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SCIENTIFIC NAME OF SOURCE ORGANISM

[Clear](#)

- Severe acute respiratory syndrome coronavirus 2 (84)
- synthetic construct (1)

TAXONOMY

[Clear](#)

- Riboviria (84)
- artificial sequences (1)

EXPERIMENTAL METHOD

[Clear](#)

- X-RAY DIFFRACTION (84)

ENTITY POLYMER TYPE

[Clear](#)

- Protein (84)

RESOLUTION (Å)

[Clear](#)

- 1.0 - 1.5 (14)
- 1.5 - 2.0 (60)
- 2.0 - 2.5 (10)

RELEASE DATE

[Clear](#)

- 2020 - 2024 (84)

ENZYME CLASSIFICATION NAME

[Clear](#)

MEMBRANE PROTEIN NAME

[Clear](#)

SYMMETRY TYPE

[Clear](#)

- Cyclic (84)
- Asymmetric (83)

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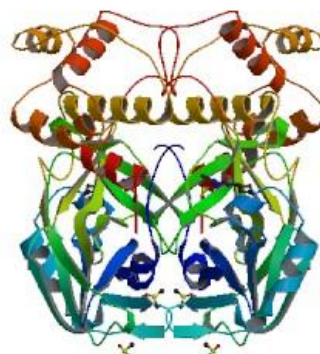
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[3D View](#)

5R84

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PanDDA analysis group deposition -- Crystal Structure of COVID-19 main protease in complex with Z31792168

Fearon, D., Powell, A.J., Douangamath, A., Owen, C.D., Wild, C., Krojer, T., Lukacik, P., Strain-Damerell, C.M., Walsh, M.A., von Delft, F.

To be published

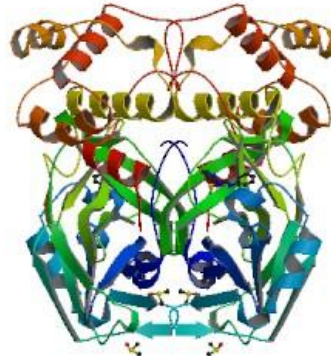
Released 2020-03-11

Method X-RAY DIFFRACTION 1.83 Å

Organisms Severe acute respiratory syndrome coronavirus 2

Macromolecule SARS-CoV-2 main protease (protein)

Unique Ligands DMS, GWS


[3D View](#)

5R83

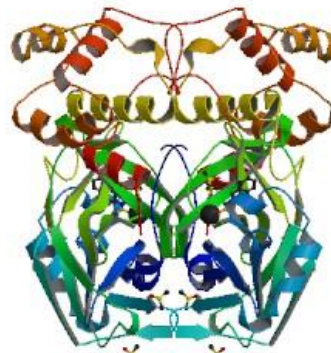
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PanDDA analysis group deposition -- Crystal Structure of SARS-CoV-2 main protease in complex with Z44592329

Fearon, D., Powell, A.J., Douangamath, A., Owen, C.D., Wild, C., Krojer, T., Lukacik, P., Strain-Damerell, C.M., Walsh, M.A., von Delft, F.

To be published

| | |
|-----------------------|---|
| Released | 2020-03-11 |
| Method | X-RAY DIFFRACTION 1.58 Å |
| Organisms | Severe acute respiratory syndrome coronavirus 2 |
| Macromolecule | SARS-CoV-2 main protease (protein) |
| Unique Ligands | DMS, K0G |


[3D View](#)

5R7Y

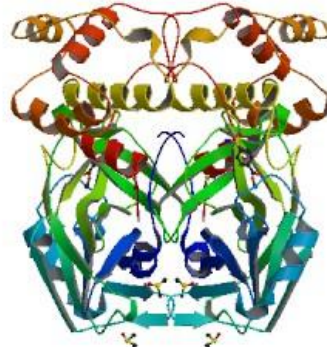
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PanDDA analysis group deposition -- Crystal Structure of COVID-19 main protease in complex with Z45617795

Fearon, D., Powell, A.J., Douangamath, A., Owen, C.D., Wild, C., Krojer, T., Lukacik, P., Strain-Damerell, C.M., Walsh, M.A., von Delft, F.

To be published

| | |
|-----------------------|---|
| Released | 2020-03-11 |
| Method | X-RAY DIFFRACTION 1.65 Å |
| Organisms | Severe acute respiratory syndrome coronavirus 2 |
| Macromolecule | SARS-CoV-2 main protease (protein) |
| Unique Ligands | CL, DMS, JFM |


[3D View](#)

5R80

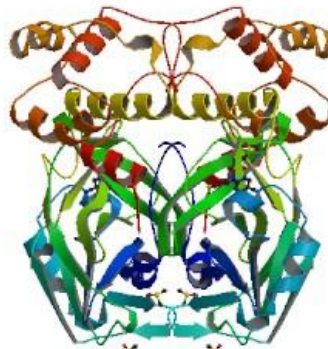
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PanDDA analysis group deposition -- Crystal Structure of SARS-CoV-2 main protease in complex with Z18197050

Fearon, D., Powell, A.J., Douangamath, A., Owen, C.D., Wild, C., Krojer, T., Lukacik, P., Strain-Damerell, C.M., Walsh, M.A., von Delft, F.

To be published

| | |
|-----------------------|---|
| Released | 2020-03-11 |
| Method | X-RAY DIFFRACTION 1.93 Å |
| Organisms | Severe acute respiratory syndrome coronavirus 2 |
| Macromolecule | SARS-CoV-2 main protease (protein) |
| Unique Ligands | DMS, RZG |


[3D View](#)

5R82

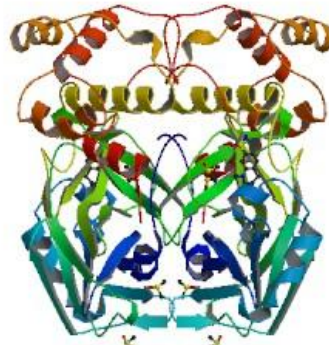
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PanDDA analysis group deposition -- Crystal Structure of COVID-19 main protease in complex with Z219104216

Fearon, D., Powell, A.J., Douangamath, A., Owen, C.D., Wild, C., Krojer, T., Lukacik, P., Strain-Damerell, C.M., Walsh, M.A., von Delft, F.

To be published

| | |
|-----------------------|---|
| Released | 2020-03-11 |
| Method | X-RAY DIFFRACTION 1.31 Å |
| Organisms | Severe acute respiratory syndrome coronavirus 2 |
| Macromolecule | SARS-CoV-2 main protease (protein) |
| Unique Ligands | DMS, RZS |


[3D View](#)

5R81

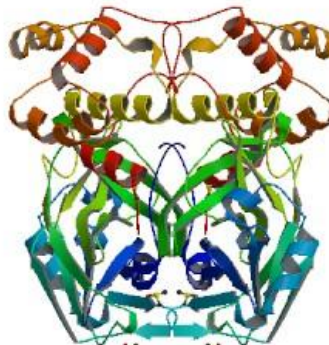
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PanDDA analysis group deposition -- Crystal Structure of COVID-19 main protease in complex with Z1367324110

Fearon, D., Powell, A.J., Douangamath, A., Owen, C.D., Wild, C., Krojer, T., Lukacik, P., Strain-Damerell, C.M., Walsh, M.A., von Delft, F.

To be published

| | |
|-----------------------|---|
| Released | 2020-03-11 |
| Method | X-RAY DIFFRACTION 1.95 Å |
| Organisms | Severe acute respiratory syndrome coronavirus 2 |
| Macromolecule | SARS-CoV-2 main protease (protein) |
| Unique Ligands | DMS, RZJ |


[3D View](#)

5R8T

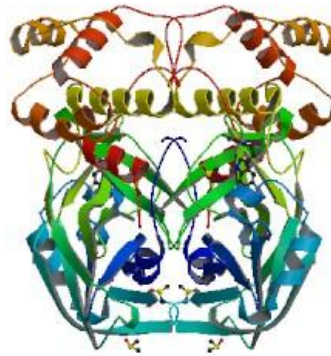
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PanDDA analysis group deposition of ground-state model of SARS-CoV-2 main protease screened against DSI poised (Enamine), Fraglites and Peplites (Newcastle university), Mini Frags (Astex), York 3D (York university), electrophile cysteine covalent (Weizman institute) fragment libraries

Fearon, D., Owen, C.D., Douangamath, A., Lukacik, P., Powell, A.J., Strain-Damerell, C.M., Resnick, E., Krojer, T., Gehrtz, P., Wild, C., Aimon, A., Brandao-Neto, J., Carbery, A., Dunnett, L., Skyner, R., Snee, M., London, N., Walsh, M.A., von Delft, F.

To be published

| | |
|-----------------------|---|
| Released | 2020-04-01 |
| Method | X-RAY DIFFRACTION 1.27 Å |
| Organisms | Severe acute respiratory syndrome coronavirus 2 |
| Macromolecule | SARS-CoV-2 main protease (protein) |
| Unique Ligands | DMS |


[3D View](#)

5R7Z

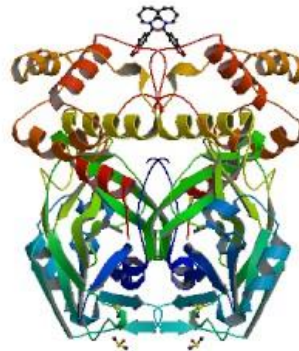
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PanDDA analysis group deposition -- Crystal Structure of SARS-CoV-2 main protease in complex with Z1220452176

Fearon, D., Powell, A.J., Douangamath, A., Owen, C.D., Wild, C., Krojer, T., Lukacik, P., Strain-Damerell, C.M., Walsh, M.A., von Delft, F.

To be published

| | |
|-----------------------|---|
| Released | 2020-03-11 |
| Method | X-RAY DIFFRACTION 1.59 Å |
| Organisms | Severe acute respiratory syndrome coronavirus 2 |
| Macromolecule | SARS-CoV-2 main protease (protein) |
| Unique Ligands | DMS, HWH |


[3D View](#)

5REA

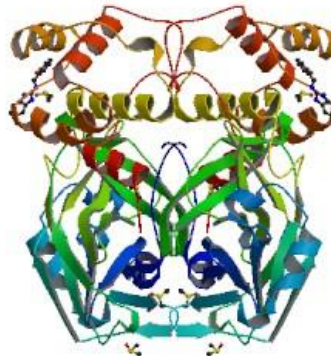
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PanDDA analysis group deposition -- Crystal Structure of SARS-CoV-2 main protease in complex with Z31432226

Fearon, D., Owen, C.D., Douangamath, A., Lukacik, P., Powell, A.J., Strain-Damerell, C.M., Resnick, E., Krojer, T., Gehrtz, P., Wild, C., Aimon, A., Brandao-Neto, J., Carbery, A., Dunnett, L., Skyner, R., Snee, M., London, N., Walsh, M.A., von Delft, F.

To be published

| | |
|-----------------------|---|
| Released | 2020-03-25 |
| Method | X-RAY DIFFRACTION 1.63 Å |
| Organisms | Severe acute respiratory syndrome coronavirus 2 |
| Macromolecule | SARS-CoV-2 main protease (protein) |
| Unique Ligands | DMS, JGP |


[3D View](#)

5REC

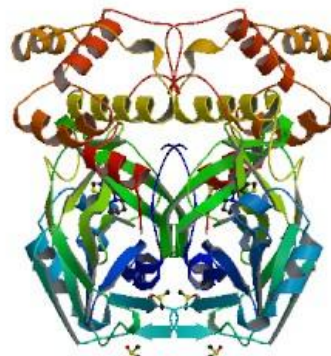
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PanDDA analysis group deposition -- Crystal Structure of SARS-CoV-2 main protease in complex with Z1587220559

Fearon, D., Owen, C.D., Douangamath, A., Lukacik, P., Powell, A.J., Strain-Damerell, C.M., Resnick, E., Krojer, T., Gehrtz, P., Wild, C., Aimon, A., Brandao-Neto, J., Carbery, A., Dunnett, L., Skyner, R., Snee, M., London, N., Walsh, M.A., von Delft, F.

To be published

| | |
|-----------------------|---|
| Released | 2020-03-25 |
| Method | X-RAY DIFFRACTION 1.73 Å |
| Organisms | Severe acute respiratory syndrome coronavirus 2 |
| Macromolecule | SARS-CoV-2 main protease (protein) |
| Unique Ligands | DMS, T1J |


[3D View](#)

5REB

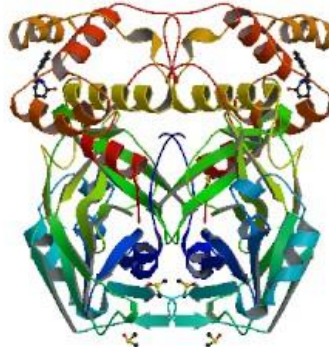
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PanDDA analysis group deposition -- Crystal Structure of SARS-CoV-2 main protease in complex with Z2856434899

Fearon, D., Owen, C.D., Douangamath, A., Lukacik, P., Powell, A.J., Strain-Damerell, C.M., Resnick, E., Krojer, T., Gehrtz, P., Wild, C., Aimon, A., Brandao-Neto, J., Carbery, A., Dunnett, L., Skyner, R., Snee, M., London, N., Walsh, M.A., von Delft, F.

To be published

| | |
|-----------------------|---|
| Released | 2020-03-25 |
| Method | X-RAY DIFFRACTION 1.68 Å |
| Organisms | Severe acute respiratory syndrome coronavirus 2 |
| Macromolecule | SARS-CoV-2 main protease (protein) |
| Unique Ligands | DMS, T0Y |


[3D View](#)

5REE

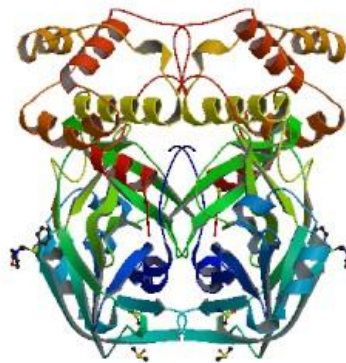
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PanDDA analysis group deposition -- Crystal Structure of SARS-CoV-2 main protease in complex with Z2217052426

Fearon, D., Owen, C.D., Douangamath, A., Lukacik, P., Powell, A.J., Strain-Damerell, C.M., Resnick, E., Krojer, T., Gehrtz, P., Wild, C., Aimon, A., Brandao-Neto, J., Carbery, A., Dunnett, L., Skyner, R., Snee, M., London, N., Walsh, M.A., von Delft, F.

To be published

| | |
|-----------------------|---|
| Released | 2020-03-25 |
| Method | X-RAY DIFFRACTION 1.77 Å |
| Organisms | Severe acute respiratory syndrome coronavirus 2 |
| Macromolecule | SARS-CoV-2 main protease (protein) |
| Unique Ligands | DMS, T1M |


[3D View](#)

5RED

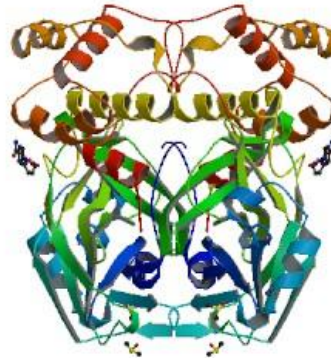
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PanDDA analysis group deposition -- Crystal Structure of SARS-CoV-2 main protease in complex with Z2856434865

Fearon, D., Owen, C.D., Douangamath, A., Lukacik, P., Powell, A.J., Strain-Damerell, C.M., Resnick, E., Krojer, T., Gehrtz, P., Wild, C., Aimon, A., Brandao-Neto, J., Carbery, A., Dunnett, L., Skyner, R., Snee, M., London, N., Walsh, M.A., von Delft, F.

To be published

| | |
|-----------------------|---|
| Released | 2020-03-25 |
| Method | X-RAY DIFFRACTION 1.47 Å |
| Organisms | Severe acute respiratory syndrome coronavirus 2 |
| Macromolecule | SARS-CoV-2 main protease (protein) |
| Unique Ligands | DMS, JJG |


[3D View](#)

5REG

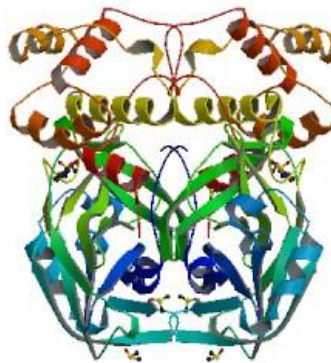
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PanDDA analysis group deposition -- Crystal Structure of SARS-CoV-2 main protease in complex with Z1545313172

Fearon, D., Owen, C.D., Douangamath, A., Lukacik, P., Powell, A.J., Strain-Damerell, C.M., Resnick, E., Krojer, T., Gehrtz, P., Wild, C., Aimon, A., Brandao-Neto, J., Carbery, A., Dunnett, L., Skyner, R., Snee, M., London, N., Walsh, M.A., von Delft, F.

To be published

| | |
|-----------------------|---|
| Released | 2020-03-25 |
| Method | X-RAY DIFFRACTION 1.67 Å |
| Organisms | Severe acute respiratory syndrome coronavirus 2 |
| Macromolecule | SARS-CoV-2 main protease (protein) |
| Unique Ligands | DMS, LWA |


[3D View](#)

5REF

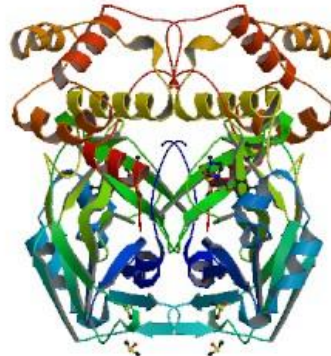
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PanDDA analysis group deposition -- Crystal Structure of SARS-CoV-2 main protease in complex with Z24758179

Fearon, D., Owen, C.D., Douangamath, A., Lukacik, P., Powell, A.J., Strain-Damerell, C.M., Resnick, E., Krojer, T., Gehrtz, P., Wild, C., Aimon, A., Brandao-Neto, J., Carbery, A., Dunnett, L., Skyner, R., Snee, M., London, N., Walsh, M.A., von Delft, F.

To be published

| | |
|-----------------------|---|
| Released | 2020-03-25 |
| Method | X-RAY DIFFRACTION 1.61 Å |
| Organisms | Severe acute respiratory syndrome coronavirus 2 |
| Macromolecule | SARS-CoV-2 main protease (protein) |
| Unique Ligands | 6SU, DMS |


[3D View](#)

5RE9

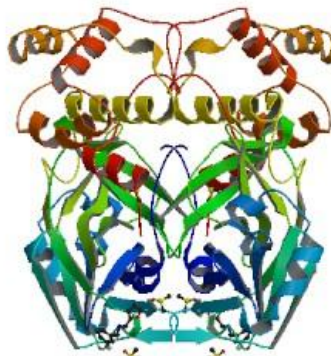
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PanDDA analysis group deposition -- Crystal Structure of SARS-CoV-2 main protease in complex with Z2856434836

Fearon, D., Owen, C.D., Douangamath, A., Lukacik, P., Powell, A.J., Strain-Damerell, C.M., Resnick, E., Krojer, T., Gehrtz, P., Wild, C., Aimon, A., Brandao-Neto, J., Carbery, A., Dunnett, L., Skyner, R., Snee, M., London, N., Walsh, M.A., von Delft, F.

To be published

| | |
|-----------------------|---|
| Released | 2020-03-25 |
| Method | X-RAY DIFFRACTION 1.72 Å |
| Organisms | Severe acute respiratory syndrome coronavirus 2 |
| Macromolecule | SARS-CoV-2 main protease (protein) |
| Unique Ligands | DMS, LPZ |


[3D View](#)

5RE8

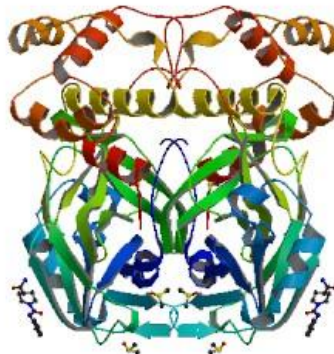
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PanDDA analysis group deposition -- Crystal Structure of SARS-CoV-2 main protease in complex with Z2737076969

Fearon, D., Owen, C.D., Douangamath, A., Lukacik, P., Powell, A.J., Strain-Damerell, C.M., Resnick, E., Krojer, T., Gehrtz, P., Wild, C., Aimon, A., Brandao-Neto, J., Carbery, A., Dunnett, L., Skyner, R., Snee, M., London, N., Walsh, M.A., von Delft, F.

To be published

| | |
|-----------------------|---|
| Released | 2020-03-25 |
| Method | X-RAY DIFFRACTION 1.81 Å |
| Organisms | Severe acute respiratory syndrome coronavirus 2 |
| Macromolecule | SARS-CoV-2 main protease (protein) |
| Unique Ligands | DMS, T0V |


[3D View](#)

5RE5

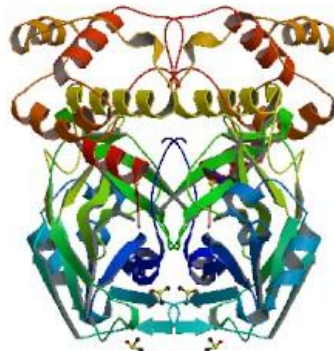
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PanDDA analysis group deposition -- Crystal Structure of SARS-CoV-2 main protease in complex with Z33545544

Fearon, D., Owen, C.D., Douangamath, A., Lukacik, P., Powell, A.J., Strain-Damerell, C.M., Resnick, E., Krojer, T., Gehrtz, P., Wild, C., Aimon, A., Brandao-Neto, J., Carbery, A., Dunnett, L., Skyner, R., Snee, M., London, N., Walsh, M.A., von Delft, F.

To be published

| | |
|-----------------------|---|
| Released | 2020-03-25 |
| Method | X-RAY DIFFRACTION 2.07 Å |
| Organisms | Severe acute respiratory syndrome coronavirus 2 |
| Macromolecule | SARS-CoV-2 main protease (protein) |
| Unique Ligands | DMS, T0J |


[3D View](#)

5RE4

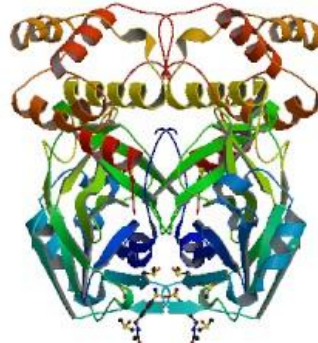
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PanDDA analysis group deposition -- Crystal Structure of SARS-CoV-2 main protease in complex with Z1129283193

Fearon, D., Owen, C.D., Douangamath, A., Lukacik, P., Powell, A.J., Strain-Damerell, C.M., Resnick, E., Krojer, T., Gehrtz, P., Wild, C., Aimon, A., Brandao-Neto, J., Carbery, A., Dunnett, L., Skyner, R., Snee, M., London, N., Walsh, M.A., von Delft, F.

To be published

| | |
|-----------------------|---|
| Released | 2020-03-25 |
| Method | X-RAY DIFFRACTION 1.88 Å |
| Organisms | Severe acute respiratory syndrome coronavirus 2 |
| Macromolecule | SARS-CoV-2 main protease (protein) |
| Unique Ligands | DMS, SZY |


[3D View](#)

5RE7

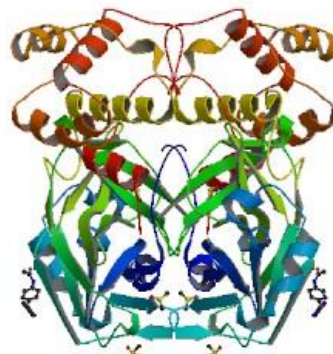
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PanDDA analysis group deposition -- Crystal Structure of SARS-CoV-2 main protease in complex with Z30932204

Fearon, D., Owen, C.D., Douangamath, A., Lukacik, P., Powell, A.J., Strain-Damerell, C.M., Resnick, E., Krojer, T., Gehrtz, P., Wild, C., Aimon, A., Brandao-Neto, J., Carbery, A., Dunnett, L., Skyner, R., Snee, M., London, N., Walsh, M.A., von Delft, F.

To be published

| | |
|-----------------------|---|
| Released | 2020-03-25 |
| Method | X-RAY DIFFRACTION 1.79 Å |
| Organisms | Severe acute respiratory syndrome coronavirus 2 |
| Macromolecule | SARS-CoV-2 main protease (protein) |
| Unique Ligands | DMS, T0S |


[3D View](#)

5RE6

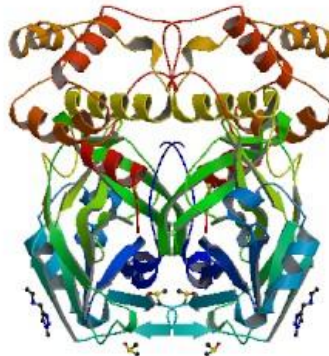
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PanDDA analysis group deposition -- Crystal Structure of SARS-CoV-2 main protease in complex with Z54571979

Fearon, D., Owen, C.D., Douangamath, A., Lukacik, P., Powell, A.J., Strain-Damerell, C.M., Resnick, E., Krojer, T., Gehrtz, P., Wild, C., Aimon, A., Brandao-Neto, J., Carbery, A., Dunnett, L., Skyner, R., Snee, M., London, N., Walsh, M.A., von Delft, F.

To be published

| | |
|-----------------------|---|
| Released | 2020-03-25 |
| Method | X-RAY DIFFRACTION 1.87 Å |
| Organisms | Severe acute respiratory syndrome coronavirus 2 |
| Macromolecule | SARS-CoV-2 main protease (protein) |
| Unique Ligands | DMS, O0S |


[3D View](#)

5RFB

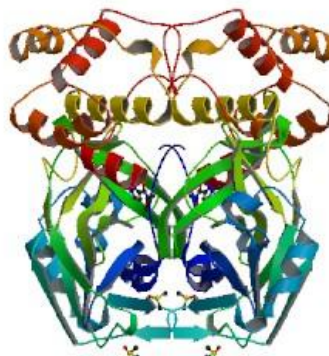
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PanDDA analysis group deposition -- Crystal Structure of SARS-CoV-2 main protease in complex with Z1271660837

Fearon, D., Owen, C.D., Douangamath, A., Lukacik, P., Powell, A.J., Strain-Damerell, C.M., Resnick, E., Krojer, T., Gehrtz, P., Wild, C., Aimon, A., Brandao-Neto, J., Carbery, A., Dunnett, L., Skyner, R., Snee, M., London, N., Walsh, M.A., von Delft, F.

To be published

| | |
|-----------------------|---|
| Released | 2020-03-25 |
| Method | X-RAY DIFFRACTION 1.48 Å |
| Organisms | Severe acute respiratory syndrome coronavirus 2 |
| Macromolecule | SARS-CoV-2 main protease (protein) |
| Unique Ligands | DMS, K3S |


[3D View](#)

5RFA

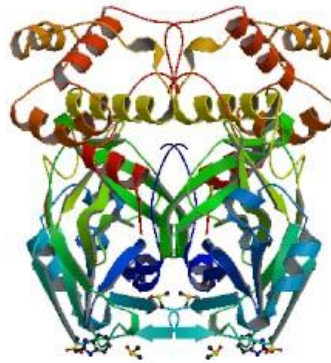
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PanDDA analysis group deposition -- Crystal Structure of SARS-CoV-2 main protease in complex with Z2643472210

Fearon, D., Owen, C.D., Douangamath, A., Lukacik, P., Powell, A.J., Strain-Damerell, C.M., Resnick, E., Krojer, T., Gehrtz, P., Wild, C., Aimon, A., Brandao-Neto, J., Carbery, A., Dunnett, L., Skyner, R., Snee, M., London, N., Walsh, M.A., von Delft, F.

To be published

| | |
|-----------------------|---|
| Released | 2020-03-25 |
| Method | X-RAY DIFFRACTION 1.52 Å |
| Organisms | Severe acute respiratory syndrome coronavirus 2 |
| Macromolecule | SARS-CoV-2 main protease (protein) |
| Unique Ligands | DMS, JGY |


[3D View](#)

5RFD

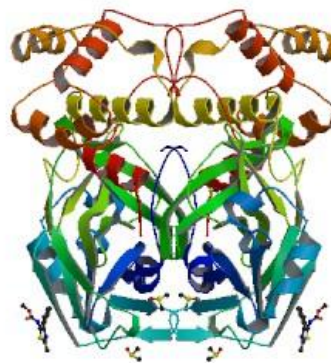
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PanDDA analysis group deposition -- Crystal Structure of SARS-CoV-2 main protease in complex with Z126932614

Fearon, D., Owen, C.D., Douangamath, A., Lukacik, P., Powell, A.J., Strain-Damerell, C.M., Resnick, E., Krojer, T., Gehrtz, P., Wild, C., Aimon, A., Brandao-Neto, J., Carbery, A., Dunnett, L., Skyner, R., Snee, M., London, N., Walsh, M.A., von Delft, F.

To be published

| | |
|-----------------------|---|
| Released | 2020-03-25 |
| Method | X-RAY DIFFRACTION 1.41 Å |
| Organisms | Severe acute respiratory syndrome coronavirus 2 |
| Macromolecule | SARS-CoV-2 main protease (protein) |
| Unique Ligands | DMS, T6J |


[3D View](#)

5RFC

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PanDDA analysis group deposition -- Crystal Structure of SARS-CoV-2 main protease in complex with Z979145504

Fearon, D., Owen, C.D., Douangamath, A., Lukacik, P., Powell, A.J., Strain-Damerell, C.M., Resnick, E., Krojer, T., Gehrtz, P., Wild, C., Aimon, A., Brandao-Neto, J., Carbery, A., Dunnett, L., Skyner, R., Snee, M., London, N., Walsh, M.A., von Delft, F.

To be published

| | |
|-----------------------|---|
| Released | 2020-03-25 |
| Method | X-RAY DIFFRACTION 1.4 Å |
| Organisms | Severe acute respiratory syndrome coronavirus 2 |
| Macromolecule | SARS-CoV-2 main protease (protein) |
| Unique Ligands | DMS, K1Y |

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