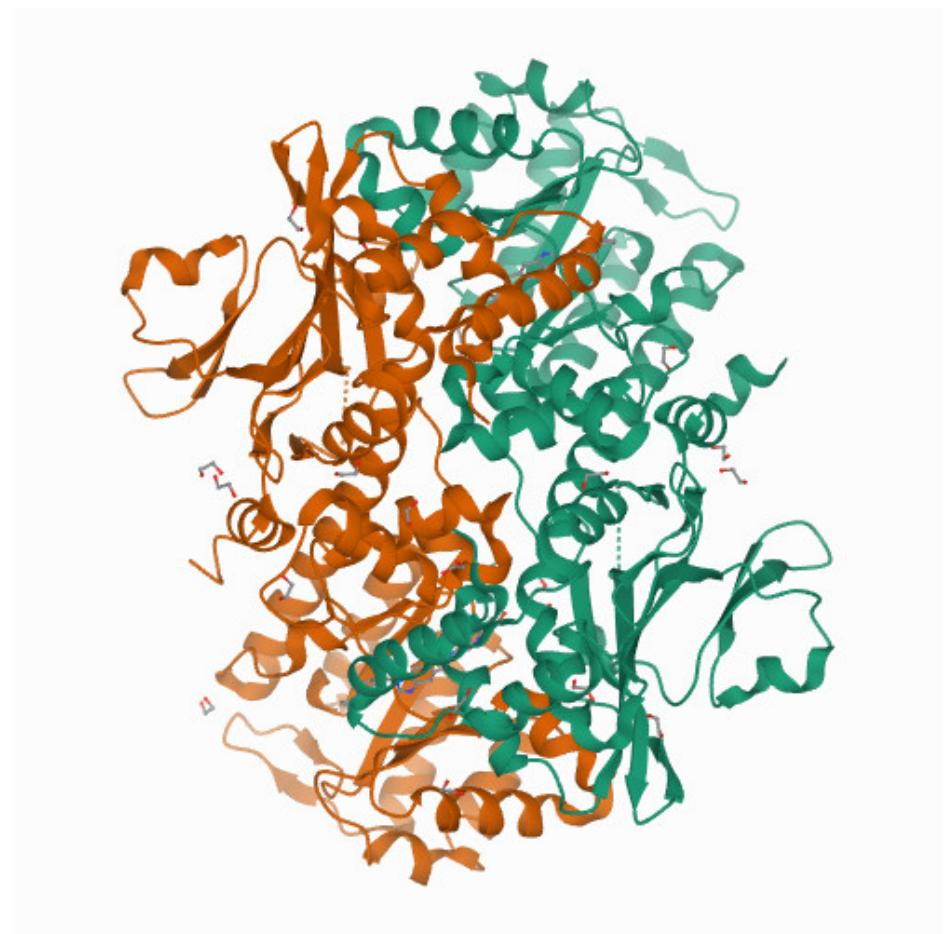
Homo sapiens

Macromolecule

Nicotinamide phosphoribosyltransferase (protein)

Unique Ligands

1EB, EDO, PO4

[3D View](#)**4N9E**[Download File](#) [View File](#)

Fragment-based Design of 3-Aminopyridine-derived Amides as Potent Inhibitors of Human Nicotinamide Phosphoribosyltransferase (NAMPT)

Dragovich, P.S., Zhao, G., Baumeister, T., Bravo, B., Giannetti, A.M., Ho, Y., Hua, R., Li, G., Liang, X., O'Brien, T., Skelton, N.J., Wang, C., Zhao, Q., Oh, A., Wang, W., Wang, Y., Xiao, Y., Yuen, P., Zak, M., Zheng, X.

(2014) Bioorg Med Chem Lett **24**: 954-962

Released

2014-02-19

Method

X-RAY DIFFRACTION 1.72 Å

Organisms

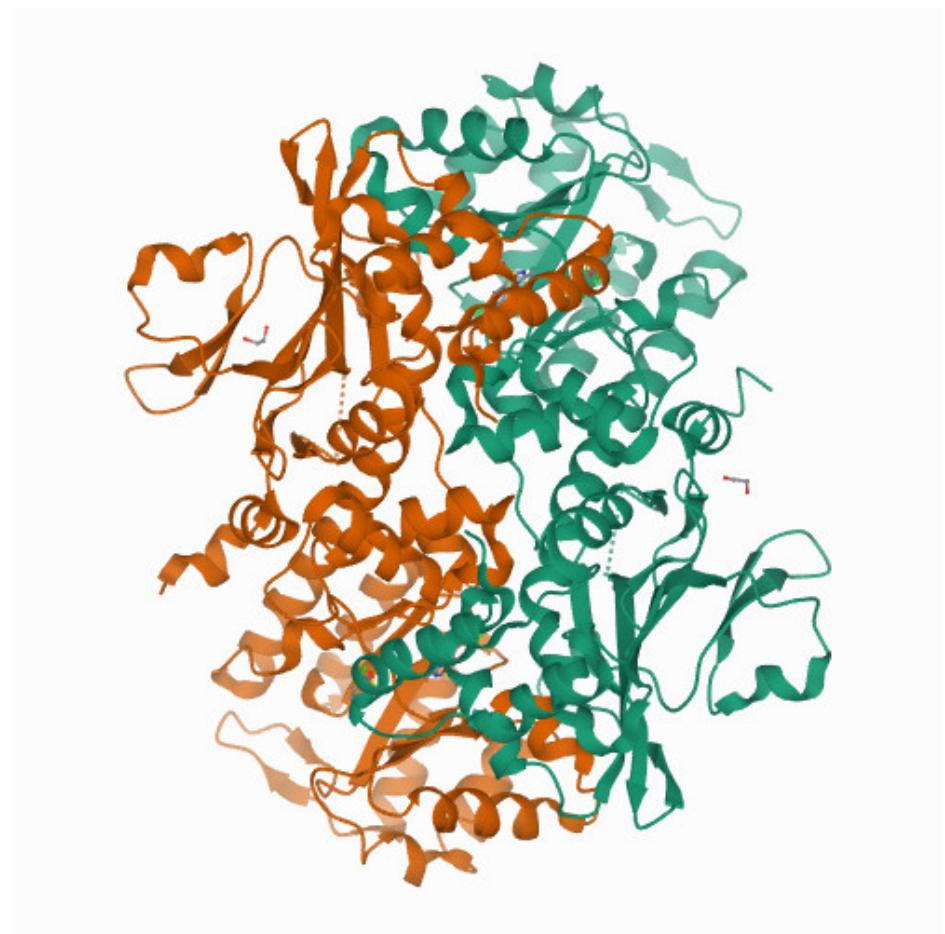
Homo sapiens

Macromolecule

Nicotinamide phosphoribosyltransferase (protein)

Unique Ligands

2HL, DTT, EDO, PO4

 3D View

4LV9

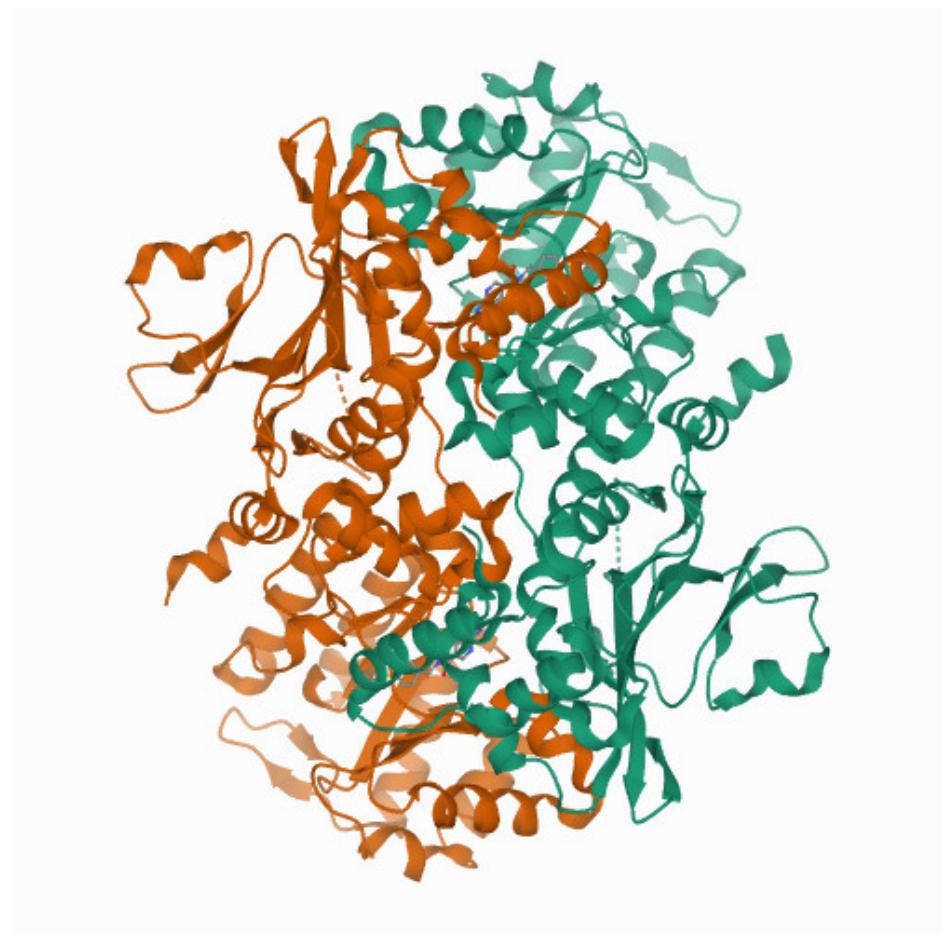
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Fragment-based Identification of Amides Derived From
trans-2-(Pyridin-3-yl)cyclopropanecarboxylic Acid as Potent
Inhibitors of Human Nicotinamide
Phosphoribosyltransferase (NAMPT)

Giannetti, A.M., Zheng, X., Skelton, N., Wang, W., Bravo, B., Feng, Y., Gunzner-Toste, J., Ho, Y., Hua, R., Wang, C., Zhao, Q., Liederer, B.M., Liu, Y., O'Brien, T., Oeh, J., Sampath, D., Shen, Y., Wang, L., Wu, H., Xiao, Y., Yuen, P., Zak, M., Zhao, G., Dragovich, P.S.

(2013) Bioorg Med Chem Lett **23**: 5488-5497

Released	2013-09-25
Method	X-RAY DIFFRACTION 1.807 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	20J, EDO, PO4

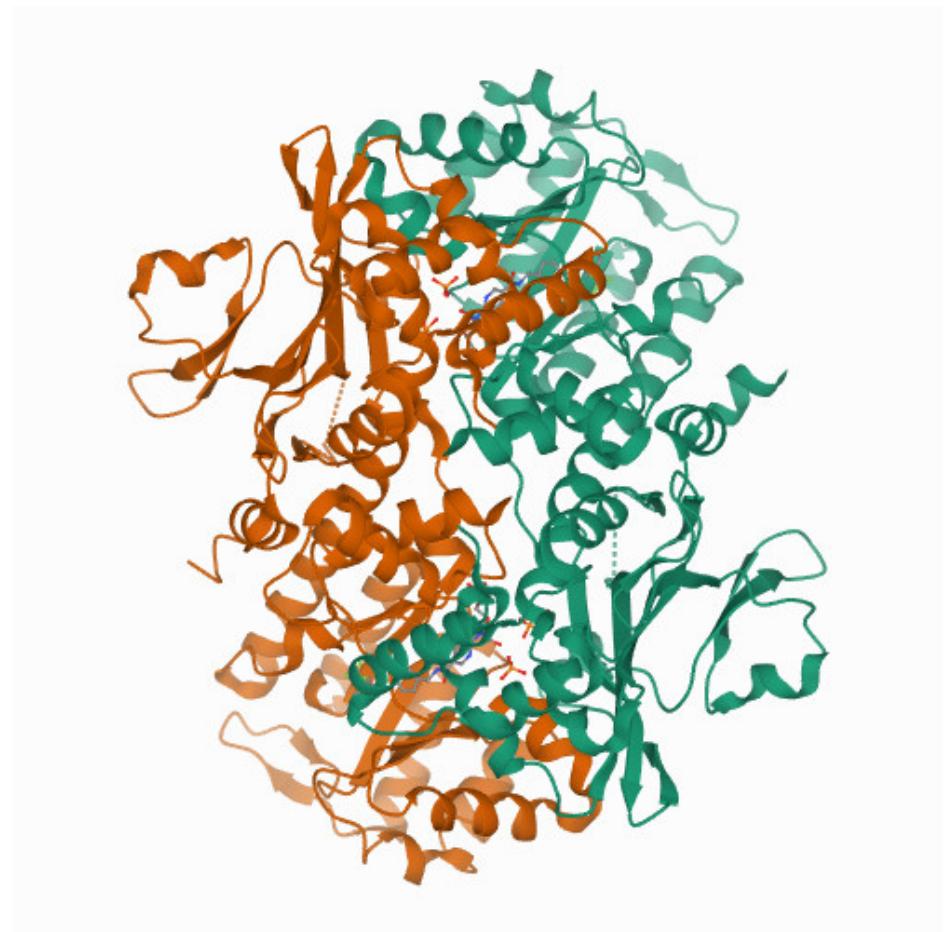
[3D View](#)**4M6P**[Download File](#)[View File](#)

Identification of Amides Derived From 1H-Pyrazolo[3,4-b]pyridine-5-carboxylic Acid as Potent Inhibitors of Human Nicotinamide Phosphoribosyltransferase (NAMPT)

Giannetti, A.M., Zheng, X., Skelton, N., Wang, W., Bravo, B., Feng, Y., Gunzner-Toste, J., Ho, Y., Hua, R., Wang, C., Zhao, Q., Liederer, B.M., Liu, Y., O'Brien, T., Oeh, J., Sampath, D., Shen, Y., Wang, L., Wu, H., Xiao, Y., Yuen, P., Zak, M., Zhao, G., Dragovich, P.S.

(2013) Bioorg Med Chem Lett **23**: 5488-5497

Released	2013-09-25
Method	X-RAY DIFFRACTION 1.75 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	20R, PO4

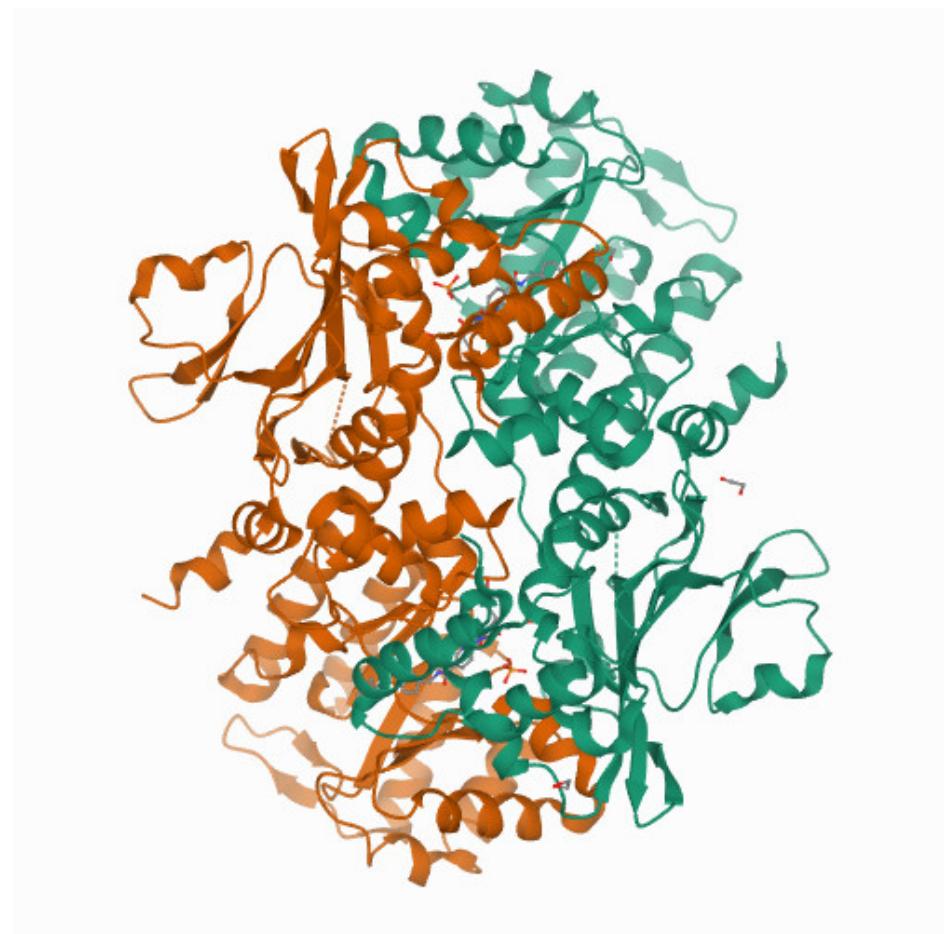
[3D View](#)**4M6Q**[Download File](#)[View File](#)

Identification of Amides Derived From 1H-Pyrazolo[3,4-b]pyridine-5-carboxylic Acid as Potent Inhibitors of Human Nicotinamide Phosphoribosyltransferase (NAMPT)

Giannetti, A.M., Zheng, X., Skelton, N., Wang, W., Bravo, B., Feng, Y., Gunzner-Toste, J., Ho, Y., Hua, R., Wang, C., Zhao, Q., Liederer, B.M., Liu, Y., O'Brien, T., Oeh, J., Sampath, D., Shen, Y., Wang, L., Wu, H., Xiao, Y., Yuen, P., Zak, M., Zhao, G., Dragovich, P.S.

(2013) Bioorg Med Chem Lett **23**: 5488-5497

Released	2013-09-25
Method	X-RAY DIFFRACTION 2.406 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	20T, PO4, POP

[3D View](#)**4L4L**[Download File](#)[View File](#)

Structural Analysis of a Phosphoribosylated Inhibitor in Complex with Human Nicotinamide Phosphoribosyltransferase

Oh, A., Ho, Y., Zak, M., Liu, Y., Yuen, P., Zheng, X., Dragovich, S.P., Wang, W.

(2014) Chembiochem **15**: 1121-1130

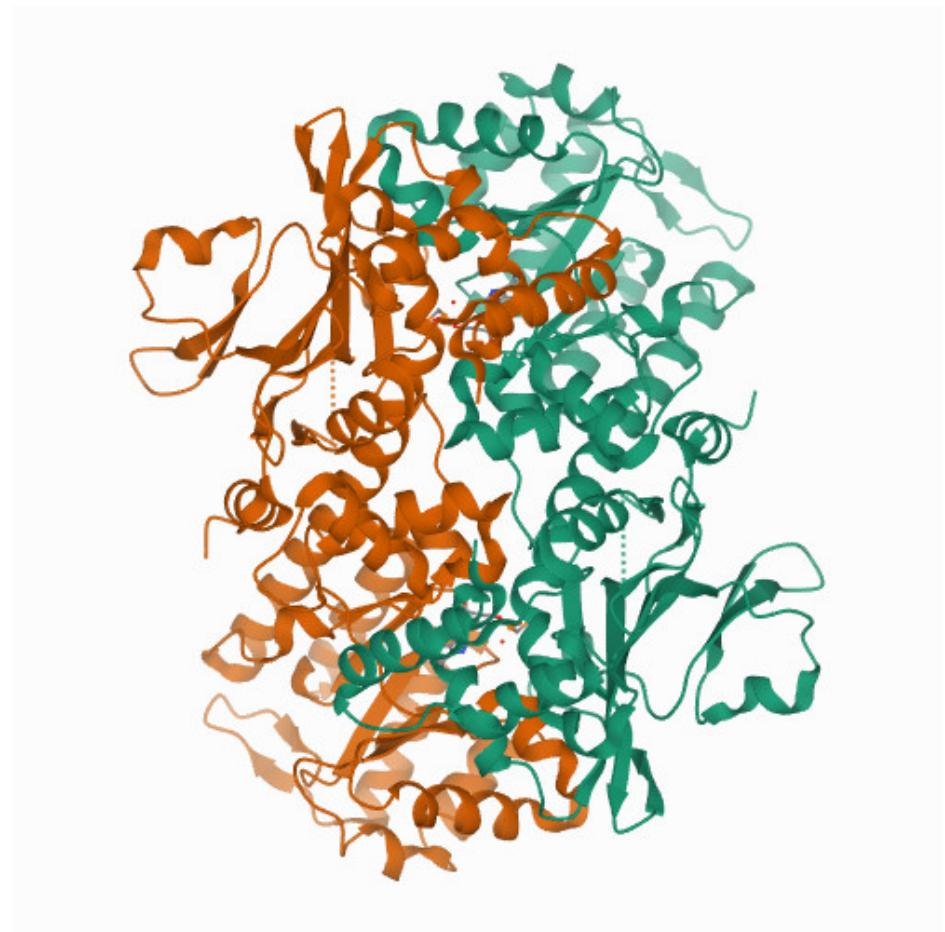
Released 2014-06-11

Method X-RAY DIFFRACTION 2.122 Å

Organisms Homo sapiens

Macromolecule Nicotinamide phosphoribosyltransferase (protein)

Unique Ligands 1XC, EDO, PO4

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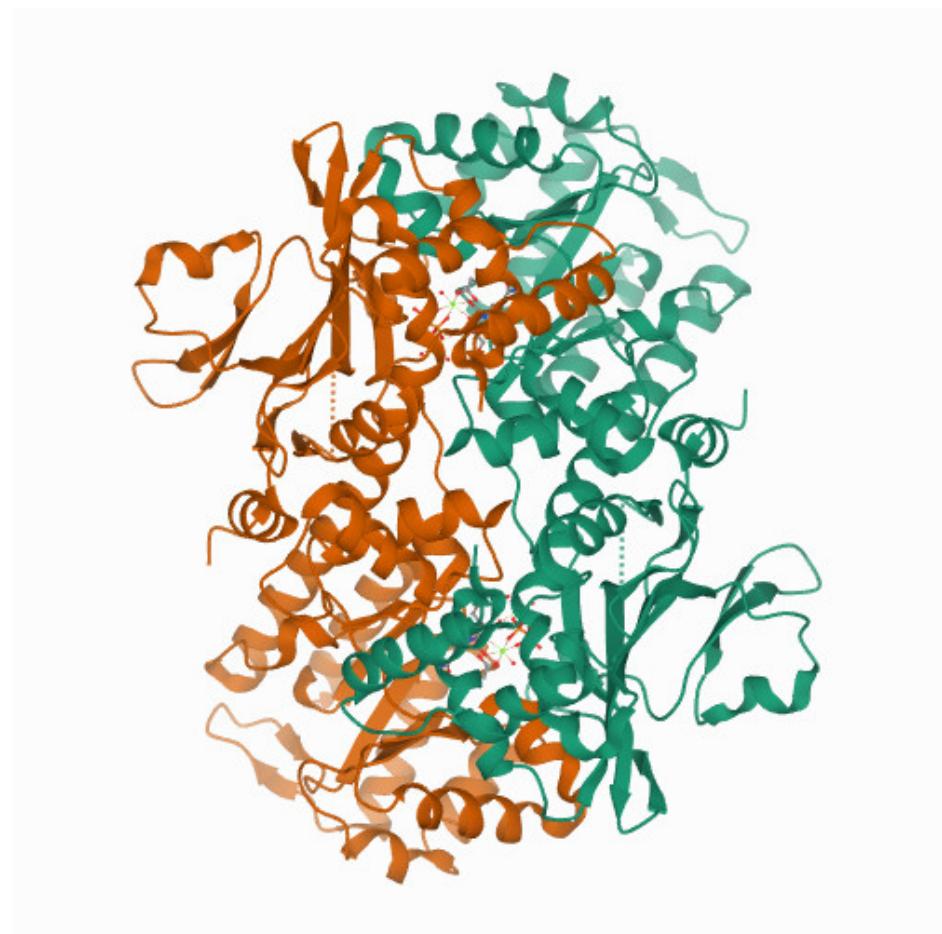
3DGR

Crystal structure of human NAMPT complexed with ADP analogue

Ho, M., Burgos, E.S., Almo, S.C., Schramm, V.L.

(2009) Proc Natl Acad Sci U S A **106**: 13748-13753

Released	2009-08-18
Method	X-RAY DIFFRACTION 2.1 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	A12

[3D View](#)

3DHD

[Download File](#) [View File](#)

Crystal structure of human NAMPT complexed with nicotinamide mononucleotide and pyrophosphate

Ho, M., Burgos, E.S., Almo, S.C., Schramm, V.L.

(2009) Proc Natl Acad Sci U S A **106**: 13748-13753

Released

2009-08-18

Method

X-RAY DIFFRACTION 2 Å

Organisms

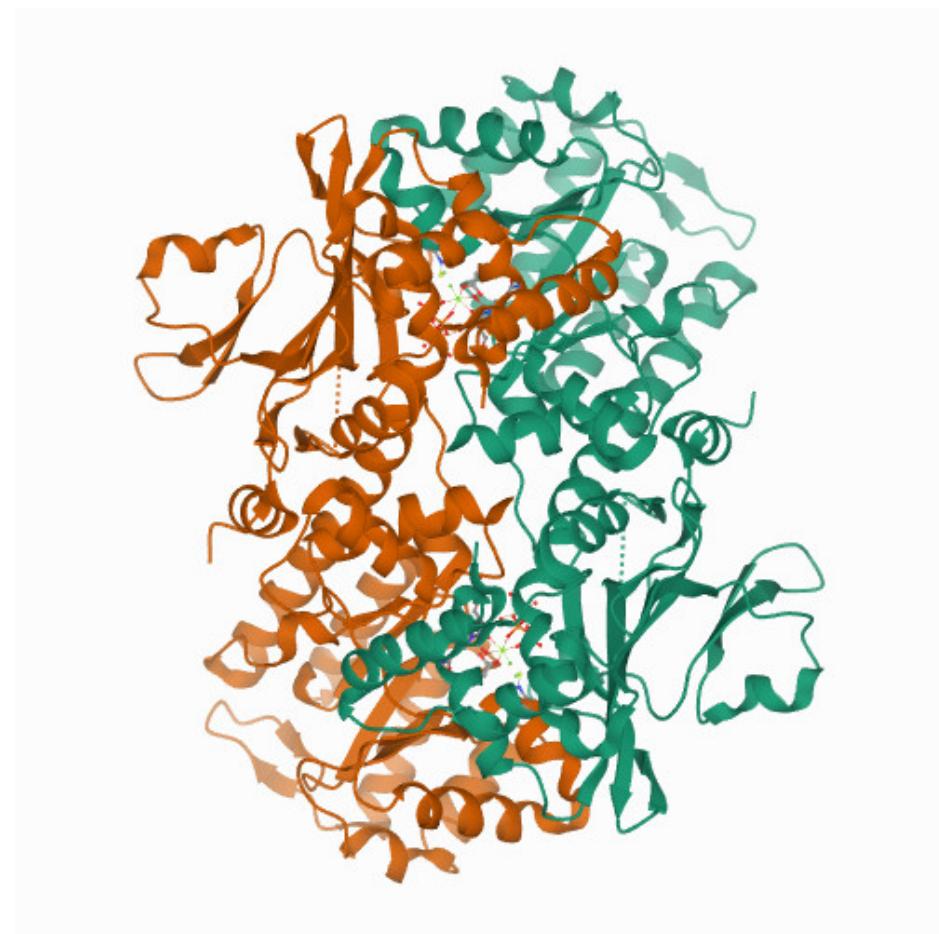
Homo sapiens

Macromolecule

Nicotinamide phosphoribosyltransferase (protein)

Unique Ligands

MG, NMN, POP

[3D View](#)

3DHF

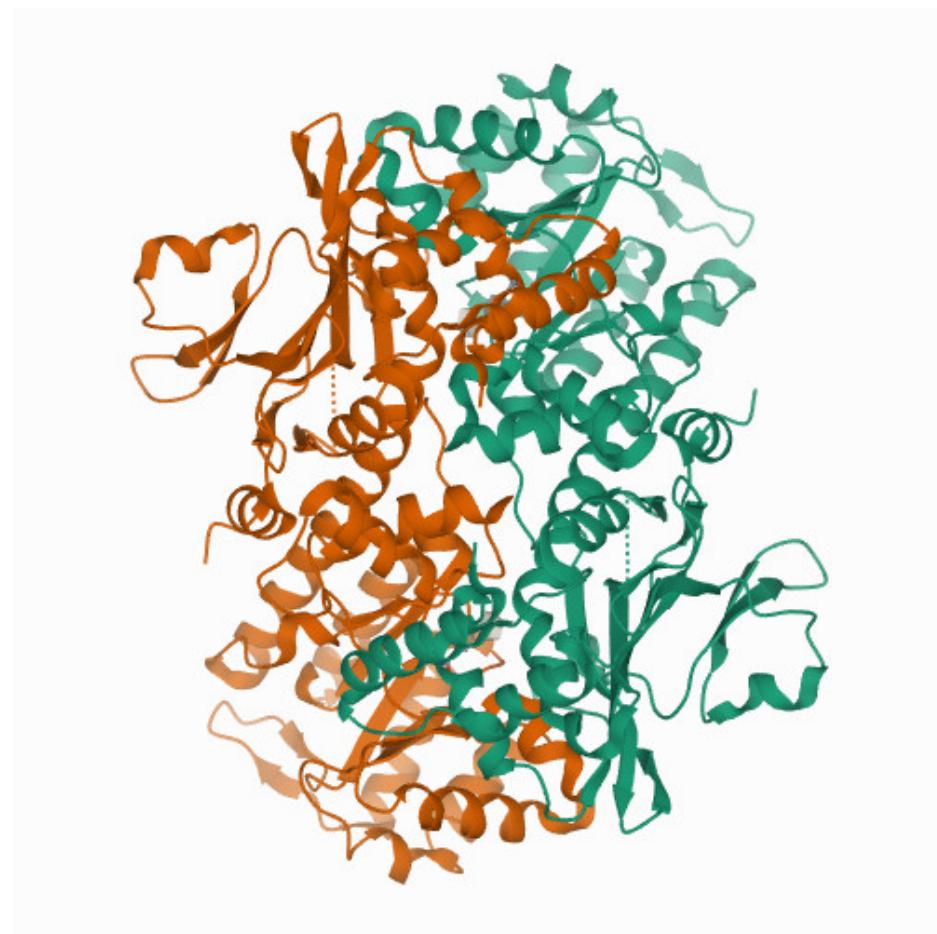
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Crystal structure of phosphorylated mimic form of human NAMPT complexed with nicotinamide mononucleotide and pyrophosphate

Ho, M., Burgos, E.S., Almo, S.C., Schramm, V.L.

(2009) Proc Natl Acad Sci U S A **106**: 13748-13753

Released	2009-08-18
Method	X-RAY DIFFRACTION 1.8 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	BEF, MG, NMN, POP

[3D View](#)

3DKJ

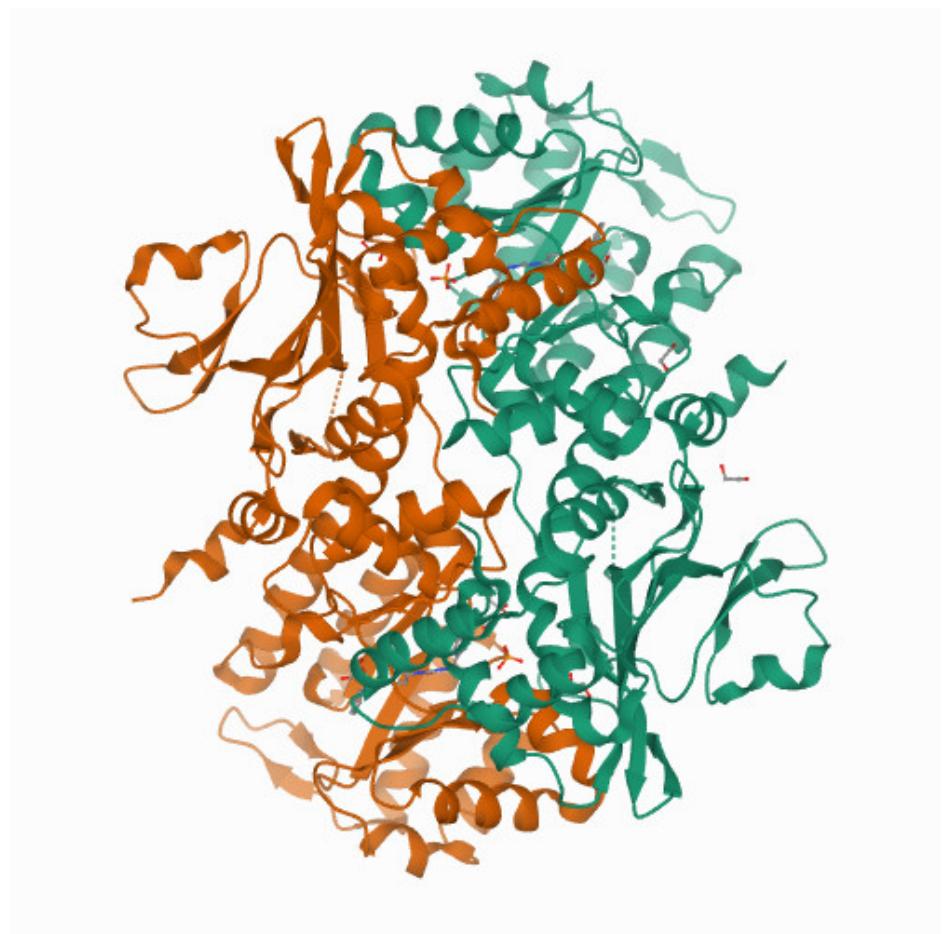
[Download File](#) [View File](#)

Crystal structure of human NAMPT complexed with benzamide and phosphoribosyl pyrophosphate

Ho, M., Burgos, E.S., Almo, S.C., Schramm, V.L.

(2009) Proc Natl Acad Sci U S A **106**: 13748-13753

Released	2009-08-18
Method	X-RAY DIFFRACTION 2 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	PRP, UNU

[3D View](#)

4JNM

[Download File](#) [View File](#)

Discovery of Potent and Efficacious Urea-containing Nicotinamide Phosphoribosyltransferase (NAMPT) Inhibitors with Reduced CYP2C9 Inhibition Properties

Gunzner-Toste, J., Zhao, G., Bauer, P., Baumeister, T., Buckmelter, A.J., Caligiuri, M., Clodfelter, K.H., Fu, B., Han, B., Ho, Y., Kley, N., Liederer, B., Lin, J., Mukadam, S., O'Brien, T., Reynolds, D.J., Sharma, G., Skelton, N., Smith, C.C., Oh, A., Wang, W., Wang, Z., Xiao, Y., Yuen, P., Zak, M., Zhang, L., Zheng, X., Bair, K.W., Dragovich, P.S.

(2013) Bioorg Med Chem Lett **23**: 3531-3538

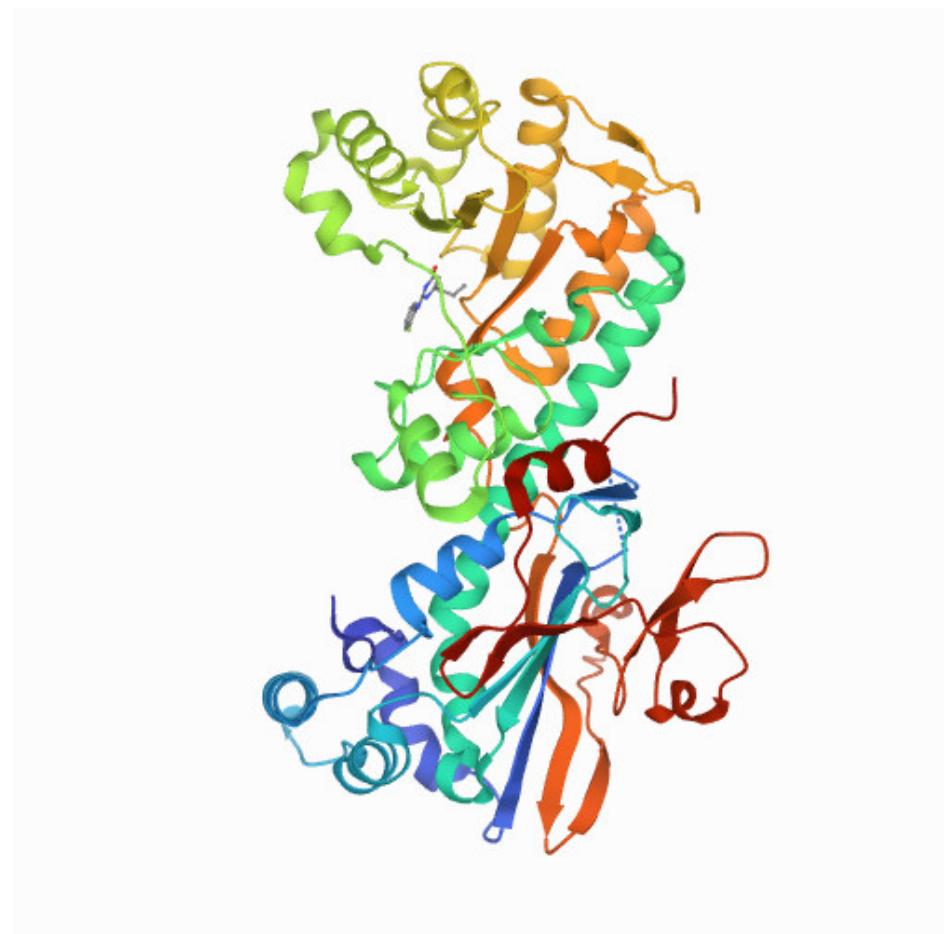
Released 2013-05-29

Method X-RAY DIFFRACTION 2.2 Å

Organisms Homo sapiens

Macromolecule Nicotinamide phosphoribosyltransferase (protein)

Unique Ligands 1LJ, EDO, PO4

[3D View](#)

5WI0

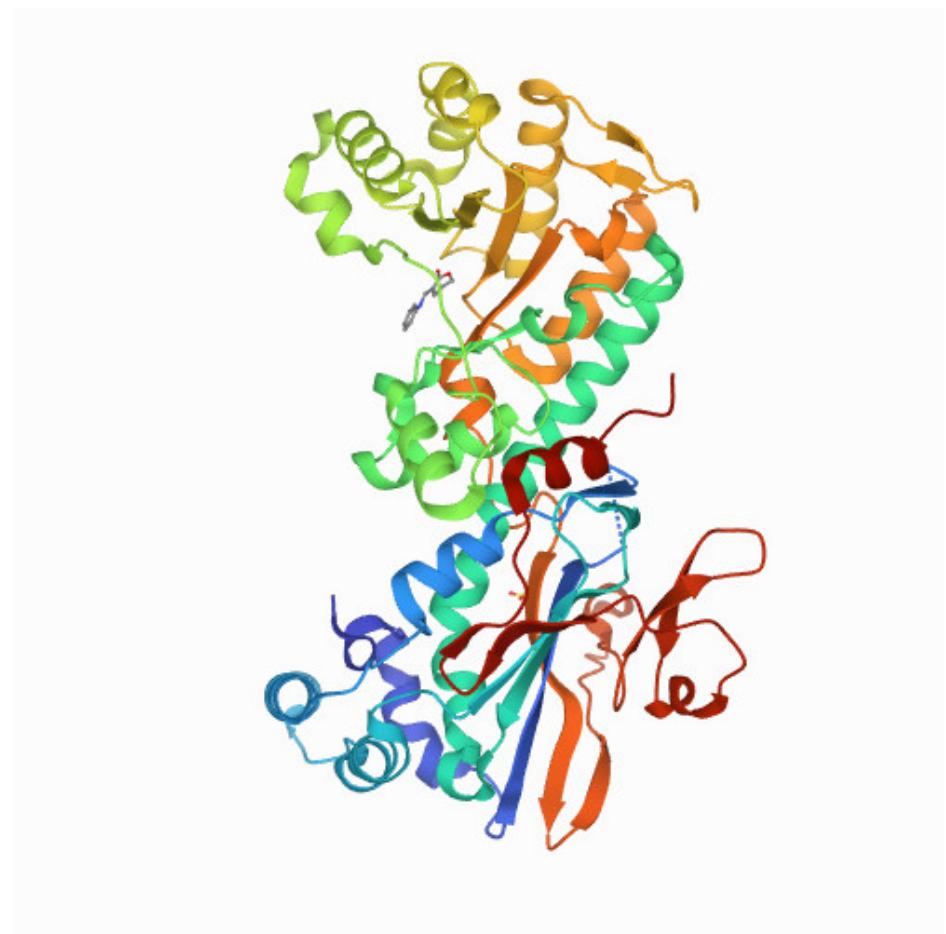
[Download File](#)[View File](#)

Crystal structure of human NAMPT with fragment 2: 2-[(2-fluorophenyl)amino]-6-propylpyrimidin-4(3H)-one

Longenecker, K.L., Raich, D., Korepanova, A.V.

(2018) Bioorg Med Chem Lett **28**: 437-440

Released	2018-01-10
Method	X-RAY DIFFRACTION 2.05 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	AQ1

[3D View](#)

5WI1

[Download File](#) [View File](#)

Crystal structure of human NAMPT with fragment 5: (3E)-3-[(phenylamino)methylidene]oxan-2-one

Longenecker, K.L., Raich, D., Korepanova, A.V.

(2018) Bioorg Med Chem Lett **28**: 437-440

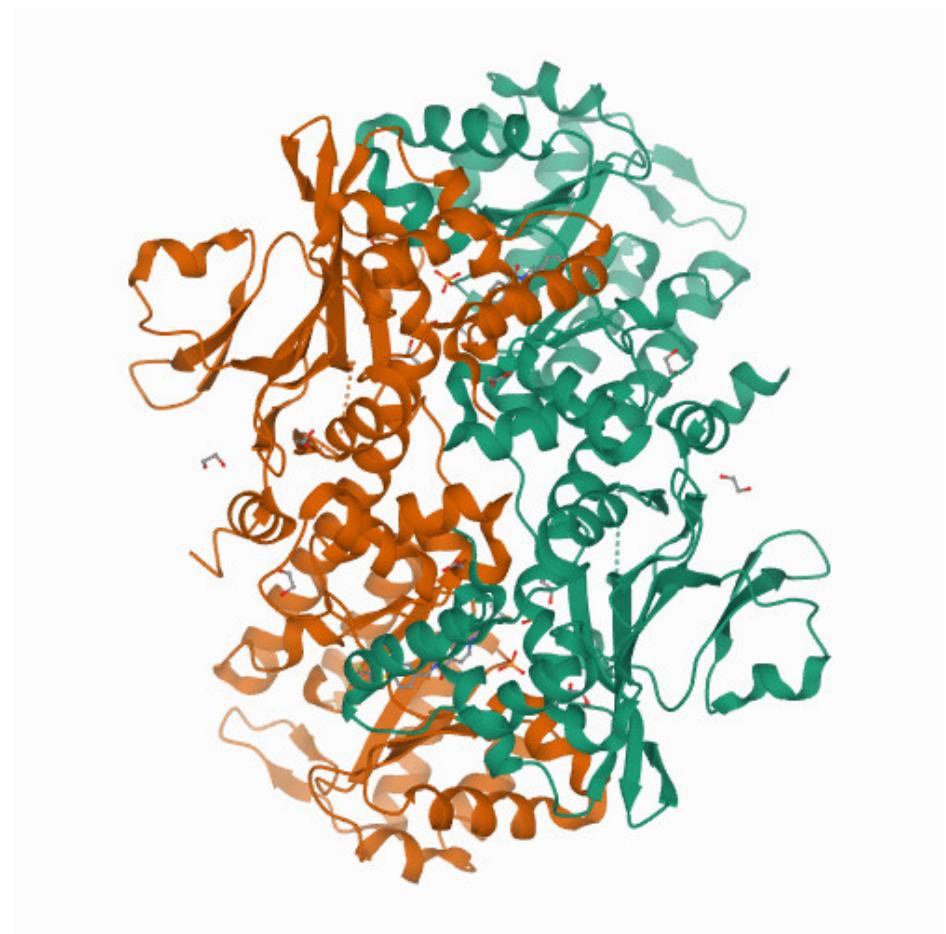
Released 2018-01-10

Method X-RAY DIFFRACTION 1.99 Å

Organisms Homo sapiens

Macromolecule Nicotinamide phosphoribosyltransferase (protein)

Unique Ligands AOY, SO4

[3D View](#)

4O10

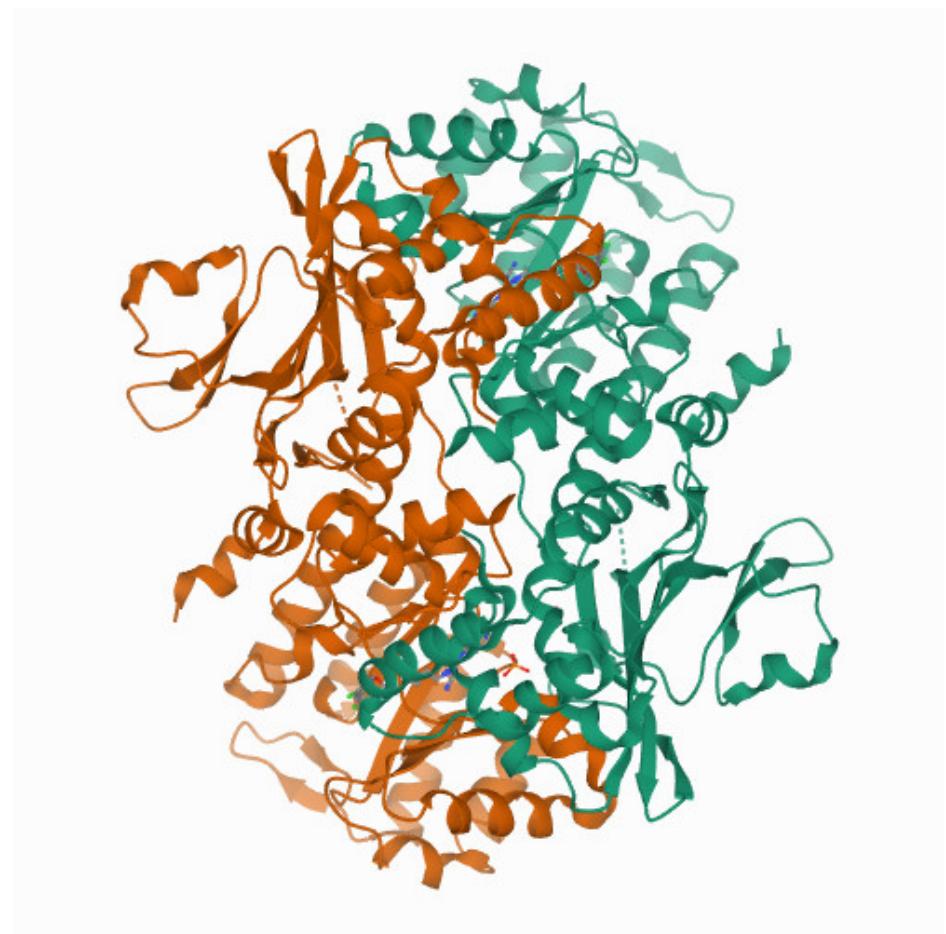
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Structural and Biochemical Analyses of the Catalysis and Potency Impact of Inhibitor Phosphoribosylation by Human Nicotinamide Phosphoribosyltransferase

Oh, A., Wang, W.

(2014) Chembiochem **15**: 1121-1130

Released	2014-06-18
Method	X-RAY DIFFRACTION 1.55 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	2QF, EDO, PO4

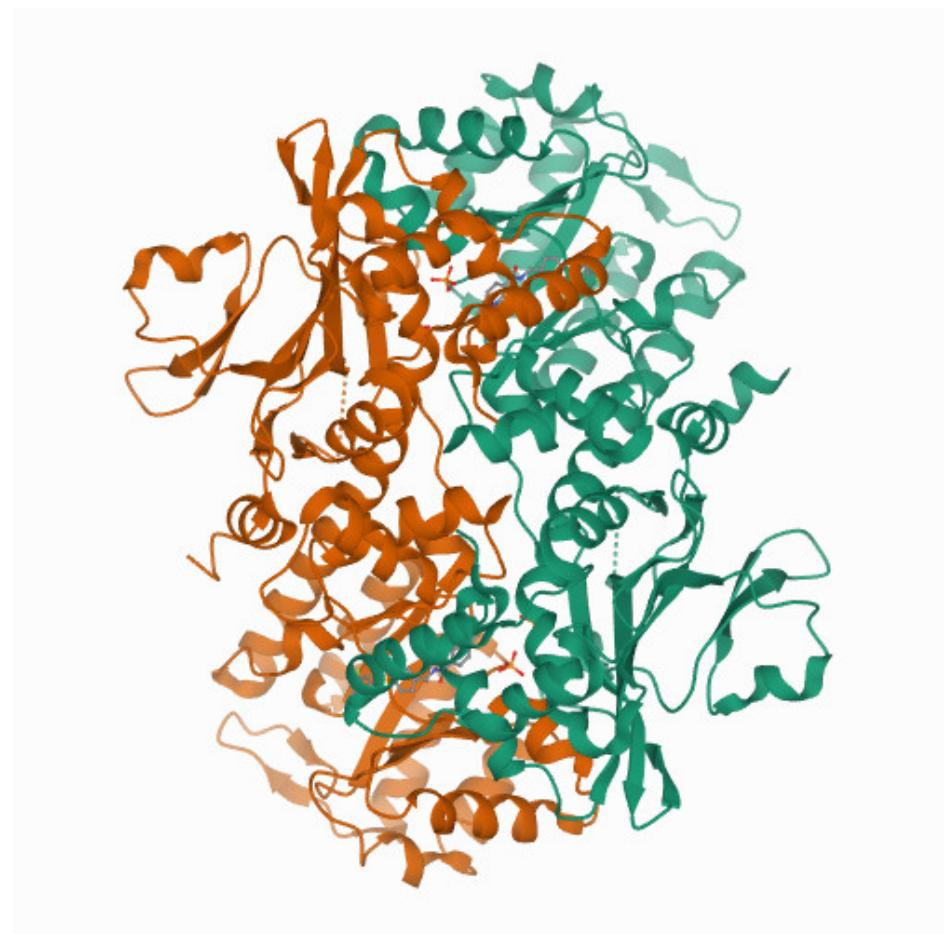
[3D View](#)**4O12**[Download File](#) [View File](#)

Structural and Biochemical Analyses of the Catalysis and Potency Impact of Inhibitor Phosphoribosylation by Human Nicotinamide Phosphoribosyltransferase

Oh, A., Wang, W.

(2014) Chembiochem **15**: 1121-1130

Released	2014-06-18
Method	X-RAY DIFFRACTION 2.498 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	2QG, PO4

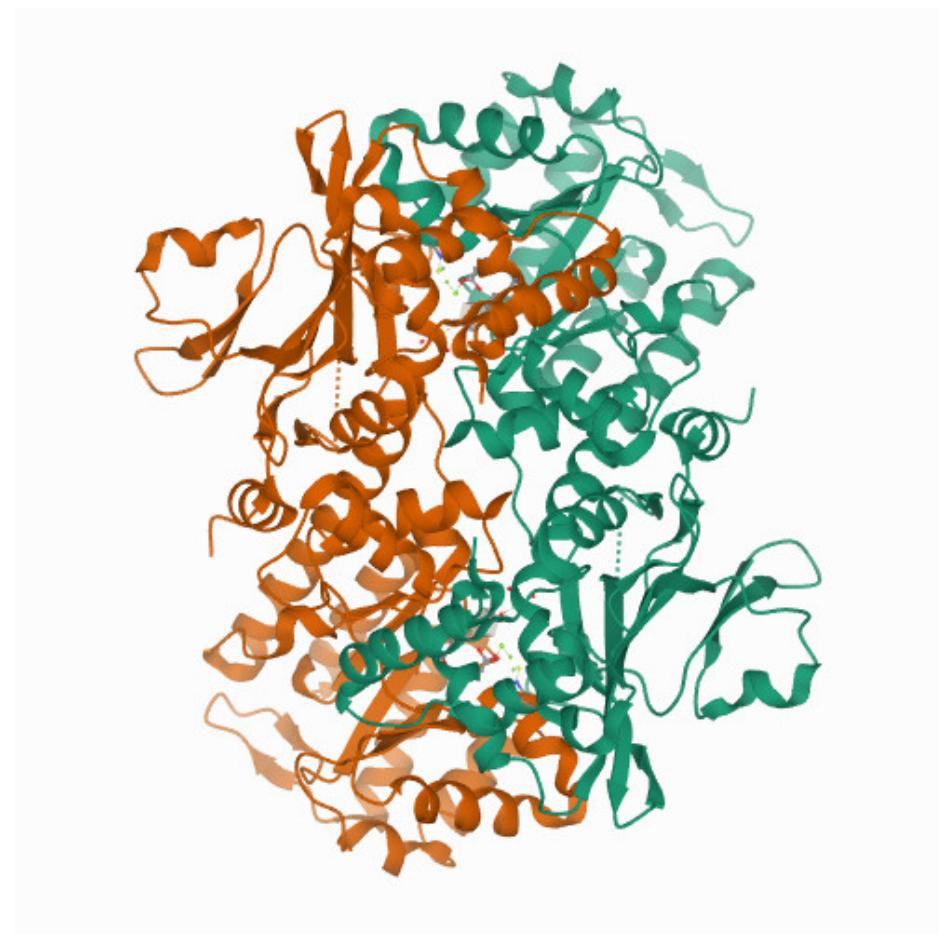
[3D View](#)**4O0Z**[Download File](#) [View File](#)

Structural and Biochemical Analyses of the Catalysis and Potency Impact of Inhibitor Phosphoribosylation by Human Nicotinamide Phosphoribosyltransferase

Oh, A., Wang, W.

(2014) Chembiochem **15**: 1121-1130

Released	2014-06-18
Method	X-RAY DIFFRACTION 2.049 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	2RM, PO4

[3D View](#)

3DKL

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Crystal structure of phosphorylated mimic form of human NAMPT complexed with benzamide and phosphoribosyl pyrophosphate

Ho, M., Burgos, E.S., Almo, S.C., Schramm, V.L.

(2009) Proc Natl Acad Sci U S A **106**: 13748-13753

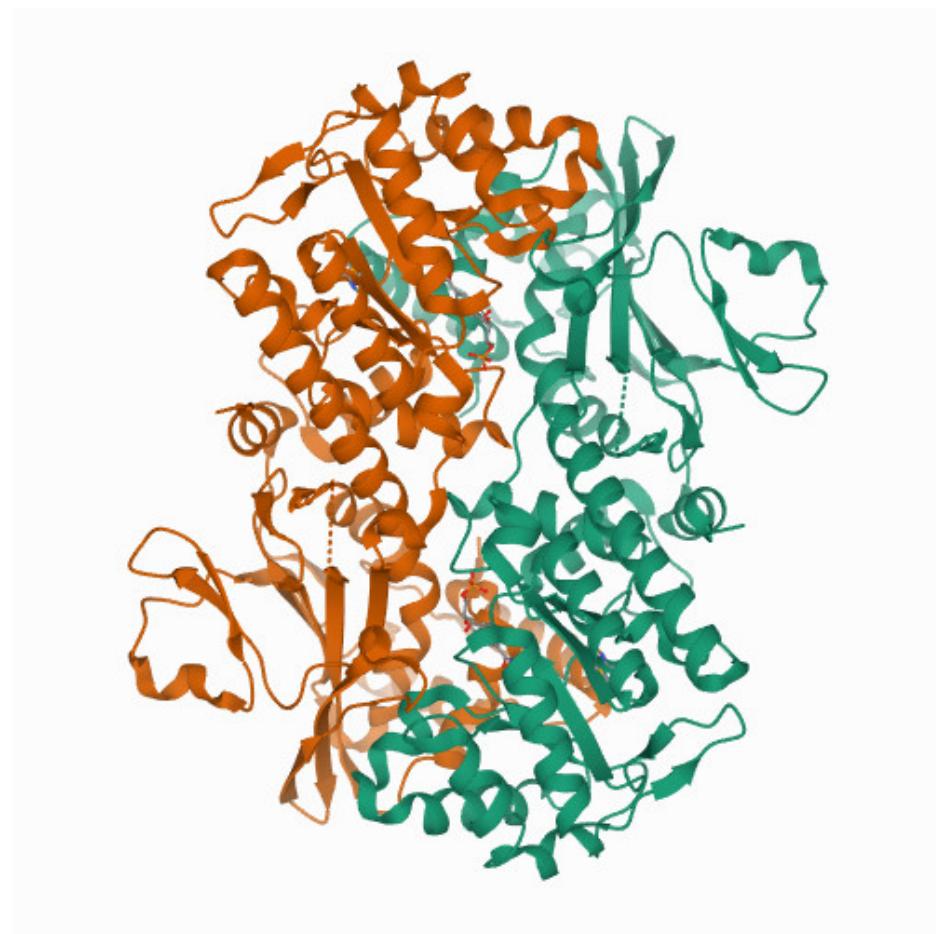
Released 2009-08-18

Method X-RAY DIFFRACTION 1.89 Å

Organisms Homo sapiens

Macromolecule Nicotinamide phosphoribosyltransferase (protein)

Unique Ligands BEF, MG, PRP, UNU

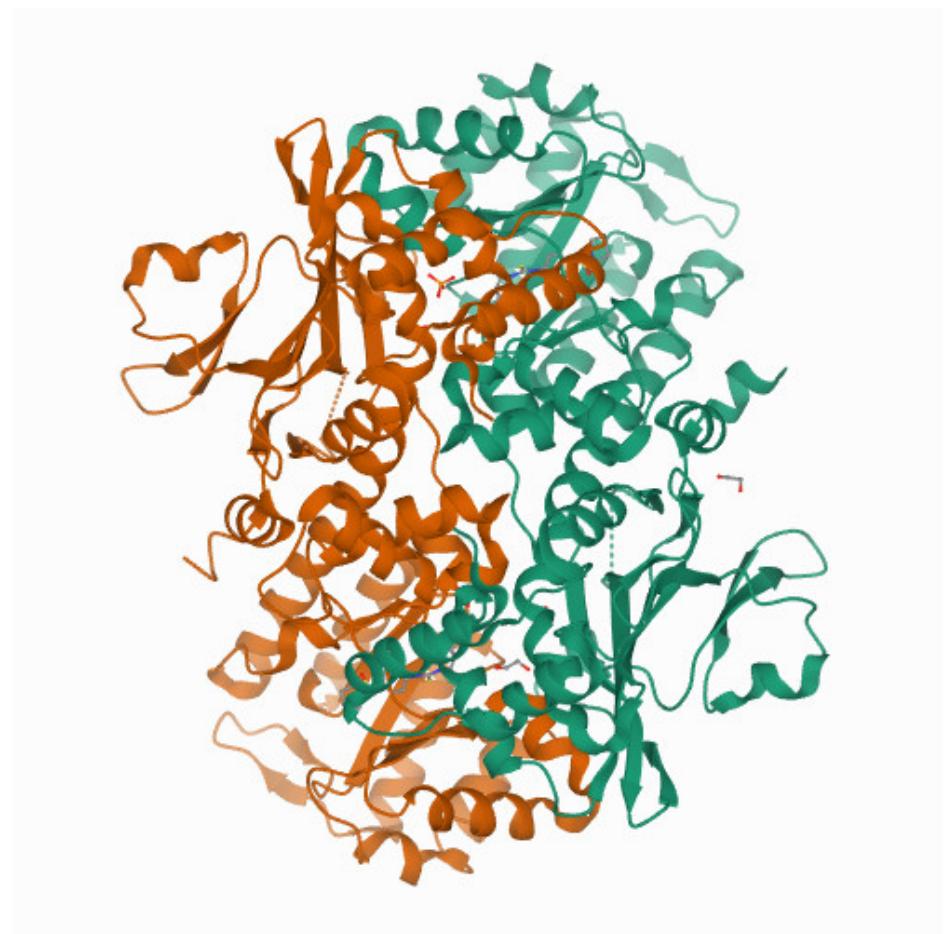
[3D View](#)**2H3D**[Download File](#) [View File](#)

Crystal Structure of Mouse Nicotinamide Phosphoribosyltransferase/Visfatin/Pre-B Cell Colony Enhancing Factor in Complex with Nicotinamide Mononucleotide

Wang, T., Zhang, X., Bheda, P., Revollo, J.R., Imai, S.I., Wolberger, C.

(2006) Nat Struct Mol Biol **13**: 661-662

Released	2006-06-20
Method	X-RAY DIFFRACTION 2.1 Å
Organisms	Mus musculus
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	NMN

[3D View](#)

4JR5

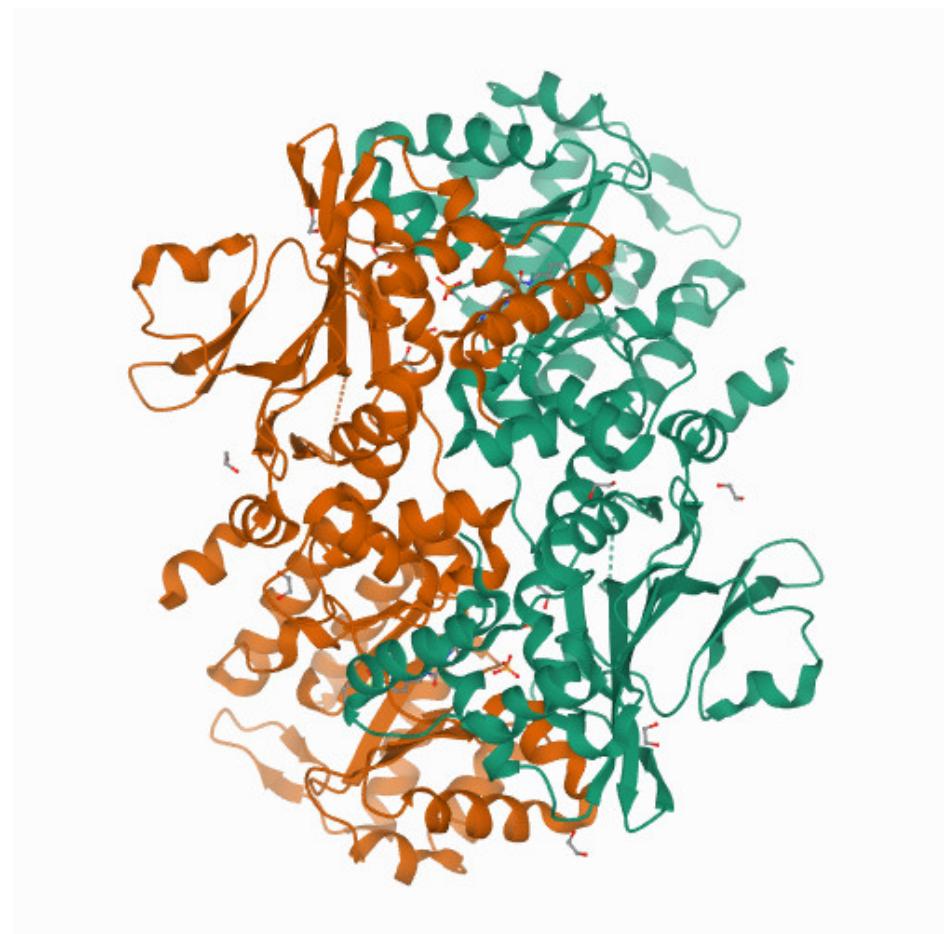
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Structure-based Identification of Ureas as Novel Nicotinamide Phosphoribosyltransferase (Nampt) Inhibitors

Zheng, X., Bauer, P., Baumeister, T., Buckmelter, A.J., Caligiuri, M., Clodfelter, K.H., Han, B., Ho, Y., Kley, N., Lin, J., Reynolds, D.J., Sharma, G., Smith, C.C., Wang, Z., Dragovich, P.S., Oh, A., Wang, W., Zak, M., Gunzner-Toste, J., Zhao, G., Yuen, P., Bair, K.W.

(2013) J Med Chem **56**: 4921-4937

Released	2013-05-08
Method	X-RAY DIFFRACTION 1.906 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	1LS, EDO, PO4

[3D View](#)

4KFN

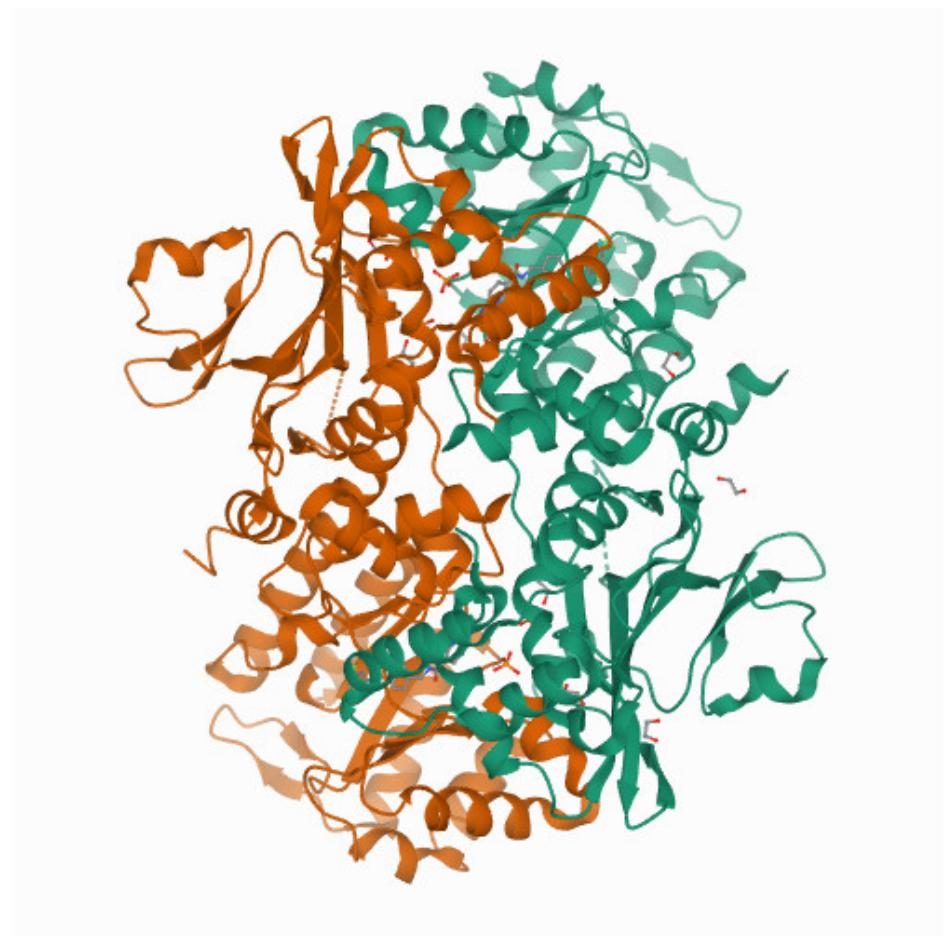
[Download File](#) [View File](#)

Structure-Based Discovery of Novel Amide-Containing Nicotinamide Phosphoribosyltransferase (Nampt) Inhibitors

Zheng, X., Bauer, P., Baumeister, T., Buckmelter, A.J., Caligiuri, M., Clodfelter, K.H., Han, B., Ho, Y., Kley, N., Lin, J., Reynolds, D.J., Sharma, G., Smith, C.C., Wang, Z., Dragovich, P.S., Gunzner-Toste, J., Liederer, B.M., Ly, J., O'Brien, T., Oh, A., Wang, L., Wang, W., Xiao, Y., Zak, M., Zhao, G., Yuen, P., Bair, K.W.

(2013) J Med Chem **56**: 4921-4937

Released	2013-05-08
Method	X-RAY DIFFRACTION 1.6 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	1QR, EDO, PO4

[3D View](#)

4KFO

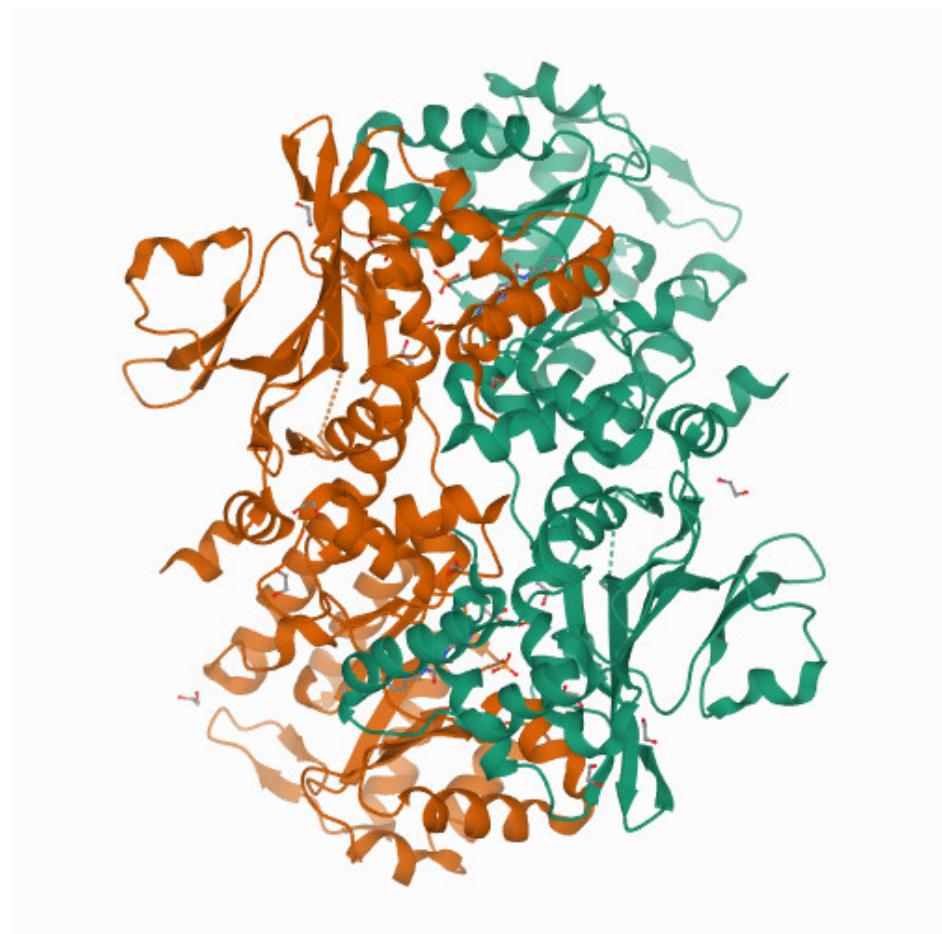
[Download File](#) [View File](#)

Structure-Based Discovery of Novel Amide-Containing Nicotinamide Phosphoribosyltransferase (Nampt) Inhibitors

Zheng, X., Bauer, P., Baumeister, T., Buckmelter, A.J., Caligiuri, M., Clodfelter, K.H., Han, B., Ho, Y., Kley, N., Lin, J., Reynolds, D.J., Sharma, G., Smith, C.C., Wang, Z., Dragovich, P.S., Gunzner-Tosteb, J., Liederer, B.M., Ly, J., O'Brien, T., Oh, A., Wang, L., Wang, W., Xiao, Y., Zak, M., Zhao, G., Yuen, P., Bair, K.W.

(2013) J Med Chem **56**: 4921-4937

Released	2013-05-08
Method	X-RAY DIFFRACTION 1.6 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	1QS, EDO, PO4

[3D View](#)**4LWW**[Download File](#)[View File](#)

Discovery of Potent and Efficacious Cyanoguanidine-containing Nicotinamide Phosphoribosyltransferase (Nampt) Inhibitors

Zheng, X., Baumeister, T., Buckmelter, A.J., Caligiuri, M., Clodfelter, K.H., Han, B., Ho, Y., Kley, N., Lin, J., Reynolds, D.J., Sharma, G., Smith, C.C., Wang, Z., Dragovich, P.S., Oh, A., Wang, W., Zak, M., Wang, L., Yuen, P., Bair, K.W.

(2014) Bioorg Med Chem Lett **24**: 337-343

Released

2013-12-25

Method

X-RAY DIFFRACTION 1.641 Å

Organisms

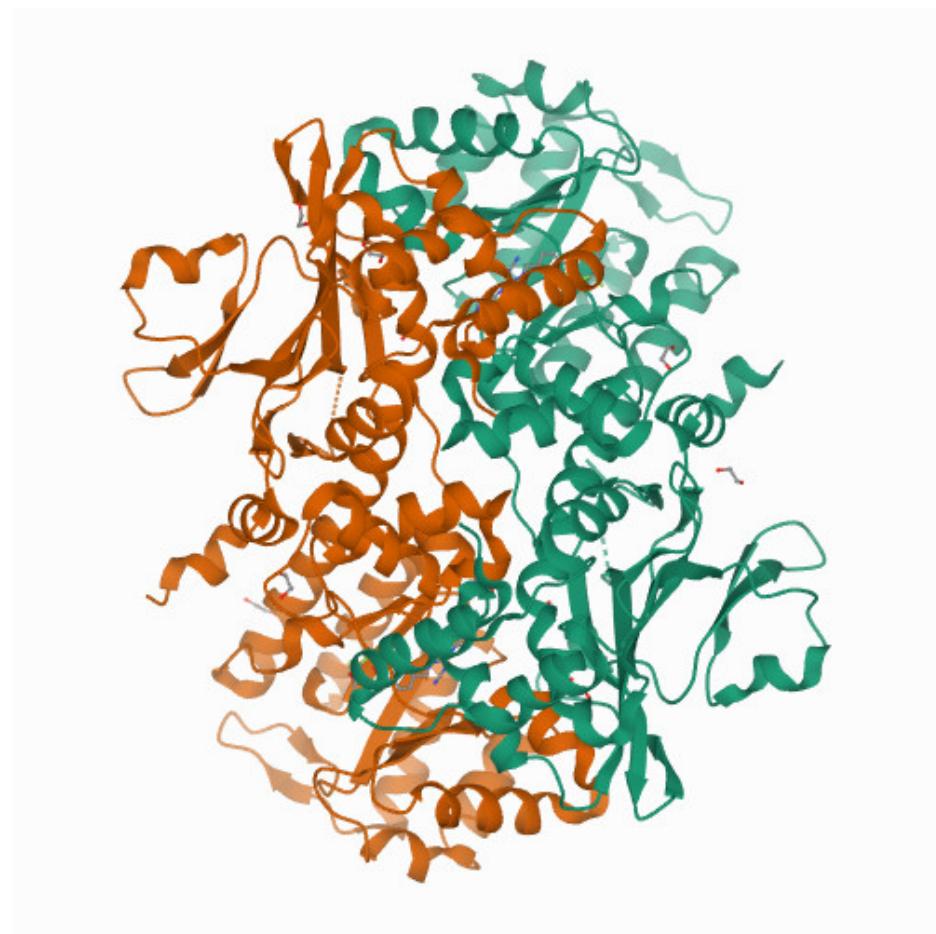
Homo sapiens

Macromolecule

Nicotinamide phosphoribosyltransferase (protein)

Unique Ligands

EDO, LWW, PO4

[3D View](#)

4LTS

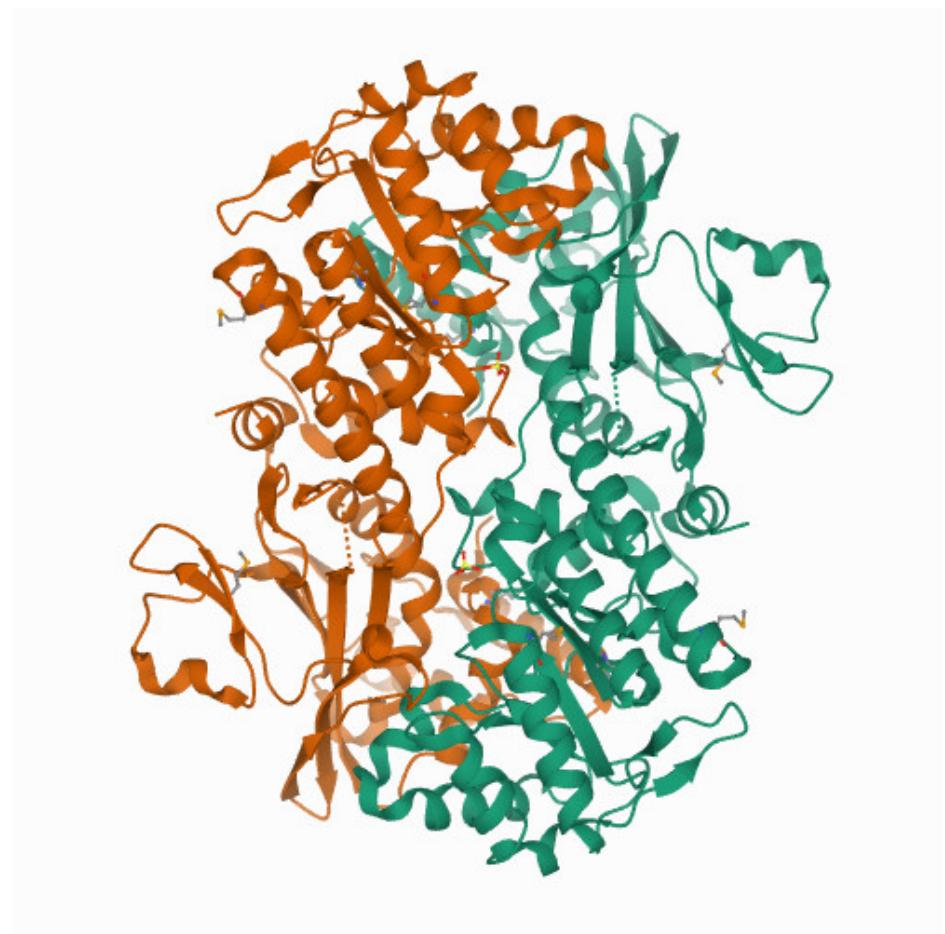
[Download File](#) [View File](#)

Discovery of Potent and Efficacious Cyanoguanidine-containing Nicotinamide Phosphoribosyltransferase (Nampt) Inhibitors

Zheng, X., Baumeister, T., Buckmelter, A.J., Caligiuri, M., Clodfelter, K.H., Han, B., Ho, Y., Kley, N., Lin, J., Reynolds, D.J., Sharma, G., Smith, C.C., Wang, Z., Dragovich, P.S., Oh, A., Wang, W., Zak, M., Wang, L., Yuen, P., Bair, K.W.

(2014) Bioorg Med Chem Lett **24**: 337-343

Released	2013-12-25
Method	X-RAY DIFFRACTION 1.692 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	EDO, LTS, PO4

[3D View](#)

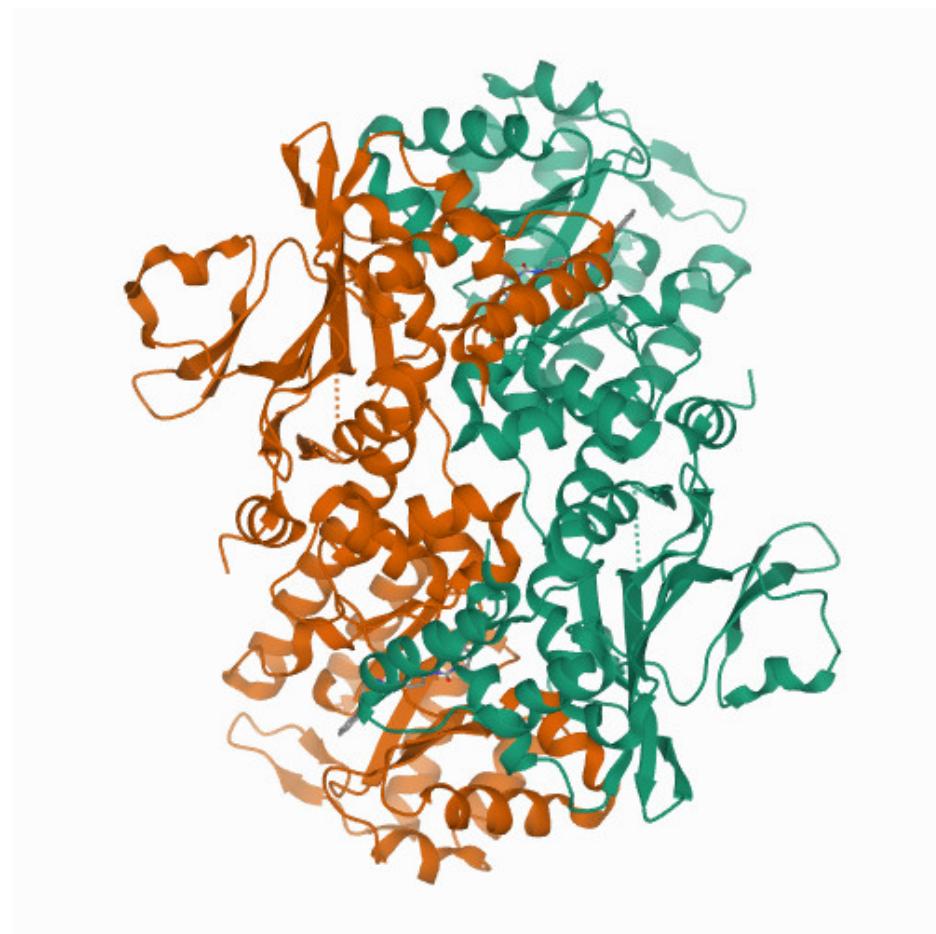
2H3B

[Download File](#) [View File](#)

Crystal Structure of Mouse Nicotinamide Phosphoribosyltransferase/Visfatin/Pre-B Cell Colony Enhancing Factor 1

Wang, T., Zhang, X., Bheda, P., Revollo, J.R., Imai, S.I., Wolberger, C.
(2006) Nat Struct Mol Biol **13**: 661-662

Released	2006-06-20
Method	X-RAY DIFFRACTION 1.95 Å
Organisms	Mus musculus
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	SO4

[3D View](#)

5UPE

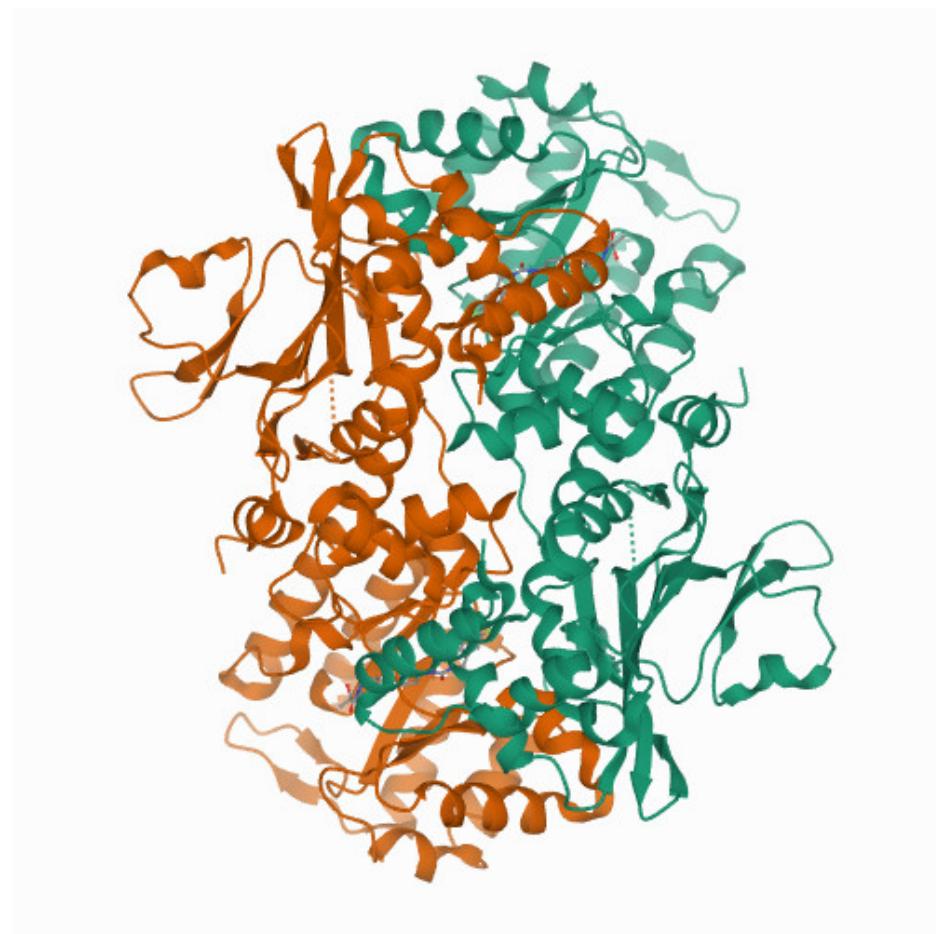
[Download File](#)[View File](#)

Crystal structure of human NAMPT with isoindoline urea inhibitor compound 5

Longenecker, K.L., Raich, D., Korepanova, A.V.

(2017) Bioorg Med Chem Lett **27**: 3317-3325

Released	2017-06-28
Method	X-RAY DIFFRACTION 1.93 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	8HY

[3D View](#)

5UPF

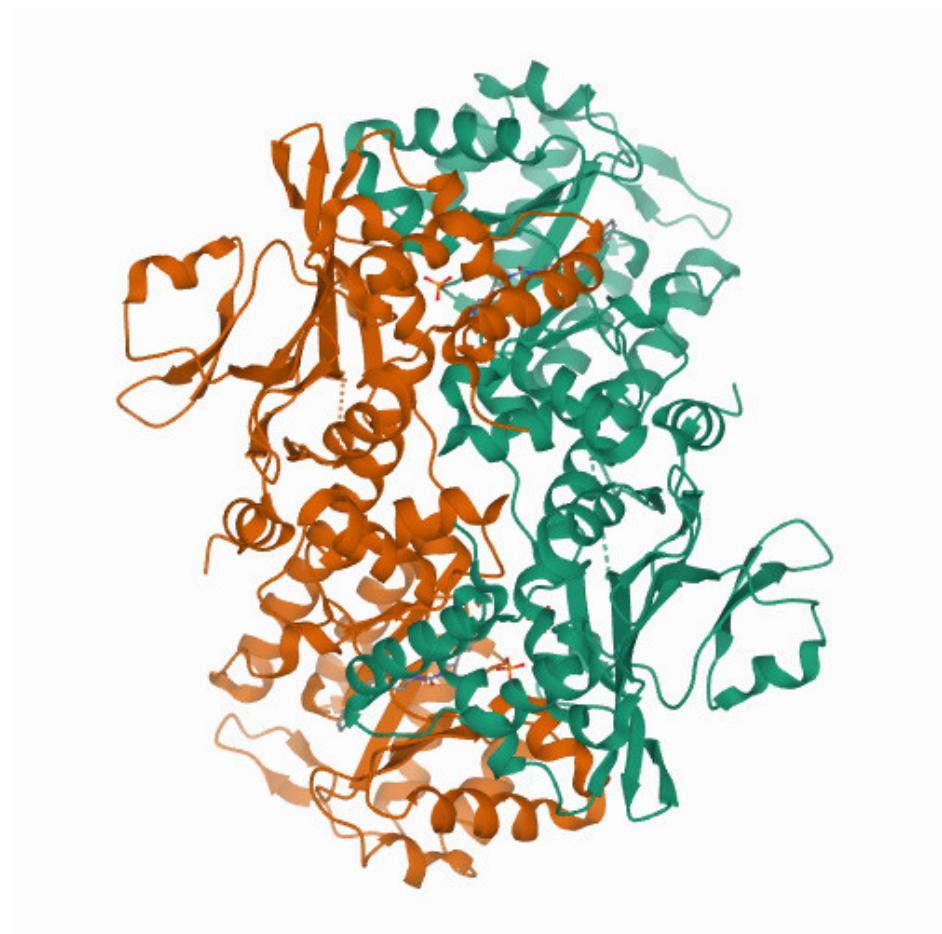
[Download File](#)[View File](#)

Crystal structure of human NAMPT with isoindoline urea inhibitor compound 53

Longenecker, K.L., Raich, D., Korepanova, A.V.

(2017) Bioorg Med Chem Lett **27**: 3317-3325

Released	2017-06-28
Method	X-RAY DIFFRACTION 1.69 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	8HV

[3D View](#)

6PEB

[Download File](#)[View File](#)

Crystal Structure of human NAMPT in complex with NVP-LTM976

Weihofen, W.A.

(2019) ACS Med Chem Lett **10**: 1524-1529

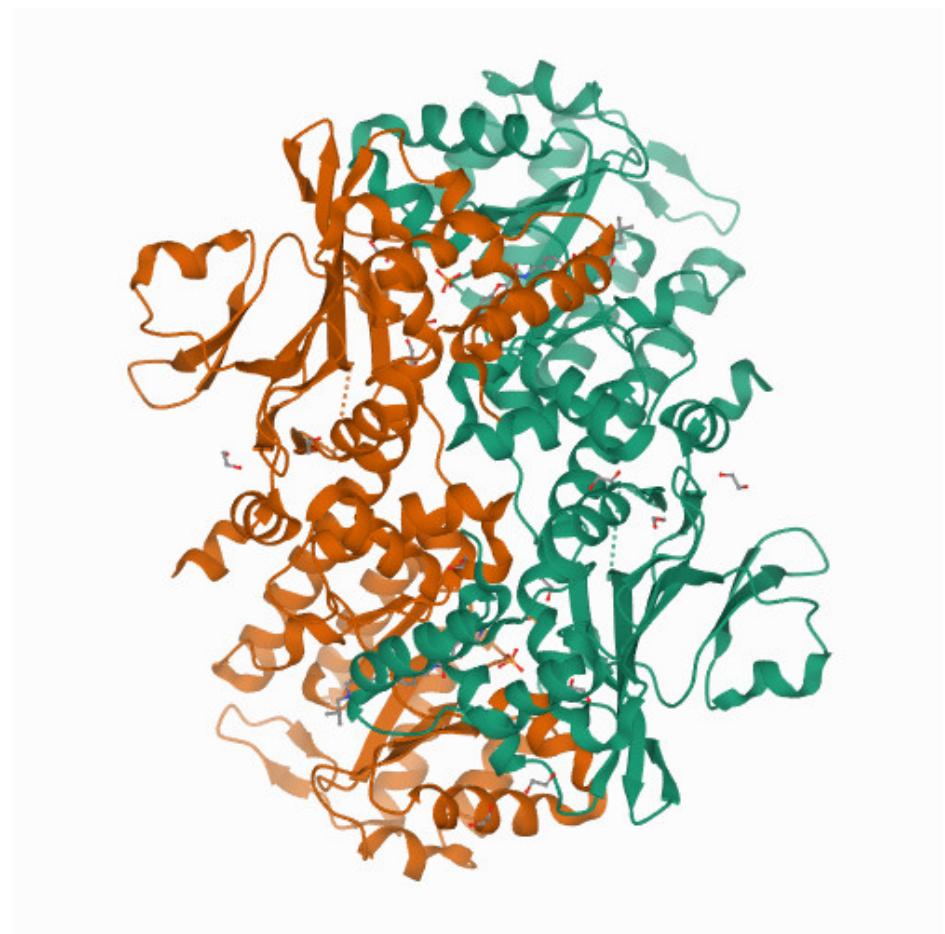
Released 2019-12-04

Method X-RAY DIFFRACTION 2.46 Å

Organisms Homo sapiens

Macromolecule Nicotinamide phosphoribosyltransferase (protein)

Unique Ligands OE4, PO4

[3D View](#)

4WQ6

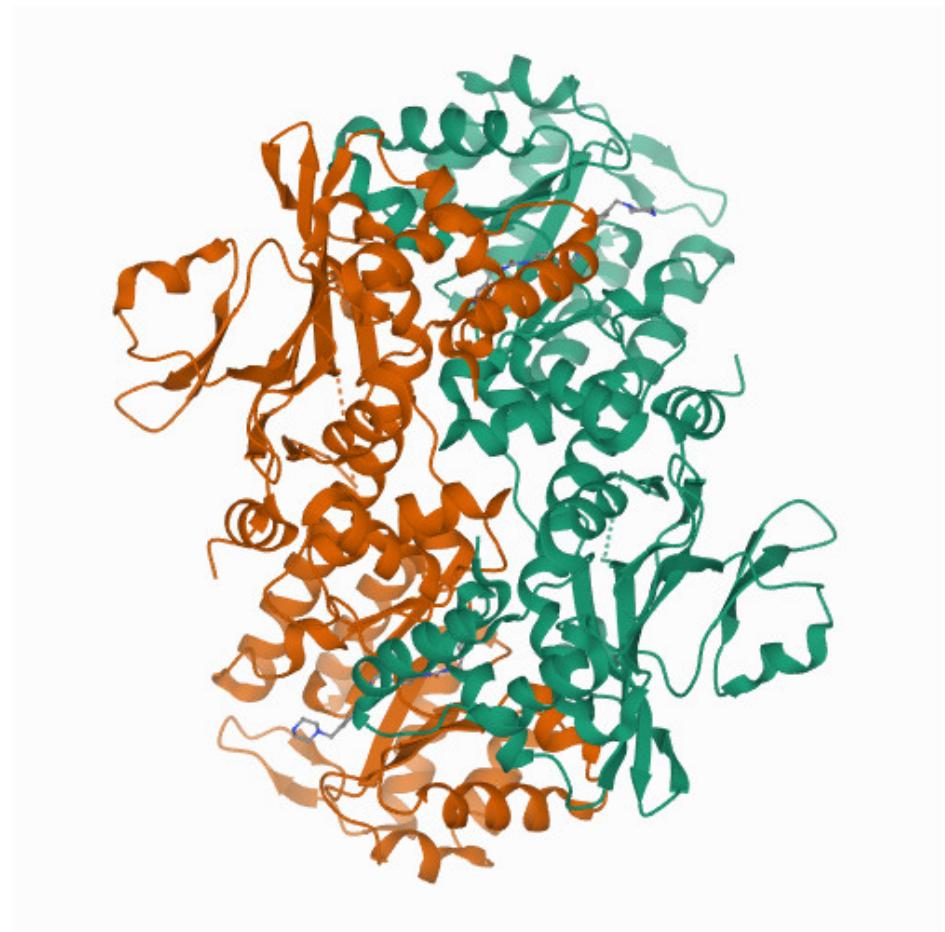
[Download File](#) [View File](#)

The crystal structure of human Nicotinamide phosphoribosyltransferase (NAMPT) in complex with N-(4-((S)-[1-(2-methylpropyl)piperidin-4-yl]sulfinyl)benzyl)furo[2,3-c]pyridine-2-carboxamide inhibitor (compound 21)

Li, D., Wang, W.

(2015) Bioorg Med Chem Lett **25**: 529-541

Released	2015-02-11
Method	X-RAY DIFFRACTION 1.72 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	3TQ, EDO, PO4

[3D View](#)

6B75

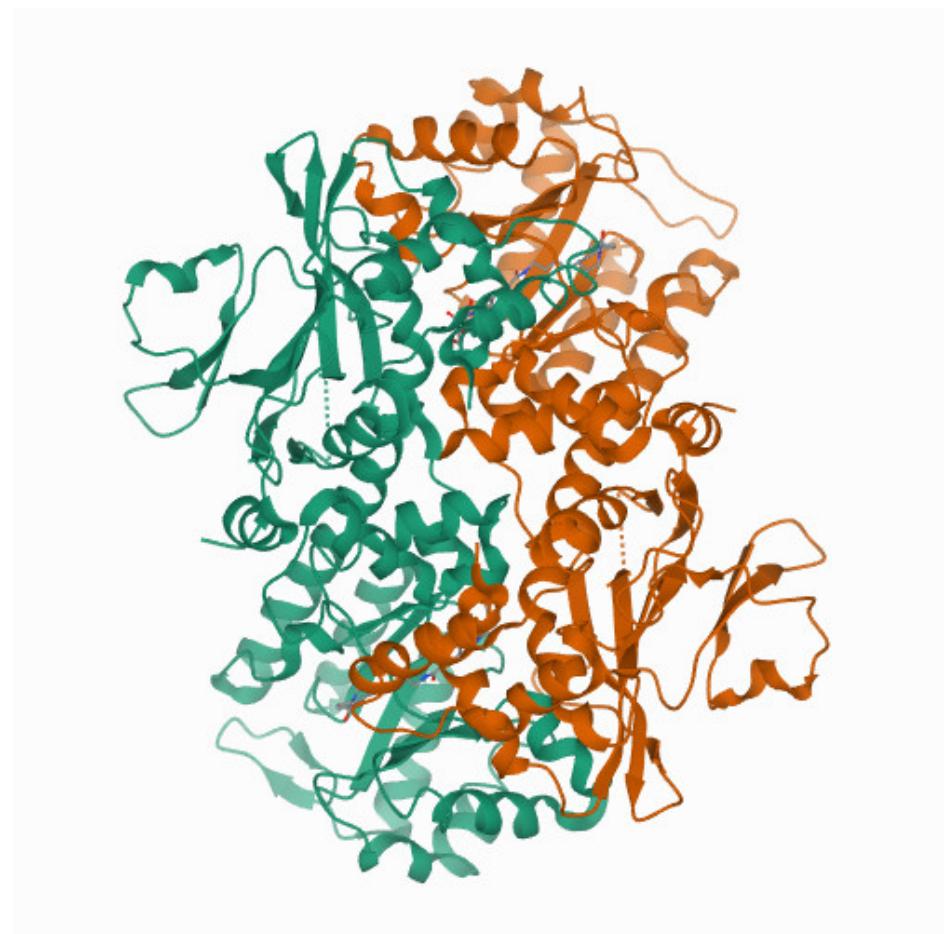
[Download File](#) [View File](#)

Crystal Structure of human NAMPT in complex with NVP-LOQ594

Weihofen, W.A., Thigale, S.

To be published

Released	2018-10-03
Method	X-RAY DIFFRACTION 2.53 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	CVP

 3D View

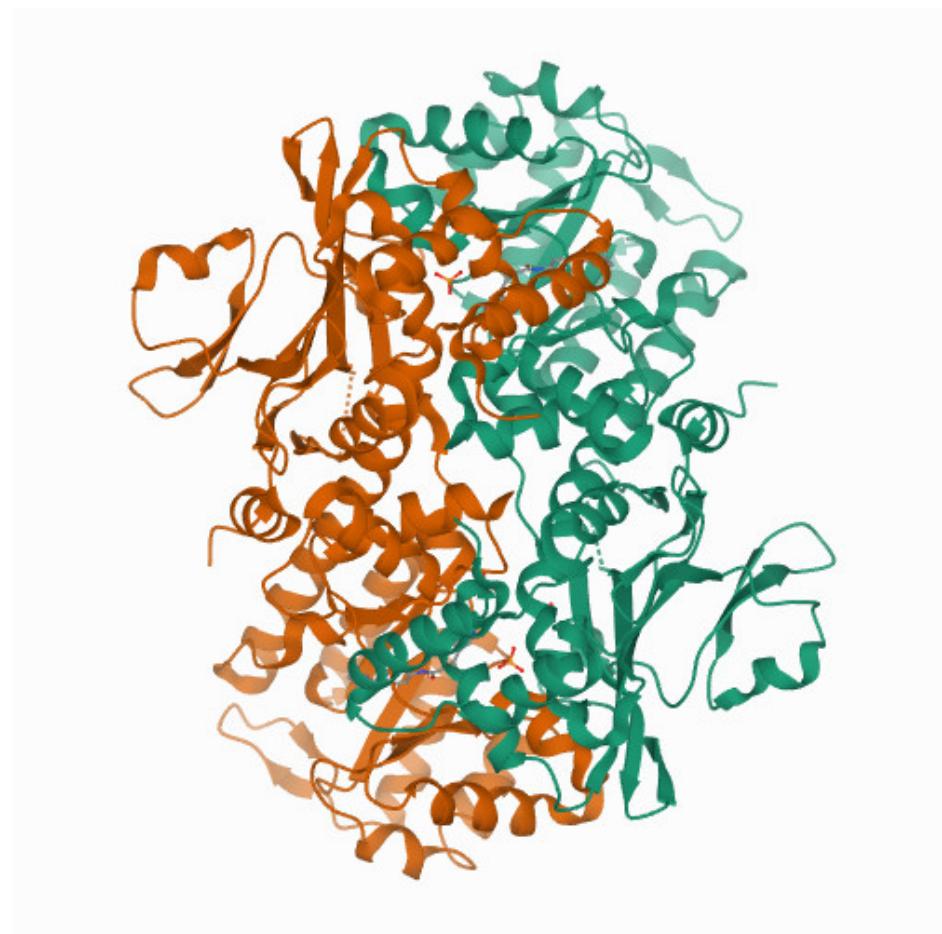
3G8E

 Download File View File **Crystal Structure of Rattus norvegicus Visfatin/PBEF/Nampt in Complex with an FK866-based inhibitor**

Kang, G.B., Bae, M.H., Kim, M.K., Im, I., Kim, Y.C., Eom, S.H.

(2009) Mol Cells **27**: 667-671

Released	2009-08-18
Method	X-RAY DIFFRACTION 3 Å
Organisms	Rattus norvegicus
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	IS1

[3D View](#)

6B76

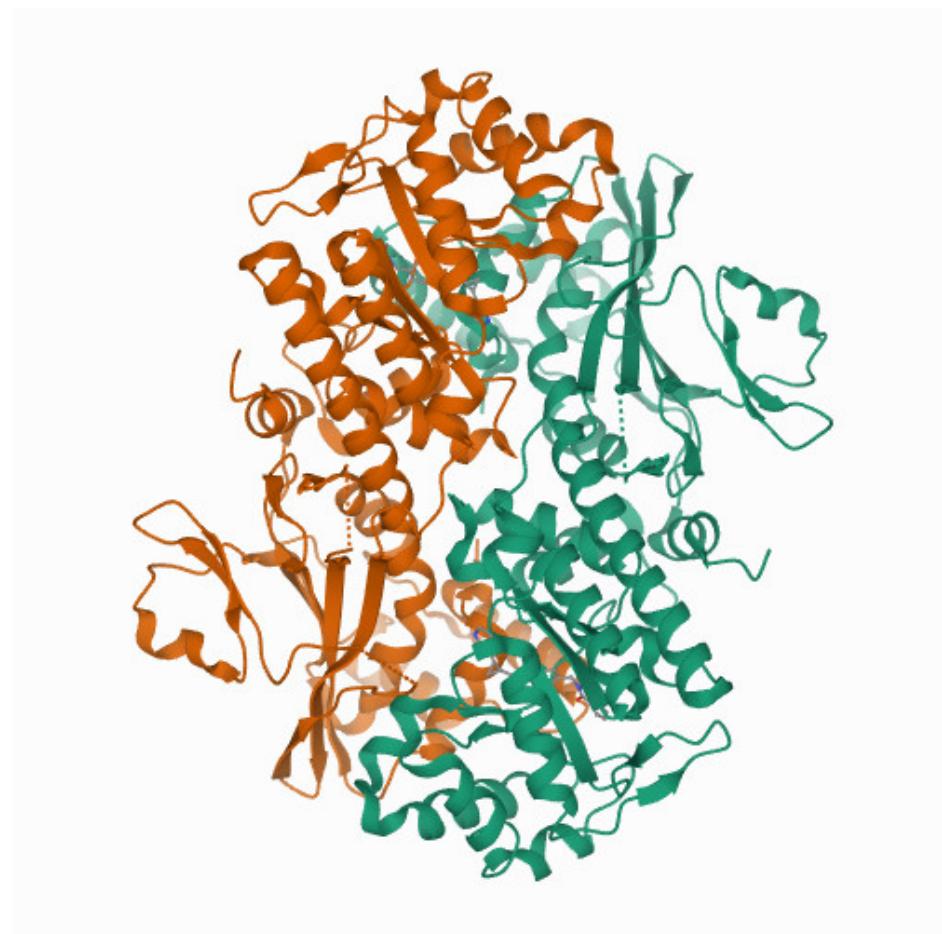
[Download File](#) [View File](#)

Crystal Structure of human NAMPT in complex with NVP-LVR596

Weihofen, W.A., Thigale, S.

To be published

Released	2018-10-03
Method	X-RAY DIFFRACTION 2.44 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	CVJ, PO4

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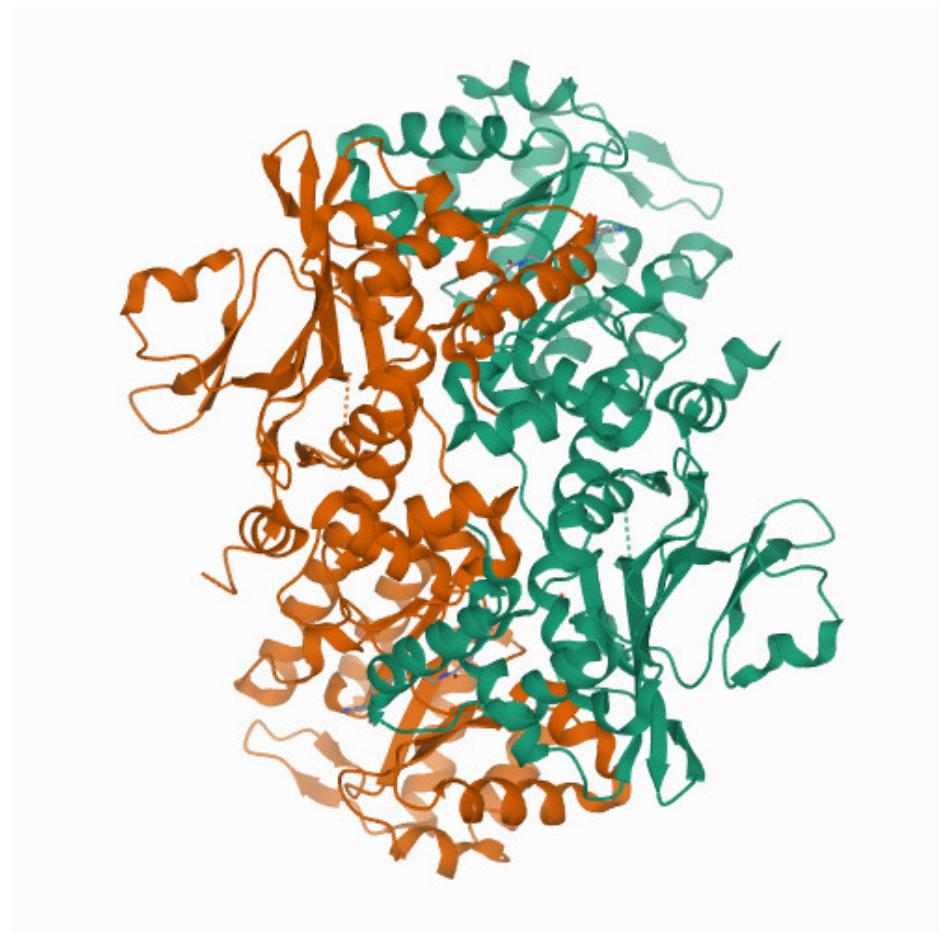
6AZJ

Crystal Structure of human NAMPT in complex with NVP-LQN520

Weihofen, W.A., Thigale, S.

To be published

Released	2018-09-12
Method	X-RAY DIFFRACTION 2.53 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	C5V

 [3D View](#)[Download File](#) [View File](#)

6E68

NAMPT co-crystal with inhibitor compound 2

Waight, A.B., Neumann, C.S.

To be published

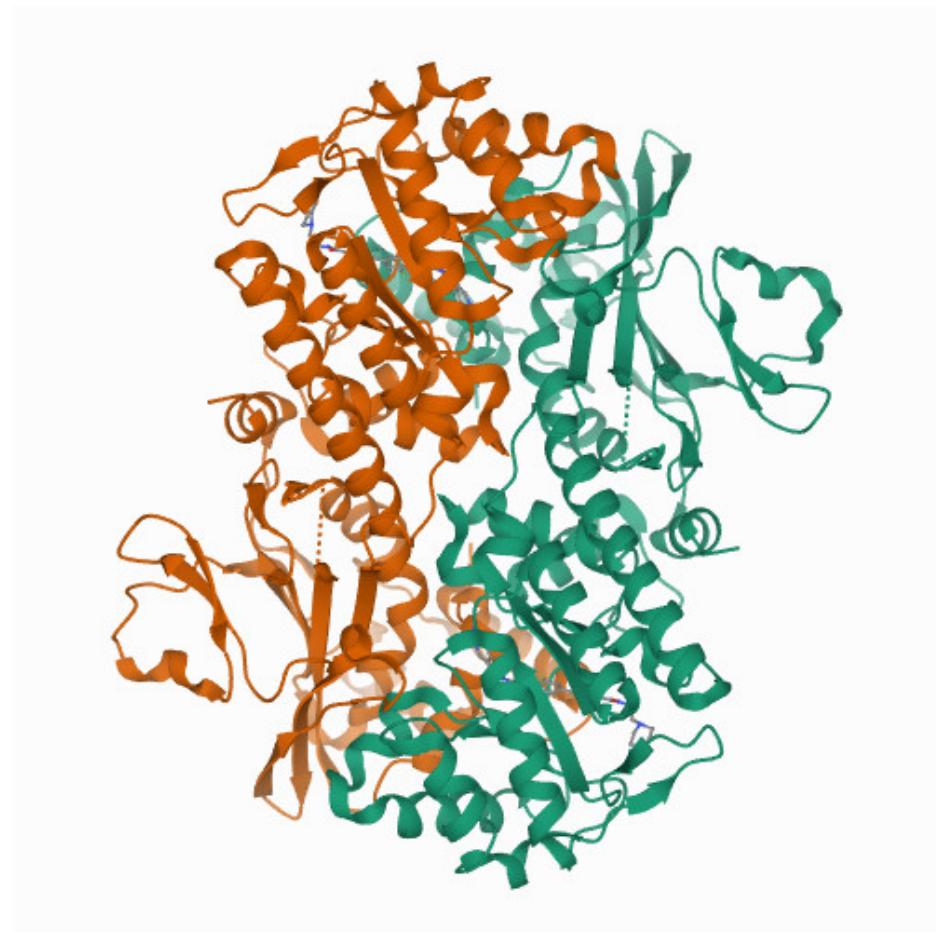
Released 2018-08-08

Method X-RAY DIFFRACTION 1.5 Å

Organisms Homo sapiens

Macromolecule Nicotinamide phosphoribosyltransferase (protein)

Unique Ligands HVM, PO4

[3D View](#)[Download File](#) [View File](#)

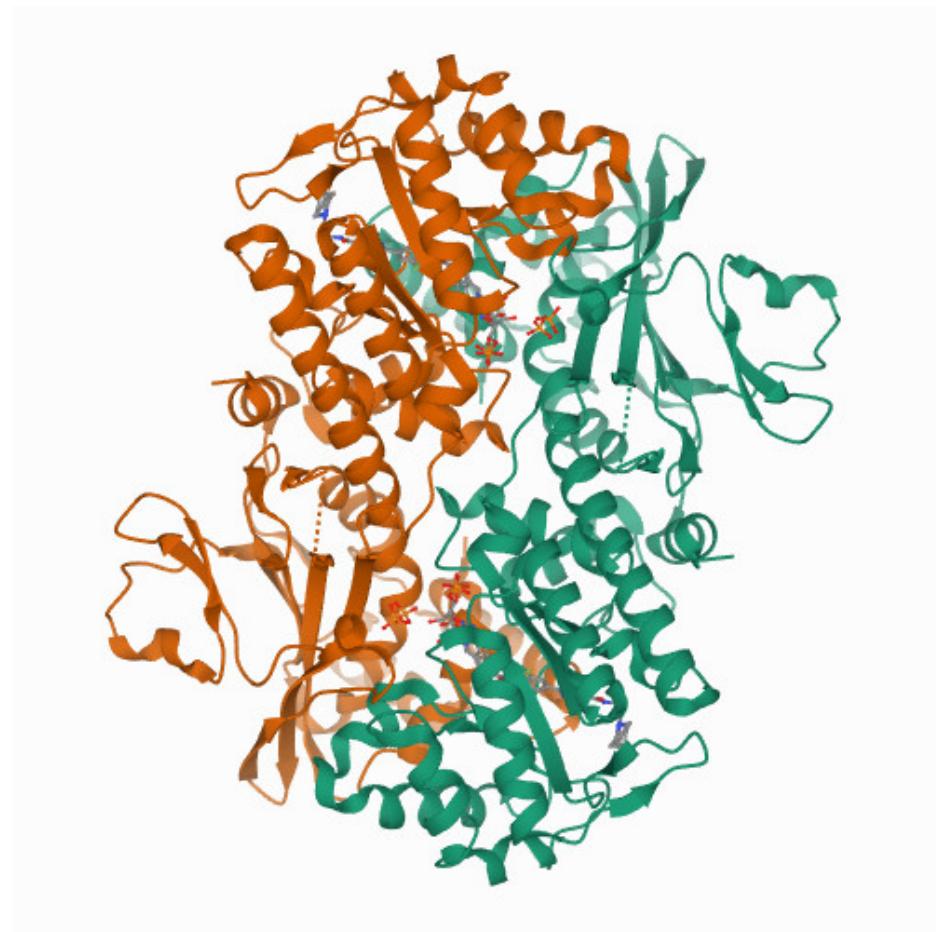
5LX3

CRYSTAL STRUCTURE OF VISFATIN IN COMPLEX WITH SAR154782.

Bertrand, T., Marquette, J.P.

To be published

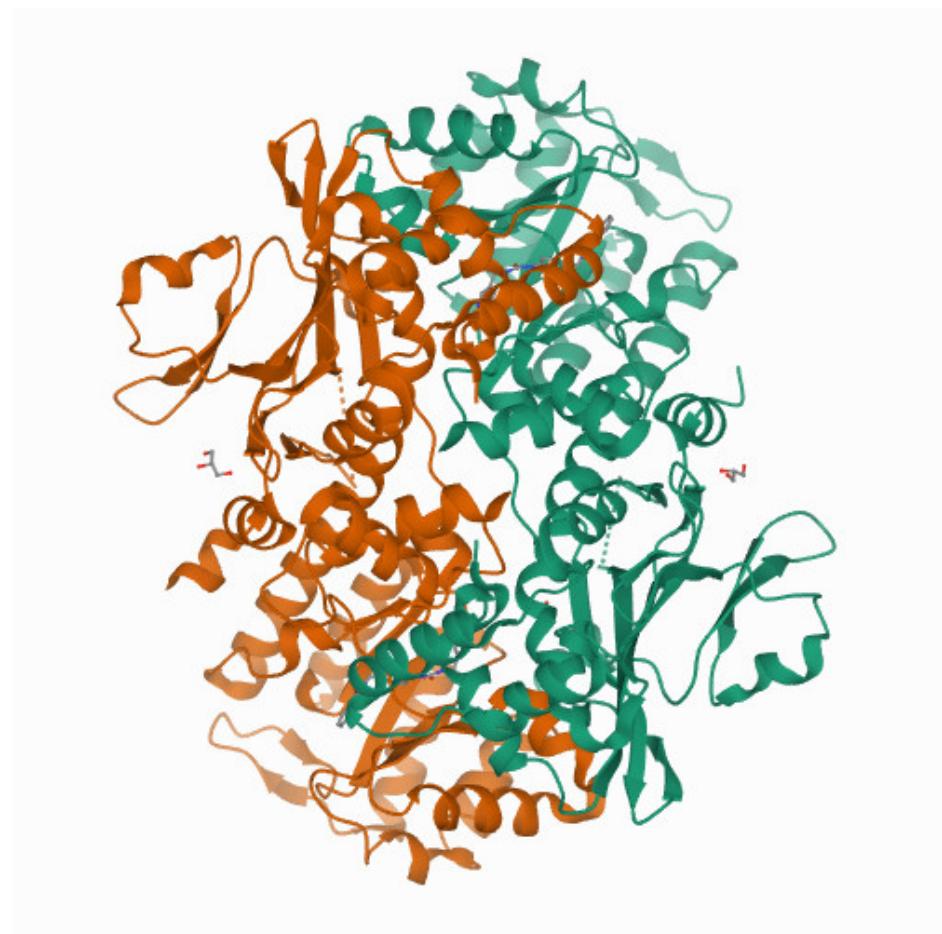
Released	2017-10-25
Method	X-RAY DIFFRACTION 2.1 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	7A1

[3D View](#)**5LX5**[Download File](#) [View File](#) **CRYSTAL STRUCTURE OF VISFATIN IN COMPLEX WITH SAR154782-RP.**

Bertrand, T., Marquette, J.P.

To be published

Released	2017-10-25
Method	X-RAY DIFFRACTION 1.88 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	7A0, DPO

[3D View](#)

6ATB

[Download File](#)[View File](#)

Crystal Structure of human NAMPT in complex with NVP-LOD812

Weihofen, W.A., Thigale, S.

To be published

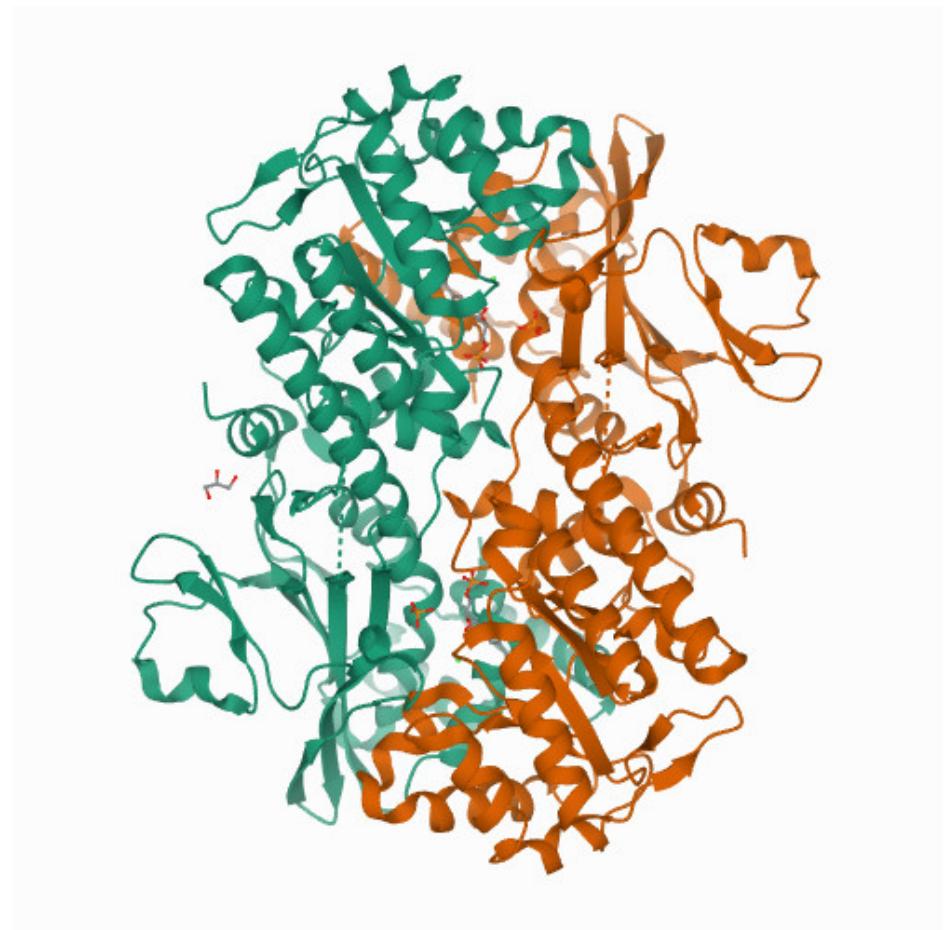
Released 2018-09-12

Method X-RAY DIFFRACTION 2.53 Å

Organisms Homo sapiens

Macromolecule Nicotinamide phosphoribosyltransferase (protein)

Unique Ligands BWA, DMS, GOL, PO4

[3D View](#)

6TA2

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Human NAMPT in complex with nicotinic acid mononucleotide and phosphate

Houry, D., Raasakka, A., Kursula, P., Ziegler, M.

To be published

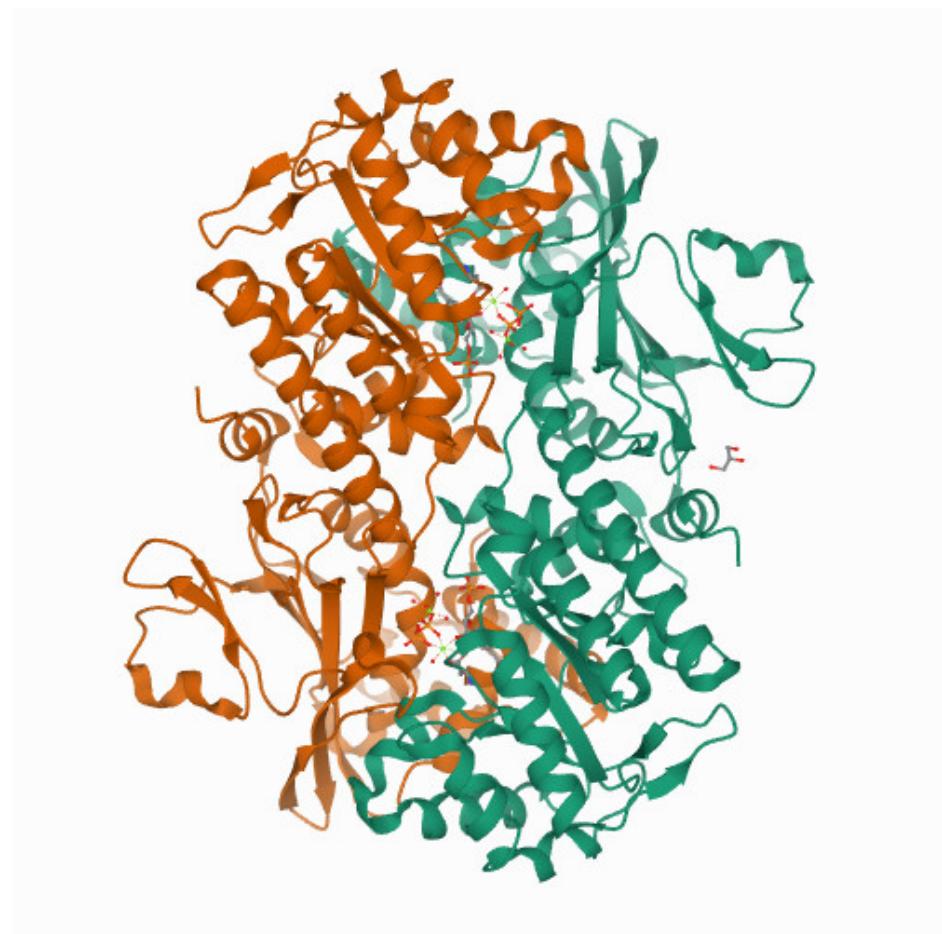
Released 2020-11-18

Method X-RAY DIFFRACTION 1.68 Å

Organisms Homo sapiens

Macromolecule Nicotinamide phosphoribosyltransferase (protein)

Unique Ligands CL, GOL, NCN, PO4

[3D View](#)

6TAC

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Human NAMPT deletion mutant in complex with
nicotinamide mononucleotide, pyrophosphate, and Mg²⁺

Houry, D., Raasakka, A., Kursula, P., Ziegler, M.

To be published

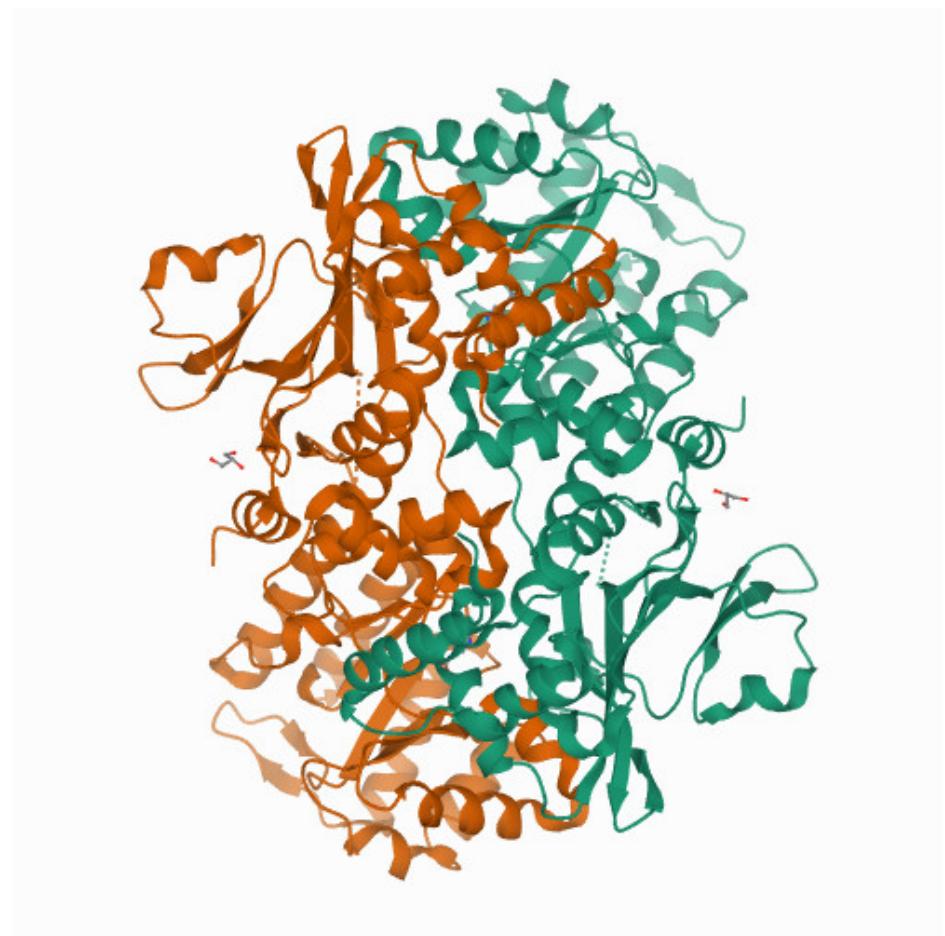
Released 2020-11-18

Method X-RAY DIFFRACTION 1.6 Å

Organisms Homo sapiens

Macromolecule Nicotinamide phosphoribosyltransferase (protein)

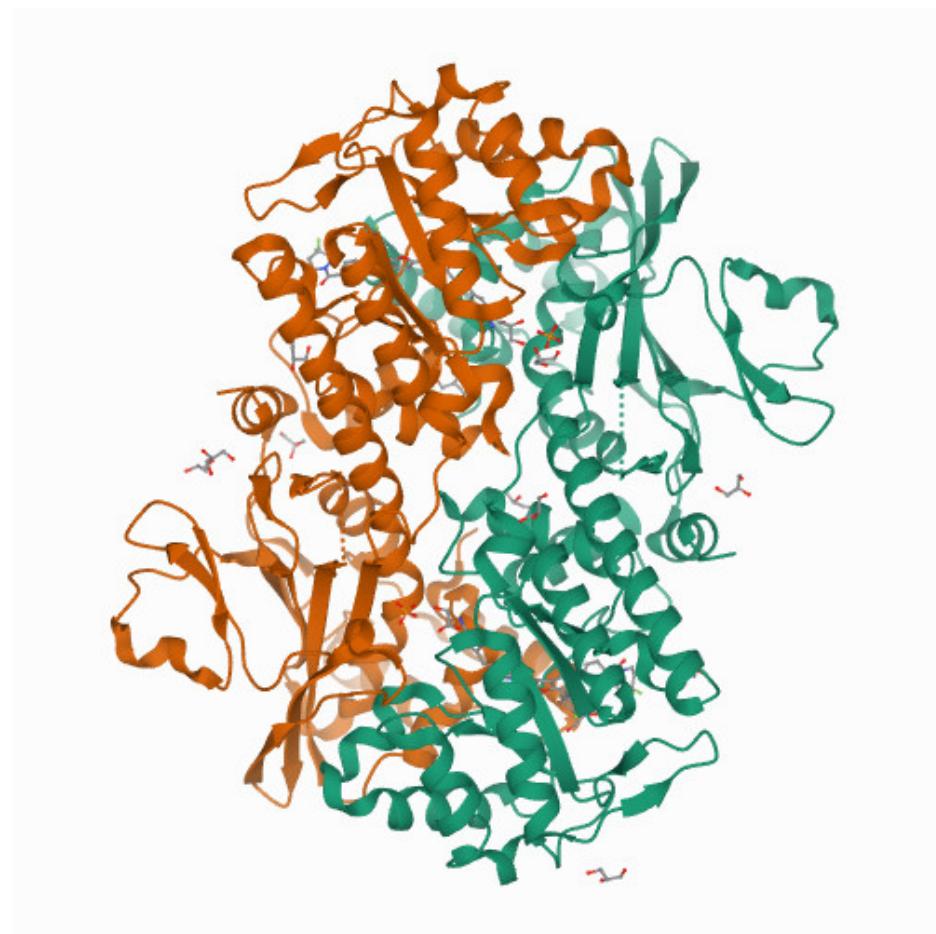
Unique Ligands GOL, MG, NMN, PPV

[3D View](#)**6TA0**[Download File](#) [View File](#) **Human NAMPT in complex with nicotinic acid and phosphoribosyl pyrophosphate**

Houry, D., Raasakka, A., Kursula, P., Ziegler, M.

To be published

Released	2020-11-18
Method	X-RAY DIFFRACTION 1.58 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	GOL, NIO, PRP

[3D View](#)

5NSD

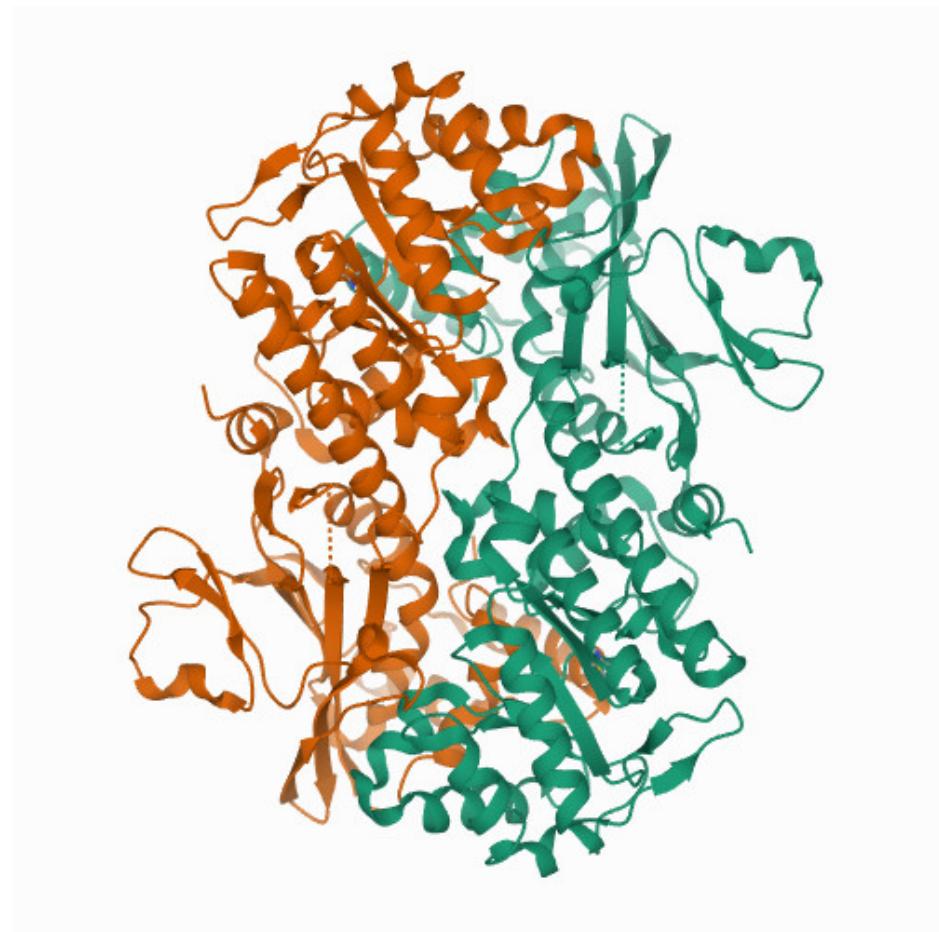
[Download File](#) [View File](#)

Co-crystal structure of NAMPT dimer with KPT-9274

Neggers, J.E., Kwanten, B., Dierckx, T., Noguchi, H., Voet, A., Vercruyse, T., Baloglu, E., Senapedis, W., Jacquemyn, M., Daelemans, D.

(2018) Nat Commun **9**: 502-502

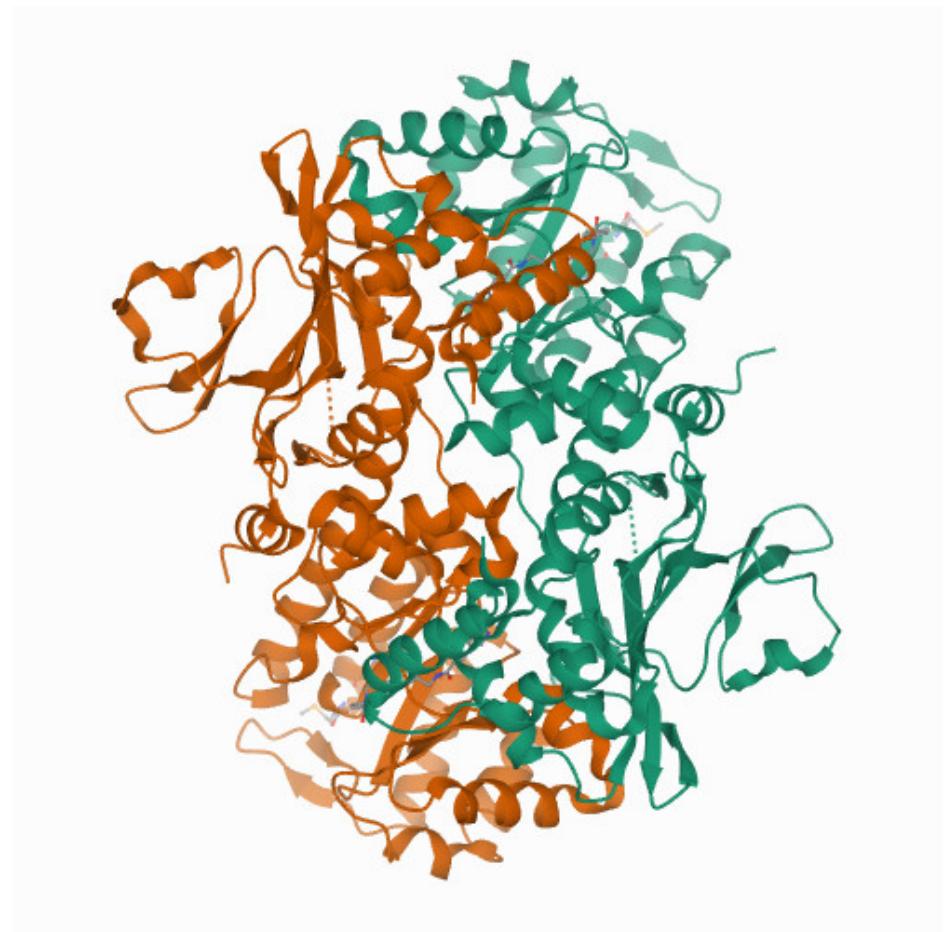
Released	2018-02-14
Method	X-RAY DIFFRACTION 2.046 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	96Q, GOL, PO4

[3D View](#)**2GVL**[Download File](#) [View File](#) **Crystal Structure of Murine NMPRTase**

Khan, J.A., Tao, X., Tong, L.

(2006) Nat Struct Mol Biol **13**: 582-588

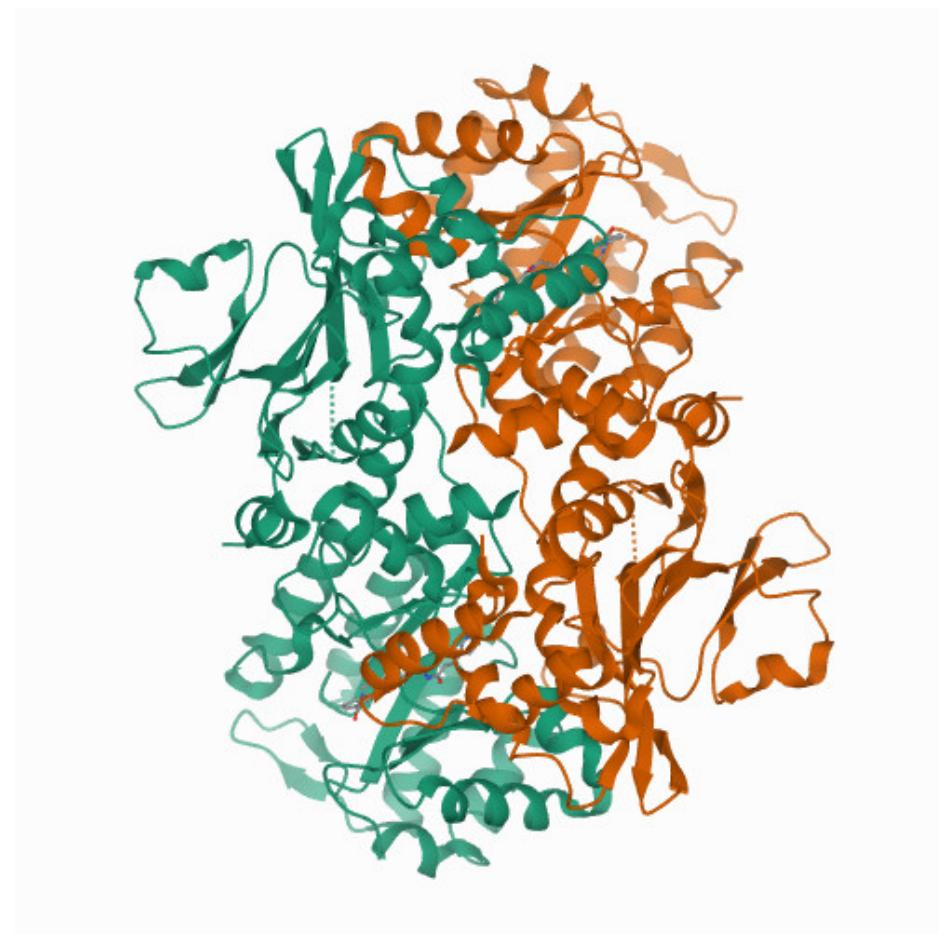
Released	2006-07-25
Method	X-RAY DIFFRACTION 2.1 Å
Organisms	Mus musculus
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)

[3D View](#)**2GVJ**[Download File](#) [View File](#) **Crystal Structure of Human NMPRTase in complex with FK866**

Khan, J.A., Tao, X., Tong, L.

(2006) Nat Struct Mol Biol **13**: 582-588

Released	2006-06-20
Method	X-RAY DIFFRACTION 2.1 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	DGB

 3D View

2G97

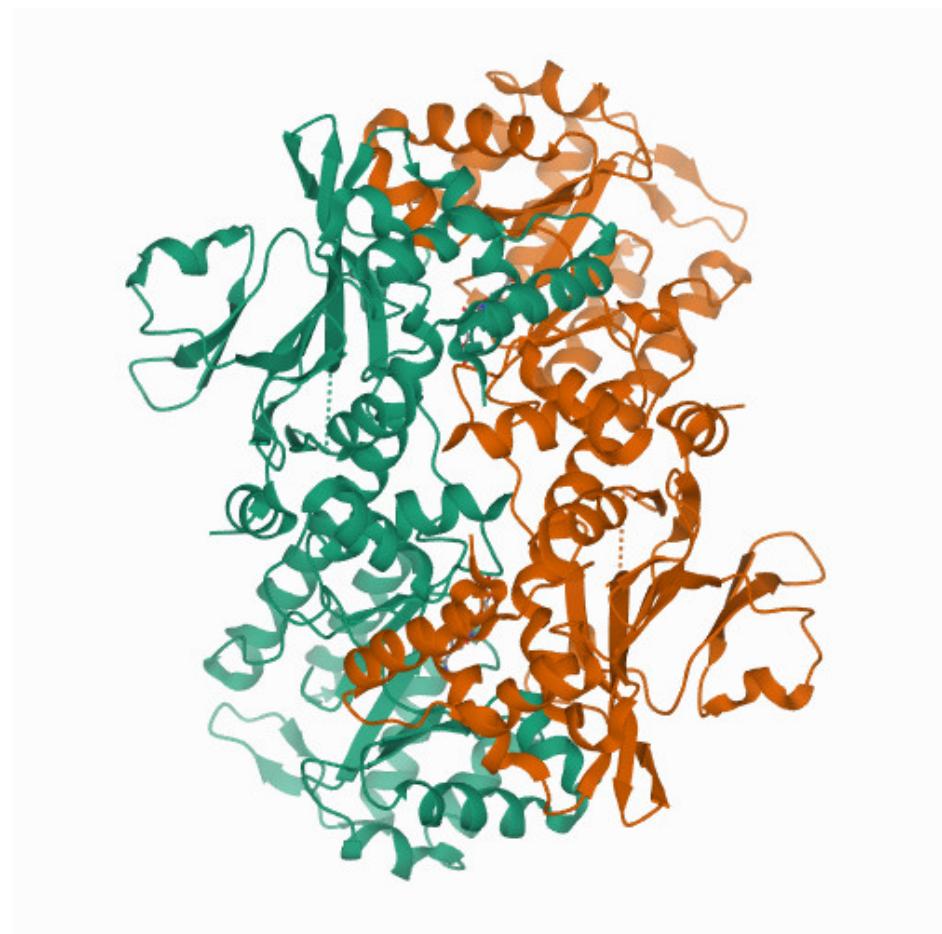
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Crystal Structure of Visfatin/Pre-B Cell Colony Enhancing Factor 1/Nicotinamide Phosphoribosyltransferase In Complex with the Specific Inhibitor FK-866

Kim, M.-K., Eom, S.H.

(2006) J Mol Biol **362**: 66-77

Released	2006-08-01
Method	X-RAY DIFFRACTION 2.9 Å
Organisms	Rattus norvegicus
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	DGB

 3D View

2G96

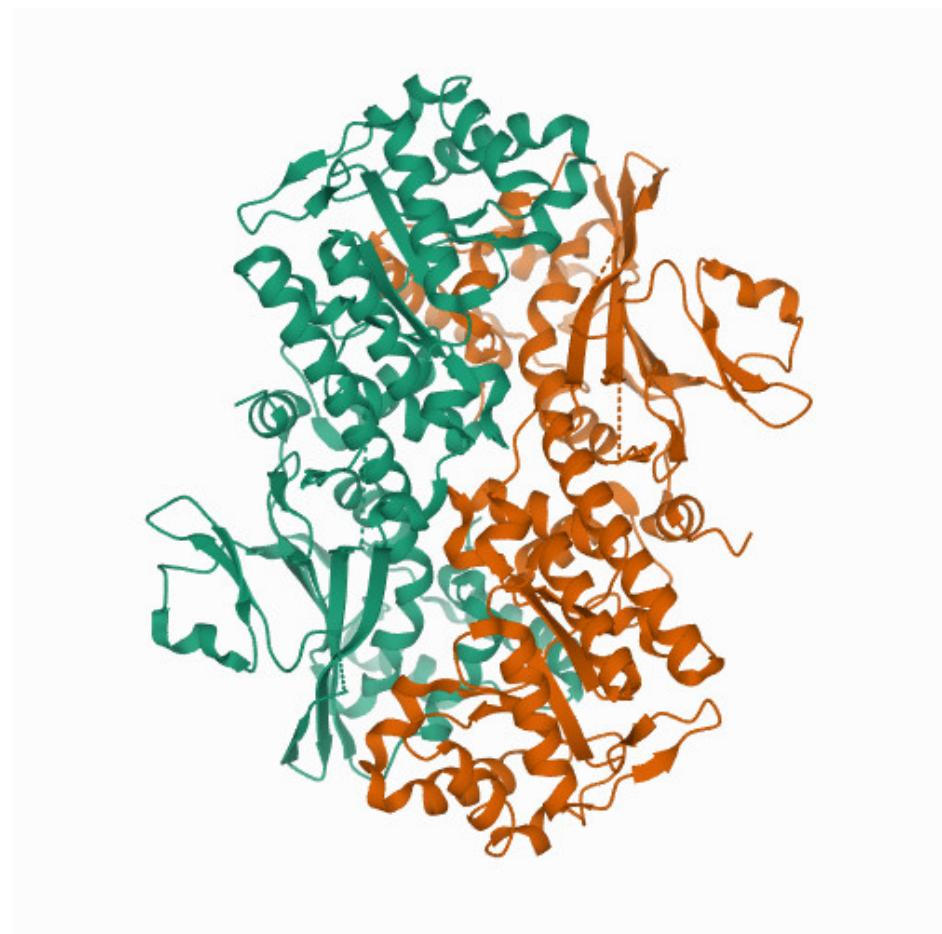
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Crystal Structure of Visfatin/Pre-B Cell Colony Enhancing Factor 1/Nicotinamide Phosphoribosyltransferase In Complex with Niconamide Mononucleotide

Eom, S.H., Kim, M.-K.

(2006) J Mol Biol **362**: 66-77

Released	2006-08-01
Method	X-RAY DIFFRACTION 2.9 Å
Organisms	Rattus norvegicus
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	NMN

 3D View

2G95

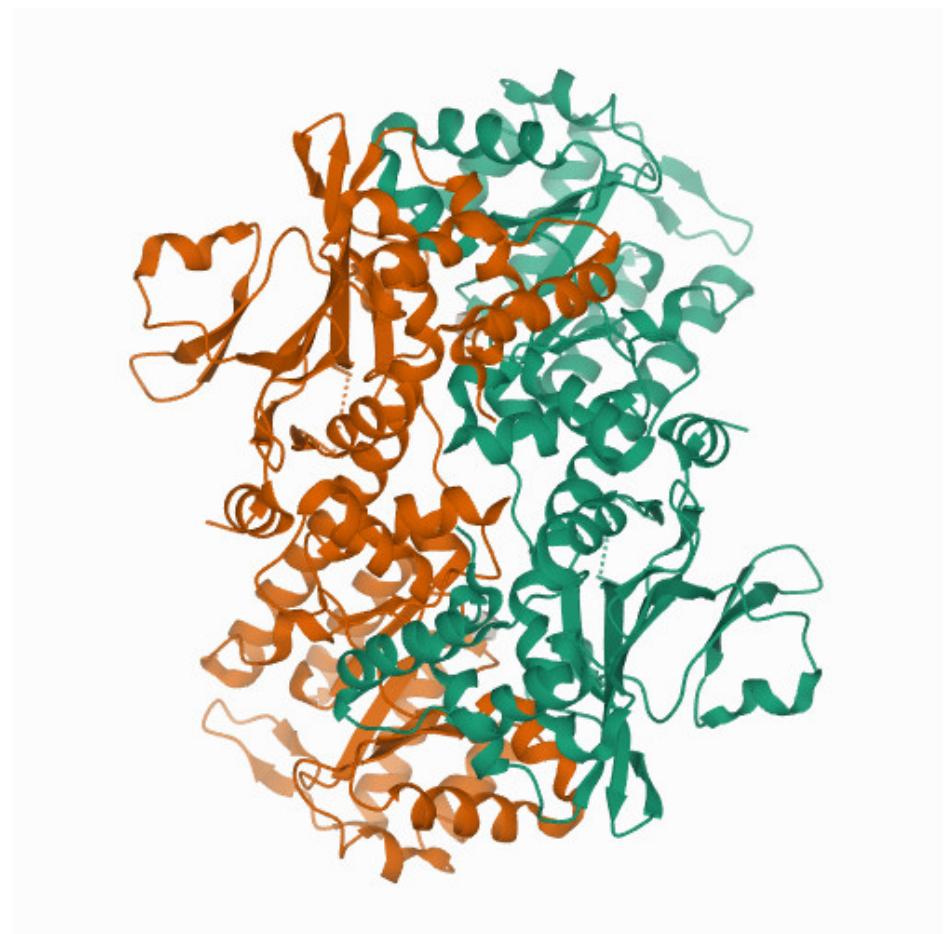
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Crystal Structure of Visfatin/Pre-B Cell Colony Enhancing Factor 1/Nicotinamide Phosphoribosyltransferase

Kim, M.-K., Eom, S.H.

(2006) J Mol Biol **362**: 66-77

Released	2006-08-01
Method	X-RAY DIFFRACTION 1.9 Å
Organisms	Rattus norvegicus
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)

[3D View](#)

2E5C

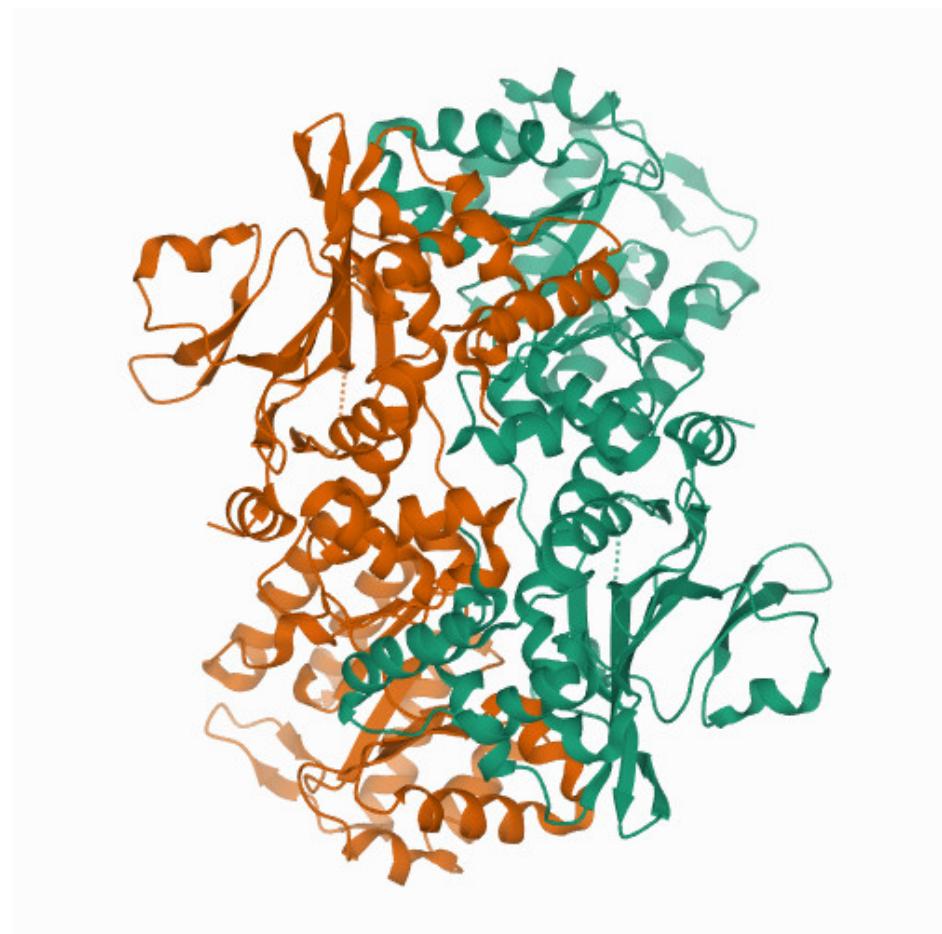
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Crystal structure of Human NMPRTase complexed with 5'-phosphoribosyl-1'-pyrophosphate

Takahashi, R., Nakamura, S., Kobayashi, Y., Ohkubo, T.

(2010) J Biochem **147**: 95-107

Released	2007-12-25
Method	X-RAY DIFFRACTION 2.2 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	PRP

[3D View](#)

2E5B

[Download File](#) [View File](#)

Crystal structure of Human NMPRTase as free-form

Takahashi, R., Nakamura, S., Kobayashi, Y., Ohkubo, T.

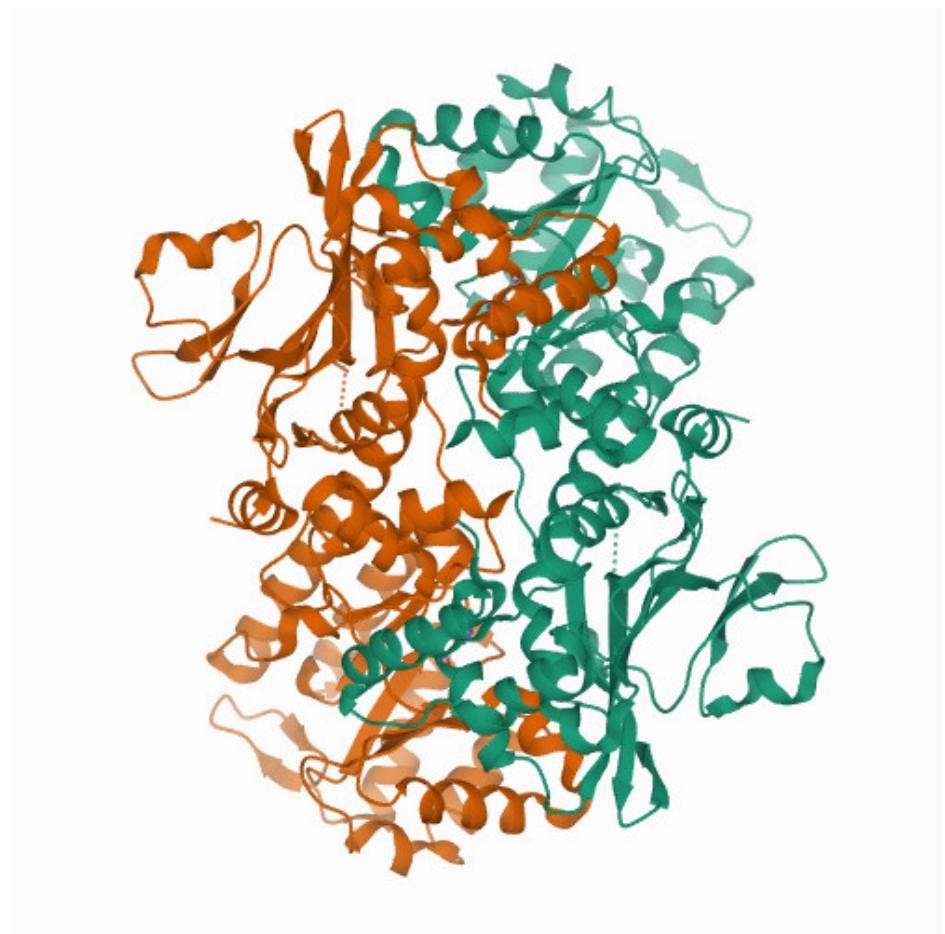
(2010) J Biochem **147**: 95-107

Released 2007-12-25

Method X-RAY DIFFRACTION 2 Å

Organisms Homo sapiens

Macromolecule Nicotinamide phosphoribosyltransferase (protein)

[3D View](#)

2E5D

[Download File](#) [View File](#)

Crystal structure of Human NMPRTase complexed with nicotinamide

Takahashi, R., Nakamura, S., Kobayashi, Y., Ohkubo, T.

(2010) J Biochem **147**: 95-107

Released

2007-12-25

Method

X-RAY DIFFRACTION 2 Å

Organisms

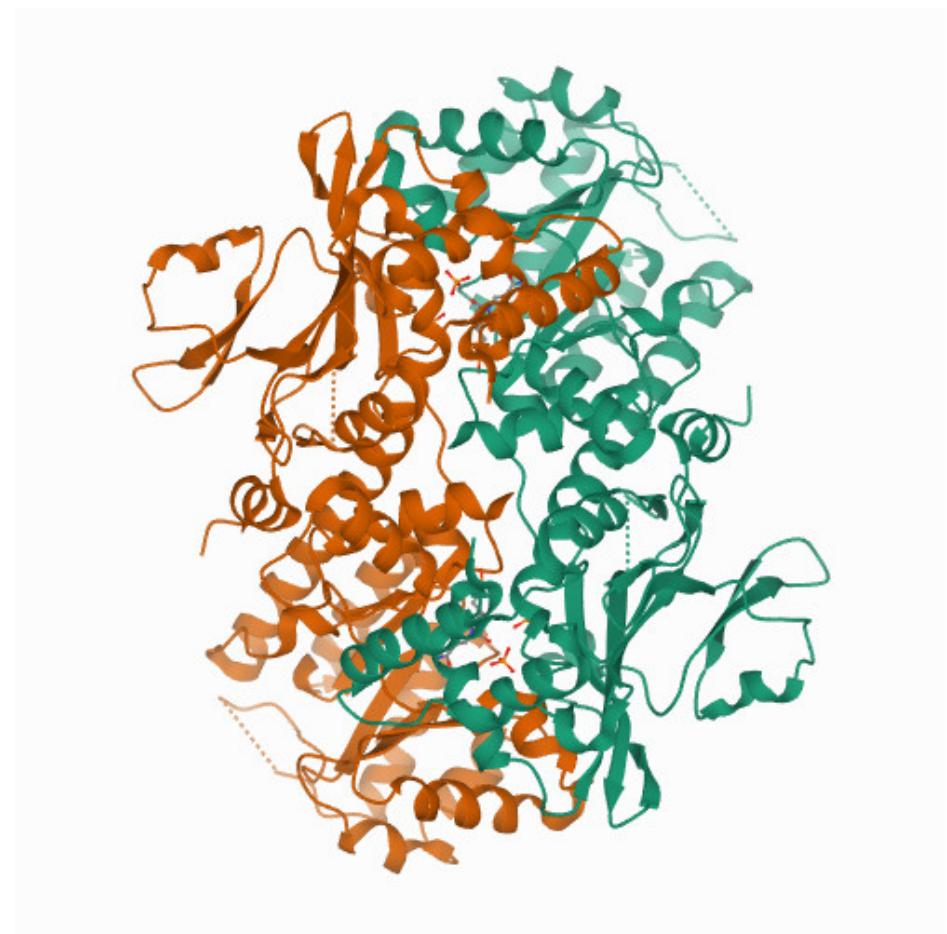
Homo sapiens

Macromolecule

Nicotinamide phosphoribosyltransferase (protein)

Unique Ligands

NCA

[3D View](#)**2GVG**[Download File](#) [View File](#) **Crystal Structure of human NMPRTase and its complex with NMN**

Khan, J.A., Tao, X., Tong, L.

(2006) Nat Struct Mol Biol **13**: 582-588

Released	2006-06-20
Method	X-RAY DIFFRACTION 2.2 Å
Organisms	Homo sapiens
Macromolecule	Nicotinamide phosphoribosyltransferase (protein)
Unique Ligands	NMN, PO4

Displaying 1 to 73 of 73 **Structures**

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Display per page

RCSB PDB is funded by the National Science Foundation (DBI-1832184), the US Department of Energy (DE-SC0019749), and the National Cancer Institute, National Institute of Allergy and Infectious Diseases, and National Institute of General Medical Sciences of the National Institutes of Health under grant R01GM133198.