

BV-BRC Test Report

D10. Protein Structures Data Tab

Item to test	Protein Structures Data Tab
URL	https://www.bv-brc.org/view/Taxonomy/194#view_tab=features
Prerequisites	None
References	https://www.bv-brc.org/docs/quick_references/organisms_taxon/protein_structures.html
Tester(s)	Rebecca Wattam, Richard Scheuermann, Ron Kenyon
Test date	6-Jan-2022 and 4-Feb-22 (original – partial success), 9-May-2022 (follow-up-passed)
Test result	Passed

Overview

- Test the Protein Structures Tab with example bacterial and viral data.
- Verify structures exist.
- Test Structure action button.
- Test example structure operations.

Test Results

- Test results were verified by examination of returned data via inspection and filters.
- All operations performed as expected.
- Future enhancement:
 - Issue: Parse gene names and resolution from PDB metadata.
 - Resolution: Updated the data loader to populate gene names and resolution from PDB metadata.

Bacteria

Mycobacterium:

Check of existence: Sum of Methods equals total count

Taxon View
 Bacteria » Actinobacteria » Actinomycetia » Corynebacteriales » Mycobacteriaceae » **Mycobacterium** (33401 Genomes)

Overview | Phylogeny | Taxonomy | Genomes | AMR Phenotypes | Sequences | Proteins | **Protein Structures** | Specialty Genes | Domains and Motifs | Epitopes | Pathways

DOWNLOAD | KEYWORDS | ADV Search | HIDE

Organism Name	Gene	Method	Institution
Mycobacterium tuberculosis H37Rv (3)	A7U43_17735 (1)	Electron microscopy (63)	(TBSGC) (1)
Archaeoglobus fulgidus (2)	BQ2027_MB1858 (1)	Solid-state nmr (1)	Accelerated Technologies Center for Gene to 3D Structure (/
Bacillus phage PBS2 (1)	BZL29_7639 (3)	Solution nmr (71)	Center for Structural Genomics of Infectious Diseases (CSG
Enterobacteria phage T4 (1)	CAB90_01754 (1)	X-ray diffraction (2927)	Integrated Center for Structure and Function Innovation (ISF
Escherichia coli (4)	CKJ66_17020 (1)		Israel Structural Proteomics Center (ISPC) (1)
Escherichia coli K-12 (1)	ESM05_02265 (1)		Midwest Center for Structural Genomics (MCSG) (3)
Homo sapiens (2)	ESM05_10720 (1)		Mycobacterium Tuberculosis Structural Proteomics Project (/
MYCOBACTERIUM AVIUM (1)	ESM05_13560 (4)		New York Consortium on Membrane Protein Structure (NYC
MYCOBACTERIUM BOVIS (1)	ESM05_13585 (1)		New York SGX Research Center for Structural Genomics (N
MYCOBACTERIUM LEPRAE (3)	ESM05_14320 (1)		New York Structural Genomics Research Consortium (NYSC
MYCOBACTERIUM MARINUM (4)	ESM05_16060 (1)		Northeast Structural Genomics Consortium (NESG) (4)
MYCOBACTERIUM TUBERCULOSIS (322)	ERS007657_00996 (2)		Seattle Structural Genomics Center for Infectious Disease (S
MYCOBACTERIUM TUBERCULOSIS H37RV (11)	ERS007661_01687 (2)		Structural Proteomics in Europe (SPINE) (5)
Mycobacterium [tuberculosis] TKK-01-0051 (1)	I547_2743 (1)		Structures of Mtb Proteins Conferring Susceptibility to Know
Mycobacterium avium (33)	J113_05350 (1)		TB Structural Genomics Consortium (TBSGC) (322)
Mycobacterium avium (strain 104) (11)	J113_23825 (1)		

PDB ID	Title	Organism Name	BRC ID	UniProtKB Accession	Gene	Product	Method	Release Date
4W1U	Crystal structure of Rv3577c/KstR2, a transcr	Mycobacterium	fig 83332.642.peg.17	P9WMB9	kstR2	HTH-type transcriptional repressor KstR2	X-ray diffraction	2015-07-29T
4WS5	Crystal structure of Mycobacterium tubercul	Mycobacterium	fig 83332.12.peg.332	P9WFO9	ung	Uracil-DNA glycosylase	X-ray diffraction	2015-07-15T
4WS6	Crystal structure of Mycobacterium tubercul	Mycobacterium	fig 83332.12.peg.332	P9WFO9	ung	Uracil-DNA glycosylase	X-ray diffraction	2015-07-15T
4WXT	X-ray crystal structure of thioredoxin from M	Mycobacterium	fig 1160712.3.peg.47	A0A067HW1	MAV3388_24025	Thioredoxin	X-ray diffraction	2014-11-26T
4X58	Anthranilate phosphoribosyl transferase vari	Mycobacterium	fig 419947.9.peg.304	A5U4M0	trpD	Anthranilate phosphoribosyltransferase	X-ray diffraction	2015-11-25T
4X59	Anthranilate phosphoribosyltransferase vari	Mycobacterium	fig 419947.9.peg.304	A5U4M0	trpD	Anthranilate phosphoribosyltransferase	X-ray diffraction	2015-11-25T
4XGQ	Crystal structure of addiction module from M	Mycobacterium	fig 83332.12.peg.696	P9WJ35,P9	vapB30,vapC30	Antitoxin VapB30,Ribonuclease VapC30	X-ray diffraction	2015-08-12T
4XGR	Crystal structure of addiction module from M	Mycobacterium	fig 83332.12.peg.696	P9WJ35,P9	vapB30,vapC30	Antitoxin VapB30,Ribonuclease VapC30	X-ray diffraction	2015-08-12T
4XXP	Crystal Structure of an Uncharacterized Pro	Mycobacterium	patric_id	Q73ZE2	MAP_1661c	GH16 domain-containing protein	X-ray diffraction	2015-02-11T
4XXX	Structure of PE-PPE domains of ESX-1 secr	Mycobacterium	fig 83332.12.peg.432	P9WJD9	espB	ESX-1 secretion-associated protein EspB	X-ray diffraction	2015-02-18T
4Y12	Crystal structure of the S/T protein kinase P	Mycobacterium	fig 83332.12.peg.452	P9WI73	pknG	Serine/threonine-protein kinase PknG	X-ray diffraction	2015-05-20T
4Y9X	Crystal structure of glucosyl-3-phosphoglyce	Mycobacterium	fig 83332.12.peg.135	P9WMMW9	gpgS	Glucosyl-3-phosphoglycerate synthase	X-ray diffraction	2015-07-15T
4YNR	DosS GAFA Domain Reduced CO Bound Cr	Mycobacterium	fig 419947.9.peg.388	P9WGK2	devS	Oxygen sensor histidine kinase response regulator Dev	X-ray diffraction	2016-02-24T
4ZFQ	Structure of M. tuberculosis (3,3) L,D-Trans	Mycobacterium	fig 83331.22.peg.538	P9WKV2	MT0501	L,D-transpeptidase 5	X-ray diffraction	2015-09-02T
4ZOK	Methylsulfonyl-containing inhibitor bound in	Mycobacterium	fig 419947.9.peg.304	A5U4M0	trpD	Anthranilate phosphoribosyltransferase	X-ray diffraction	2016-05-11T
4ZTV	Non-anthranilate-like inhibitor (TAMU-A7) cc	Mycobacterium	fig 419947.9.peg.304	A5U4M0	trpD	Anthranilate phosphoribosyltransferase	X-ray diffraction	2016-05-25T
5BO3	Bianthranilate-like inhibitor with 5 atom "line"	Mycobacterium	fig 419947.9.peg.304	A5U4M0	trpD	Anthranilate phosphoribosyltransferase	X-ray diffraction	2016-06-01T
5BTC	Crystal structure of a topoisomerase II com	Mycobacterium	fig 83332.115.peg.5	P9WG47,P9	gyrA,gyrB	DNA gyrase subunit A,DNA gyrase subunit B	X-ray diffraction	2016-03-02T
5BTF	Crystal structure of a topoisomerase II com	Mycobacterium	fig 419947.63.peg.6	P9WG45,P9	gyrB,gyrA	DNA gyrase subunit B,DNA gyrase subunit A	X-ray diffraction	2016-03-02T
5BYT	PRPP complexed with a single Mg in the act	Mycobacterium	fig 419947.9.peg.304	P9WFX5	trpD	Anthranilate phosphoribosyltransferase	X-ray diffraction	2016-07-20T
5CJN	Crystal structure of Mycobacterium tubercul	Mycobacterium	fig 83332.12.peg.204	P9WK17	glcB	Malate synthase G	X-ray diffraction	2016-08-10T

1 - 200 of 3062 results

« 1 2 3 ... 16 »

Structure display:

<input type="checkbox"/>	PDB ID	Title	Organism Name	BRC ID	UniProtKB Accession	Gene	Product	Method	Release Date
<input type="checkbox"/>	4W1U	Crystal structure of Rv3557c/KstR2, a trans	Mycobacterium tuberculosis	fig 83332.642.peg.17	P9WMB9	kstR2	HTH-type transcriptional repressor KstR2	X-ray diffraction	2015-07-29T
<input type="checkbox"/>	4WS5	Crystal structure of Mycobacterium tuberculosis	Mycobacterium tuberculosis	fig 83332.12.peg.332	P9WFG9	ung	Uracil-DNA glycosylase	X-ray diffraction	2015-07-15T
<input checked="" type="checkbox"/>	4WS6	Crystal structure of Mycobacterium tuberculosis	Mycobacterium tuberculosis	fig 83332.12.peg.332	P9WFG9	ung	Uracil-DNA glycosylase	X-ray diffraction	2015-07-15T
<input type="checkbox"/>	4WXT	X-ray crystal structure of thioredoxin from M	Mycobacterium tuberculosis	fig 1160712.3.peg.47	A0A067HW	MAV3388_24025	Thioredoxin	X-ray diffraction	2014-11-26T
<input type="checkbox"/>	4X58	Anthranilate phosphoribosyl transferase vari	Mycobacterium tuberculosis	fig 419947.9.peg.304	A5U4M0	trpD	Anthranilate phosphoribosyltransferase	X-ray diffraction	2015-11-25T
<input type="checkbox"/>	4X59	Anthranilate phosphoribosyltransferase vari	Mycobacterium tuberculosis	fig 419947.9.peg.304	A5U4M0	trpD	Anthranilate phosphoribosyltransferase	X-ray diffraction	2015-11-25T

4WS6

PDB ID 4WS6

Title Crystal structure of Mycobacterium tuberculosis uracil-DNA glycosylase in complex with 5-aminouracil, Form I

Organism Name Mycobacterium tuberculosis

Taxon ID 83332

Genome 83332.12

ID

Feature ID PATRIC.83332.12_NC_000962.CDS.3332071.3332754

BRC ID fig|83332.12.peg.3321

UniProtKB Accession P9WFG9

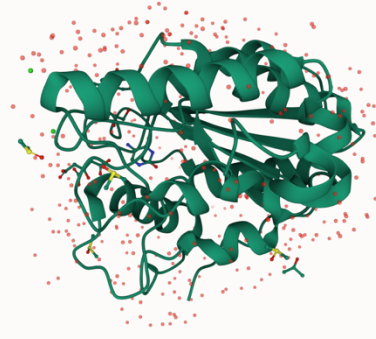
Gene ung

Ligands

Highlight Ligands ■

Sequence of 4WS6 | Cryst... Chain 1: Uracil-DNA... A

MSHHHHHGGASHTARPLELVEKGAALAEFVAQVAMGQFLRAEIAAGRRVLPAGENVLRAFTFFSNVRLVVGQDFPTTGHAVGLSFVAPOVRFPRSLANIFDEYTAADLYLPSPNGD
 120 130 140 150 160 170 180 190 200 210
 LTFNAQRGVLLLNRLVTRPNSFASIRGKGEAVTECAIRALAAKAAFLVALMGRDASTLKLPLAAGNCVAIESPHFSPLASRGFTFSRFRFRANELLVGMGAEPIDKRLP



Structure Tools

Structure

4WS6 | 2 structures

Nothing Focused

Measurements

+ Add

Superposition

Chains Atoms

Components 4WS6 | 2 structures

Preset + Add

Polymer No repr.

Ligand No repr.

Water No repr.

Ion Ball & Stick

Virus

Influenza: H7 HA

Taxon View

Viruses » Negamaviricota » Insthovicetes » Articulavirales » Orthomyxoviridae » Alphainfluenzavirus » **Influenza A virus** (810384 Genomes)

Overview Taxonomy Strains Genomes Proteins **Protein Structures** Domains and Motifs Epitopes Experiments Surveillance Serology



"H7"
KEYWORDS x



HA
GENE x

Organism Name	Gene	Method
Homo sapiens (10)	HA (52)	Electron microscopy (2)
INFLUENZA VIRUS (A/TURKEY/ITALY/214845/2002 (H7N9)) (1)	NA (11)	X-ray diffraction (50)
INFLUENZA VIRUS A/ANHUI/1/2013 (H7N9) (6)	NS1 (1)	
Influenza A virus (38)	PA (2)	
Influenza A virus (A/Anhui/1-BALF_RG45/2013(H7N9)) (1)	PB1 (1)	
Influenza A virus (A/Netherlands/219/2003(H7N7)) (3)	PB2 (1)	
Influenza A virus (A/New York/107/2003(H7N2)) (1)	ns1 (4)	

PDB ID	Title	Organism Name	BRC ID	UniProtKB Accession	Gene	Product
6WXL	Cryo-EM structure of the VRC315 clinical trial, vaccine-	Influenza A virus (/	fig 1395980.6.CDS.1	A0A067Y6L0,AI	HA	Hemagglutinin
6UIG	Crystal structure of human monoclonal antibody H7.201	Influenza A virus,H	fig 1481988.3.CDS.1	A0A4Y5QYN9	HA	Hemagglutinin
6N5A	Crystal structure of an equine H7 hemagglutinin from A	Influenza A virus	fig 387227.6.peg.1	A0A348FV55,A	HA	Hemagglutinin
6MLM	H7 HA0 in complex with Fv from H7.5 IgG	Influenza A virus (/	fig 519082.5.CDS.1	B2LVD7,B2LVD	HA	Hemagglutinin
6II9	Crystal structure of H7 hemagglutinin from A/Anhui/1/2013	Influenza A virus,H	fig 1332244.17.CDS.1	A0A0K1LUI9,AI	HA	Hemagglutinin
6II8	Crystal structure of H7 hemagglutinin from A/Anhui/1/2013	Influenza A virus,H	fig 1663875.3.CDS.1	A0A024CX39,A	HA	Hemagglutinin
6II4	Crystal structure of H7 hemagglutinin from A/Anhui/1/2013	Influenza A virus,H	fig 1332244.17.CDS.1	A0A0K1LUI9,AI	HA	Hemagglutinin
6IDZ	Crystal structure of H7 hemagglutinin mutant H7-SVTC	Influenza A virus	fig 1481988.3.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
6IDD	Crystal structure of H7 hemagglutinin mutant SH1-AVP	Influenza A virus	fig 1332244.17.CDS.1	A0A088BEK2	HA	Hemagglutinin
6IDB	Crystal structure of H7 hemagglutinin mutant H7-SVTC	Influenza A virus	fig 1332244.17.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
6IDA	Crystal structure of H7 hemagglutinin mutant H7-SVTC	Influenza A virus	fig 1481988.3.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
6ID9	Crystal structure of H7 hemagglutinin mutant H7-SGTL	Influenza A virus	fig 1332244.17.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
6ID8	Crystal structure of H7 hemagglutinin mutant H7-SVTL	Influenza A virus	fig 1332244.17.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
6ID5	Crystal structure of H7 hemagglutinin mutant H7-SVPL	Influenza A virus	fig 1332244.17.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
6ID3	Crystal structure of H7 hemagglutinin mutant H7-SGPL	Influenza A virus	fig 1332244.17.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
6ID2	Crystal structure of H7 hemagglutinin mutant H7-AVTL	Influenza A virus	fig 1481988.3.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
6ICY	Crystal structure of H7 hemagglutinin mutant H7-AGTL	Influenza A virus	fig 1481988.3.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
6ICX	Crystal structure of H7 hemagglutinin mutant AH-AGPL	Influenza A virus	fig 1332244.17.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
6ICW	Crystal structure of H7 hemagglutinin mutant AH-SGTC	Influenza A virus	fig 1481988.3.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
6FYU	Structure of H7(A/Shanghai/2/2013) Influenza Hemagg	Influenza A virus,L	fig 1332244.17.CDS.1	A0A4Y5QYN9	HA	Hemagglutinin
6D8B	The crystal structure of hemagglutinin from A/Hong Kor	Influenza A virus	fig 11320.72129.CDS.1	A0A218MY65,A	HA	Hemagglutinin
6D7U	The crystal structure of hemagglutinin from A/Guangdo	Influenza A virus	fig 11320.72161.CDS.1	A0A1S6R2B6,A	HA	Hemagglutinin
6D7C	The crystal structure of hemagglutinin from A/Hong Kor	Influenza A virus	fig 1593637.6.CDS.1	S4V1Z7,A0A0C	HA	Hemagglutinin
5VJM	Crystal structure of H7 hemagglutinin mutant (V186K, F	Influenza A virus	fig 1332244.17.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
5VJL	Crystal structure of H7 hemagglutinin mutant (V186K, F	Influenza A virus	fig 1332244.17.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
5VJK	Crystal structure of H7 hemagglutinin mutant (V186K, F	Influenza A virus	fig 1332244.17.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
5VAG	Crystal structure of H7-specific antibody m826 in comp	Influenza A virus,H	fig 1332244.17.CDS.1	R4NN21	HA	Hemagglutinin
5V2A	Crystal structure of Fab H7.167 in complex with influen	Influenza A virus (/	fig 1560294.3.CDS.1	A0A0R5TXT5,A	HA	Hemagglutinin
5T6S	Crystal structure of the A/Shanghai/2/2013 (H7N9) influ	Influenza A virus	fig 1332244.17.CDS.1	R4NN21,R4NN	HA	Hemagglutinin

1 - 52 of 52 results

Structure:

6NSA

PDB ID 6NSA

Title Crystal structure of an equine H7 hemagglutinin from A/equine/NY/49/73 (H7N7)

Organism Name Influenza A virus

Taxon ID 387227

Genome ID 387227.6

Feature ID PATRIC_387227.6.LC414434.CDS.8.1720

BRC ID fig|387227.6.peg.1

UniProtKB A0A348FV55, A0A348FV55

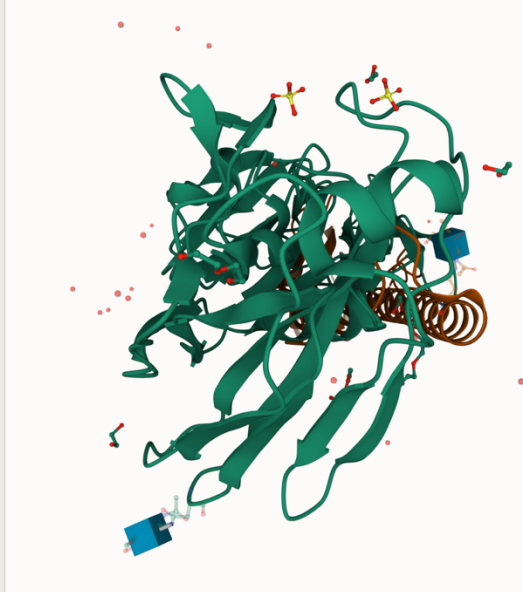
Accession

Ligands

Highlight Ligands ■

Sequence of 6NSA | Crysta... Chain 1: HEMAGGL... A ASM_1

ADPGDKICIGHHVA...
GKFDNEETLRKIL...
TRLYGSGNKLITV...



16:26:44 Updated Carbohydrate in 1ms.
16:26:44 Updated Ball & Stick in 2ms.
16:26:44 Updated Ball & Stick in 3ms.

Structure Tools

Structure

6NSA | 2 structures

Nothing Focused

Measurements

+ Add

Superposition

Chains Atoms

Components 6NSA | 2 structures

Preset + Add

Polymer No repr.

Ligand No repr.

Water No repr.

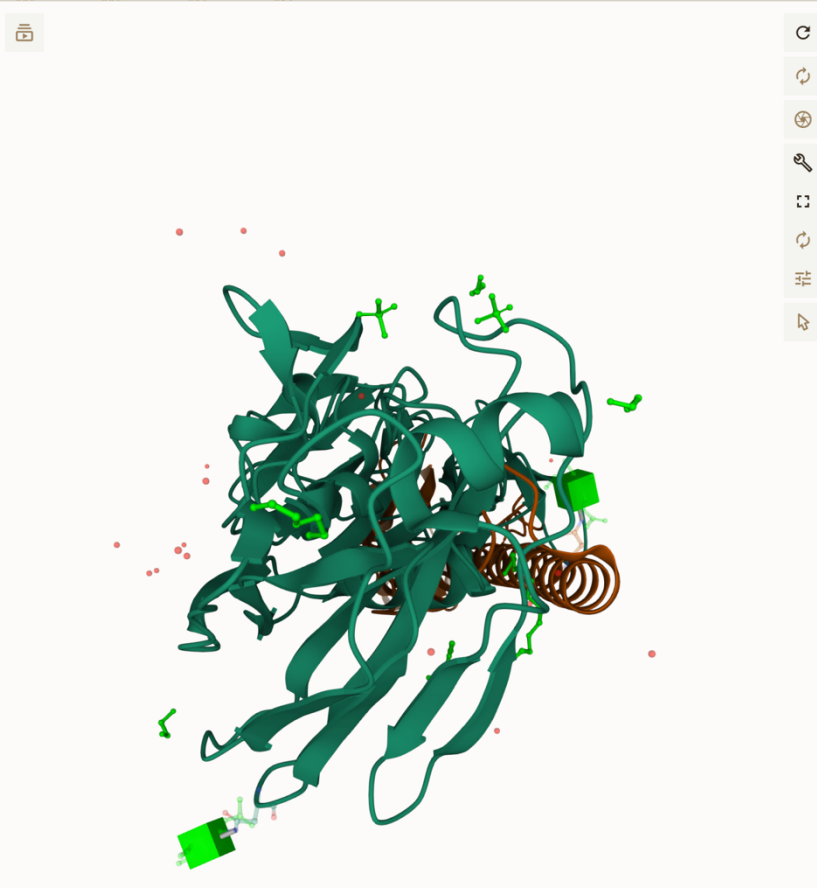
Carbohydrate 2 reprs.

Ion Ball & Stick

Highlight ligands:

Sequence of 6N5A | Crysta... Chain 1: HEMAGGL... A ASM_1

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ADFGDKICLGHAVSNGTKVDLTLEKIEVVNATETVEQKNIPKICSKGKQTDLGGCGLLGTIGPPQCDQFLEFSANLIERREGDDICYP
GKFDNEETLRKILRKSSGGIKENMGFTYTGVRNGETSACRRSRSSFYAEMKWLNSNTDNGVFPQMTKSYKNTKREPALIIWGIHHSGSTAEQ
TRLYGSGNKLIIVWSSKYQQSFAPSPGPRPQINGQSGRIDFYWLMLDPNDVTVFSFNGAIPDRASFRLRGLSLGIQSDAQLDNNCEGECYHI
```



Structure Tools

Structure

6N5A | 2 structures

Nothing Focused

30 Chains Selected

Measurements

+ Add

Superposition

Chains Atoms

Add 2 or more selections (toggle mode) from separate structures. Selections must be limited to single polymer chains or residues therein.

Components 6N5A | 2 structures

	Preset	+ Add		
Polymer	No repr.			...
Ligand	No repr.			...
Water	No repr.			...
Carbohydrate	2 reprs			...
Ion	Ball & Stick			...