Full wwPDB EM Validation Report (i)

Mar 8, 2026 – 06:37 AM UTC

PDB ID	:	9FLU / pdb_00009flu
EMDB ID	:	EMD-50539
Title	:	CryoEM structure of the fragment-1 (3402-3733) in the grappling hook protein A (GhpA) in the bacterium Aureispira sp. CCB-QB1
Authors	:	Lien, Y.-W.; Amendola, D.; Lee, K.S.; Bartlau, N.; Xu, J.; Furusawa, G.; Polz, M.F.; Stocker, R.; Weiss, G.L.; Pilhofer, M.
Deposited on	:	2024-06-05
Resolution	:	3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

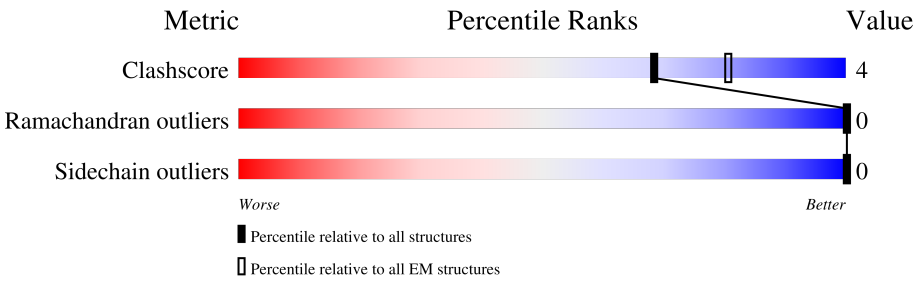
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

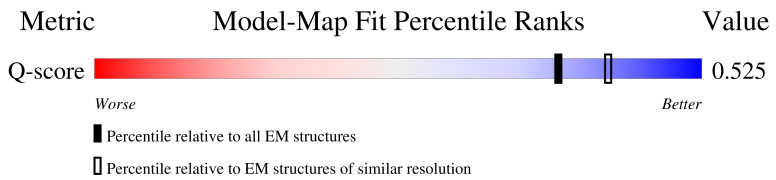
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	5898	5% 94%
1	B	5898	5% 94%
1	C	5898	5% 94%
1	D	5898	5% 94%

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Mol	Chain	Length	Quality of chain
1	E	5898	5% 94%
1	F	5898	5% 94%
1	G	5898	5% 94%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 16520 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

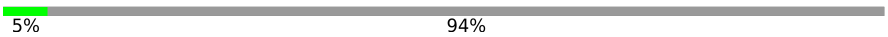
- Molecule 1 is a protein called The grappling hook protein A (GhpA) in the bacterium Aureispira sp. CCB-QB1.

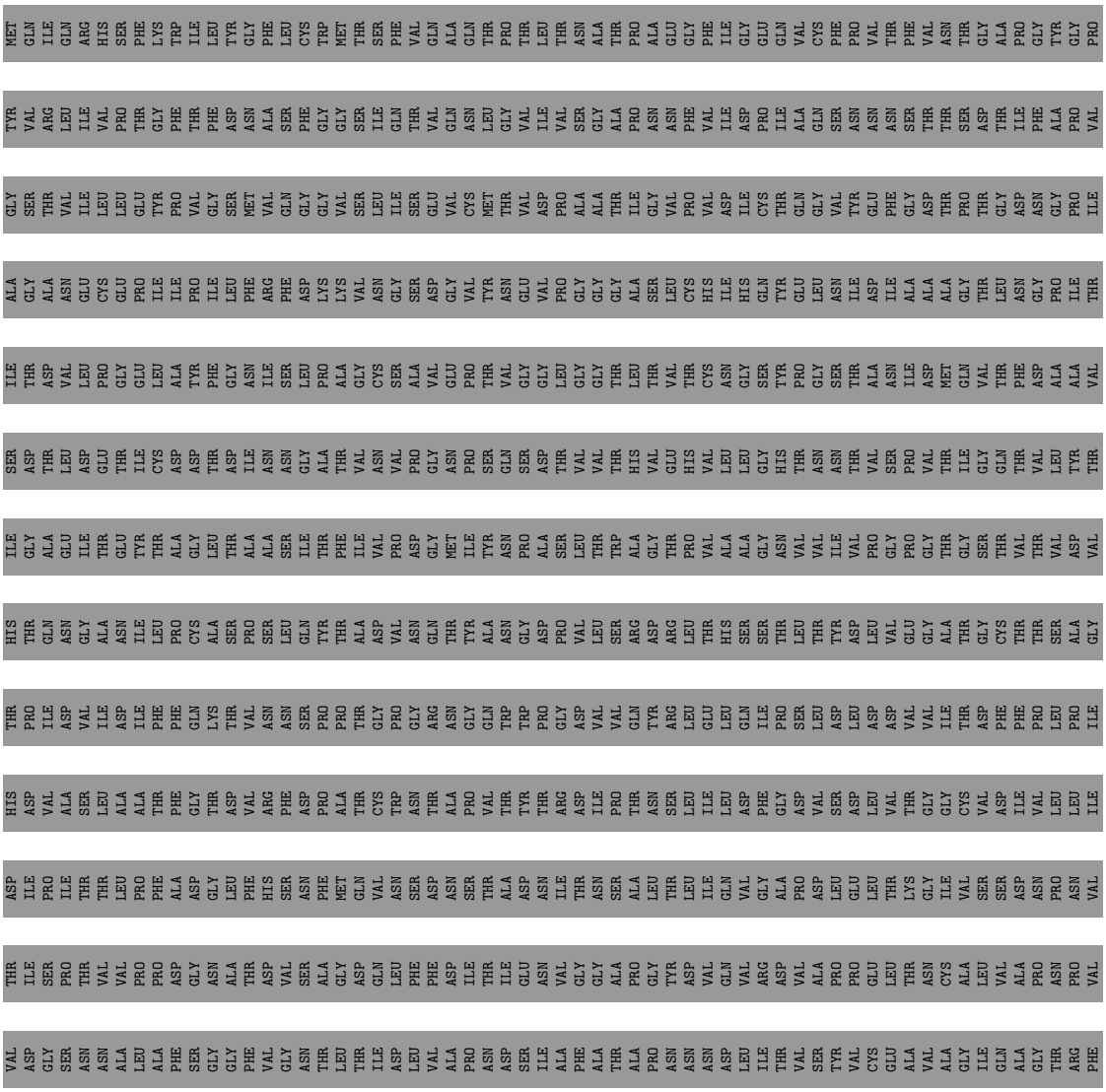
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	332	2360	1453	380	516	11	0	0
1	B	332	2360	1453	380	516	11	0	0
1	C	332	2360	1453	380	516	11	0	0
1	D	332	2360	1453	380	516	11	0	0
1	E	332	2360	1453	380	516	11	0	0
1	F	332	2360	1453	380	516	11	0	0
1	G	332	2360	1453	380	516	11	0	0

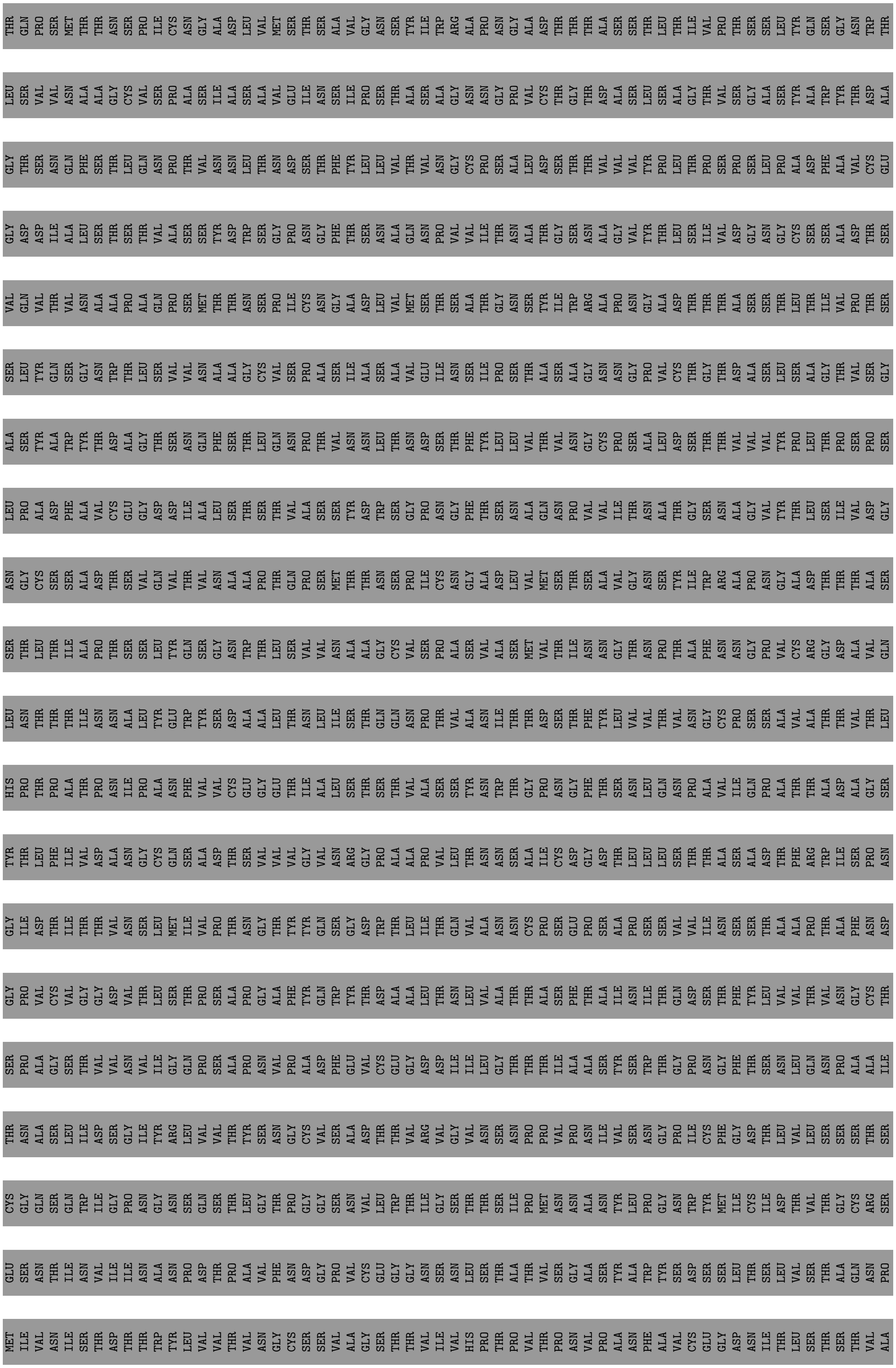
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: The grappling hook protein A (GhpA) in the bacterium Aureispira sp. CCB-QB1

Chain A: 

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LEU SER VAL VAL ASN ALA ALA GLY CYS VAL SER PRO ALA SER ILE ALA SER ALA VAL GLU ILE ASN SER ILE PRO SER THR ALA SER ALA GLY ASN ASN GLY PRO VAL CYS THR GLY THR ASP ALA SER LEU SER ALA GLY THR VAL SER GLY ALA SER TYR ALA TRP TYR THR ASP ALA
GLY THR SER ASN GLN PHE SER THR LEU GLN ASN PRO THR VAL ASN ASN LEU THR ASN ASP SER THR PHE TYR LEU LEU VAL THR VAL ASN GLY CYS PRO SER ALA LEU ASP SER THR THR VAL VAL VAL TYR PRO LEU THR PRO SER PRO SER LEU PRO ALA ASP PHE ALA VAL CYS GLU
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VAL GLN VAL THR VAL ASN ALA ALA PRO ALA GLN PRO SER MET THR THR ASN SER PRO ILE CYS ASN GLY ALA ASP LEU VAL MET SER THR SER ALA THR GLY ASN SER TYR ILE TRP ARG ALA PRO ASN GLY ALA ASP THR THR THR ALA SER SER THR LEU THR ILE VAL PRO THR SER
SER LEU TYR GLN SER GLY ASN TRP THR LEU SER VAL VAL ASN ALA ALA GLY CYS VAL SER PRO ALA SER ILE ALA SER ALA VAL GLU ILE ASN SER ILE PRO SER THR ALA SER ALA GLY ASN ASN GLY PRO VAL CYS THR GLY THR ASP ALA SER LEU SER ALA GLY THR VAL SER GLY
ALA SER TYR ALA TRP TYR THR ASP ALA GLY THR SER ASN GLN PHE SER THR LEU GLN ASN PRO THR VAL ASN ASN LEU THR ASN ASP SER THR PHE TYR LEU LEU VAL THR VAL ASN GLY CYS PRO SER ALA LEU ASP SER THR THR VAL VAL VAL TYR PRO LEU THR PRO SER PRO SER
LEU PRO ALA ASP PHE ALA VAL CYS GLU GLY ASP ASP ILE ALA LEU SER THR SER THR VAL ALA SER SER TYR ASP TRP SER GLY PRO ASN GLY PHE THR SER ASN ALA GLN ASN PRO VAL VAL ILE THR ASN ALA THR GLY SER ASN ALA GLY VAL TYR THR LEU SER ILE VAL ASP GLY
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TYR THR LEU PHE ILE VAL ASP ALA ASN GLY CYS GLN SER ALA ASP THR SER VAL VAL VAL GLY VAL ASN ARG GLY PRO ALA ALA PRO VAL LEU THR ASN ASN SER ALA ILE CYS ASP GLY ASP THR LEU LEU LEU SER THR THR ALA SER ALA ASP THR PHE ARG TRP ILE SER PRO ASN
GLY ILE ASP THR ILE THR THR VAL ASN SER LEU MET ILE VAL PRO THR ASN GLY THR TYR TYR GLN SER GLY ASP TRP THR LEU ILE THR GLN VAL ALA ASN ASN CYS PRO SER GLU PRO SER ALA PRO SER SER VAL VAL ILE ASN SER SER THR ALA ALA PRO THR ALA PHE ASN ASP
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CYS GLY GLN SER GLN TRP ILE GLY PRO ASN GLY ASN SER GLN SER THR LEU GLY THR PRO GLY GLY SER ASN VAL LEU TRP THR ILE GLY SER THR THR SER ILE PRO MET ASN ASN ALA ASN TYR LEU PRO GLY ASN TRP TYR MET ILE CYS ILE ASP THR VAL THR GLY CYS ARG SER
GLU SER ASN THR ILE ASN VAL ILE ILE ASN ALA ASN PRO ASP THR PRO ALA VAL PHE ASN ASP GLY PRO VAL CYS GLU GLY GLY ASN SER ASN LEU SER THR ALA THR VAL SER GLY ALA SER TYR ALA TRP TYR SER ASP SER SER LEU THR SER LEU VAL SER THR ALA GLN ASN PRO
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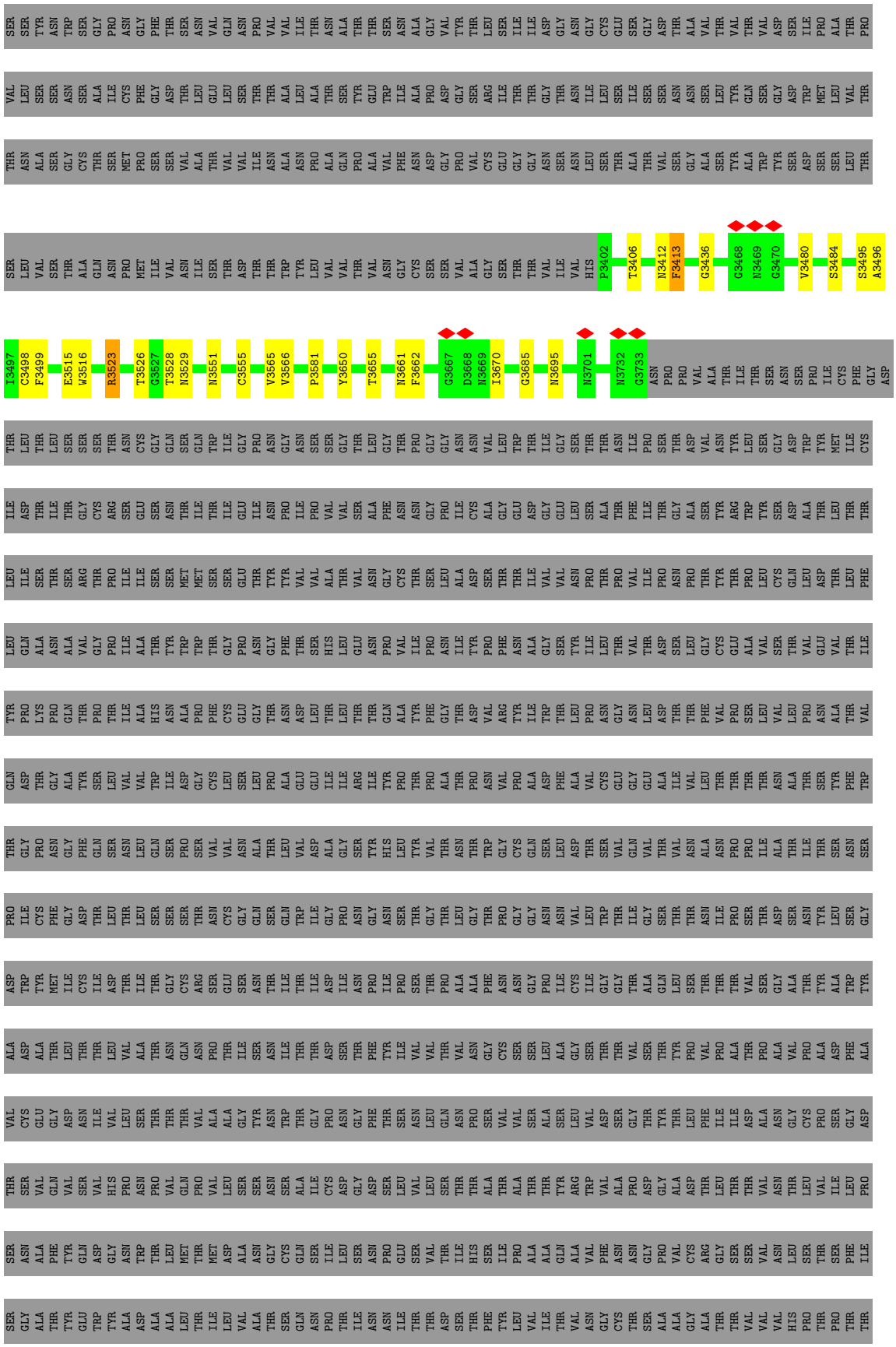
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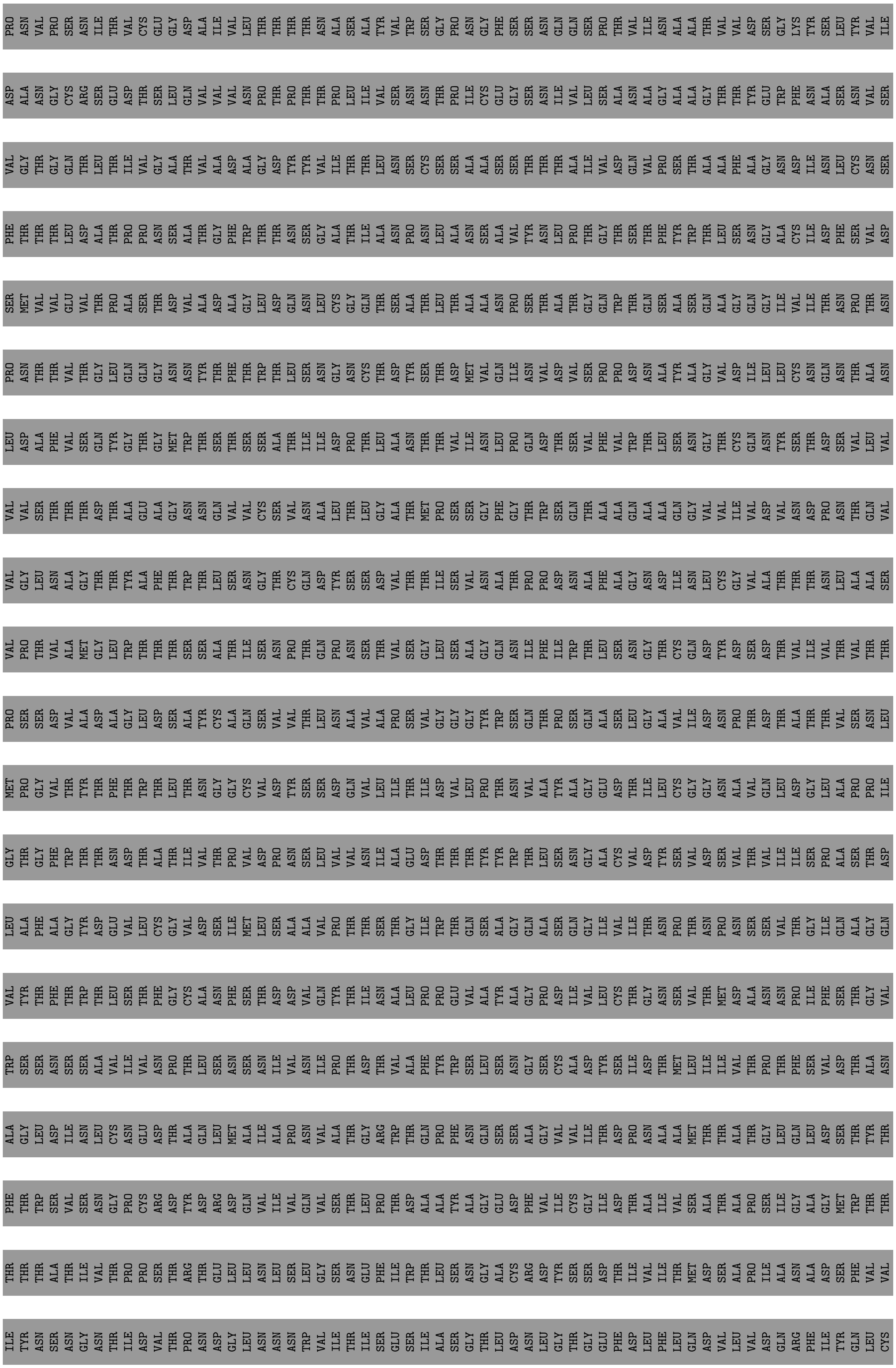
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ASP ALA ASN GLY CYS ARG SER GLU ASP THR SER LEU GLN VAL VAL VAL ASN PRO THR PRO THR THR PRO LEU ILE VAL SER ASN ASN THR PRO ILE CYS GLU GLY SER ASN ILE VAL LEU SER ALA ASN ALA GLY ALA ALA GLY THR THR TYR GLU TRP PHE ASN ALA SER ASN VAL SER
VAL GLY THR GLY GLN THR LEU THR ILE VAL GLY ALA THR VAL ALA ASP ALA GLY ASP TYR TYR VAL ILE THR THR LEU ASN SER CYS SER SER ALA ALA SER SER THR THR THR ALA ILE VAL ASP GLN VAL PRO SER THR ALA ALA PHE ALA GLY ASN ASP ILE ASN LEU CYS ASN SER
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PRO SER SER ASP VAL ALA ASP ALA GLY LEU ASP SER ALA TYR CYS ALA GLN SER VAL VAL THR LEU ASN ALA VAL ALA PRO SER VAL GLY GLY GLY TYR TRP SER GLN THR PRO SER GLN ALA SER LEU GLY ALA VAL ILE ASP ASN PRO THR ASP THR ALA THR THR VAL SER ASN LEU
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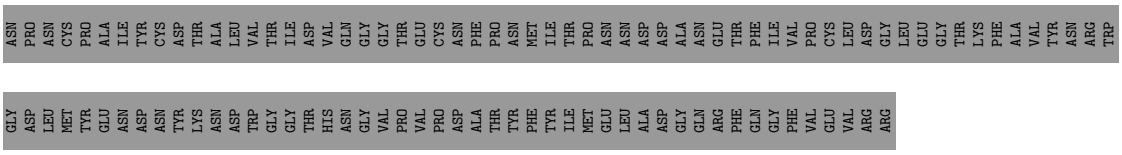
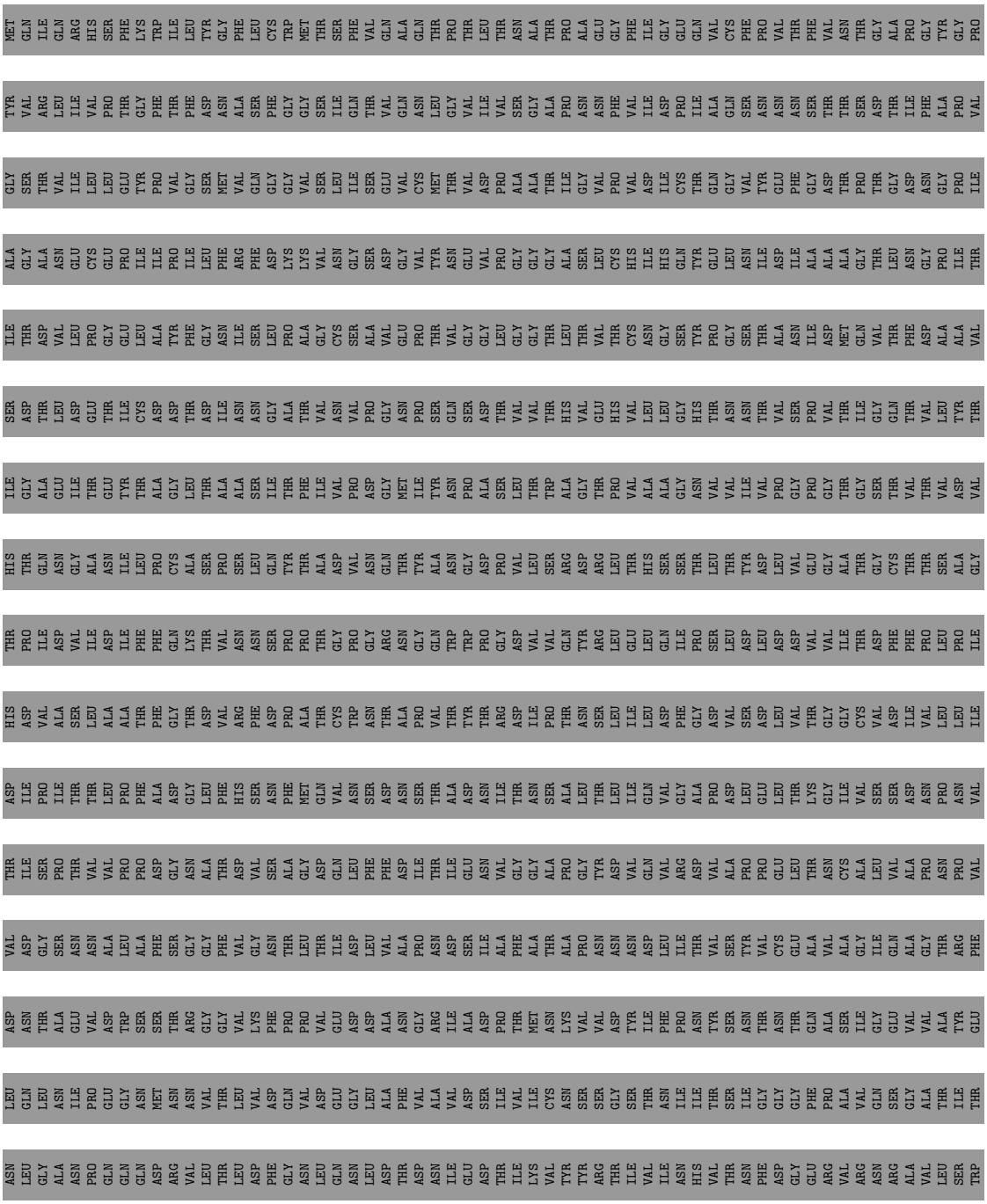
ILE TYR ASN SER ASN GLY ASN THR ILE ASP VAL THR PRO ASN ASP GLY LEU ASN ASN ASN TRP VAL ILE THR ILE SER GLU SER ILE ALA SER GLY THR LEU ASP ASN LEU GLY THR GLY GLU PHE ASP LEU PHE LEU GLN ASP VAL LEU VAL ASP GLN ARG PHE ILE TYR GLN LEU CYS



• Molecule 1: The grappling hook protein A (GhpA) in the bacterium Aureispira sp. CCB-QB1

Chain B: 5% 94%



GLY ASP ASP ILE ALA LEU SER THR SER THR VAL ALA SER SER TYR ASP TRP SER GLY PRO ASN GLY PHE THR SER ASN ALA GLN ASN PRO VAL VAL ILE THR ASN ALA THR GLY SER ASN ALA GLY VAL TYR THR LEU SER ILE VAL ASP GLY ASN GLY CYS SER SER ALA ASP THR SER

VAL GLN VAL THR VAL ASN ALA ALA PRO ALA GLN PRO SER MET THR THR ASN SER PRO ILE CYS ASN GLY ALA ASP LEU VAL MET SER THR SER ALA THR GLY ASN SER TYR ILE TRP ARG ALA PRO ASN GLY ALA ASP THR THR THR ALA SER SER THR LEU THR ILE VAL PRO THR SER

SER LEU TYR GLN SER GLY ASN TRP THR LEU SER VAL VAL ASN ALA ALA GLY CYS VAL SER PRO ALA SER ILE ALA SER ALA VAL GLU ILE ASN SER ILE PRO SER THR ALA SER ALA GLY ASN ASN GLY PRO VAL CYS THR GLY THR ASP ALA SER LEU SER ALA GLY THR VAL SER GLY

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LEU PRO ALA ASP PHE ALA VAL CYS GLU GLY ASP ASP ILE ALA LEU SER THR SER THR VAL ALA SER SER TYR ASP TRP SER GLY PRO ASN GLY PHE THR SER ASN ALA GLN ASN PRO VAL VAL ILE THR ASN ALA THR GLY SER ASN ALA GLY VAL TYR THR LEU SER ILE VAL ASP GLY

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SER THR LEU THR ILE ALA PRO THR SER SER LEU TYR GLN SER GLY ASN TRP THR LEU SER VAL VAL ASN ALA ALA GLY CYS VAL SER PRO ALA SER VAL ALA SER MET VAL THR ILE ASN ASN GLY THR ASN PRO THR ALA PHE ASN ASN GLY PRO VAL CYS ARG GLY ASP ALA VAL GLN

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TYR THR LEU PHE ILE VAL ASP ALA ASN GLY CYS GLN SER ALA ASP THR SER VAL VAL VAL GLY VAL ASN ARG GLY PRO ALA ALA PRO VAL LEU THR ASN ASN SER ALA ILE CYS ASP GLY ASP THR LEU LEU LEU SER THR THR ALA SER ALA ASP THR PHE ARG TRP ILE SER PRO ASN

GLY ILE ASP THR ILE THR THR VAL ASN SER LEU MET ILE VAL PRO THR ASN GLY THR TYR TYR GLN SER GLY ASP TRP THR LEU ILE THR GLN VAL ALA ASN ASN CYS PRO SER GLU PRO SER ALA PRO SER SER VAL VAL ILE ASN SER SER THR ALA ALA PRO THR ALA PHE ASN ASP

GLY PRO VAL CYS VAL GLY GLY ASP VAL THR LEU SER THR PRO SER ALA PRO GLY ALA PHE TYR GLN TRP TYR THR ASP ALA ALA LEU THR ASN LEU VAL ALA THR THR ALA SER PHE THR ALA ILE ASN ILE THR GLN ASP SER THR PHE TYR LEU VAL VAL THR VAL ASN GLY CYS THR

SER PRO ALA GLY SER THR VAL VAL ASN VAL ILE GLY GLN PRO SER ALA PRO ASN VAL PRO ALA ASP PHE GLU VAL CYS GLU GLY ASP ASP ILE ILE LEU GLY THR THR THR ILE ALA ALA SER TYR SER TRP THR GLY PRO ASN GLY PHE THR SER ASN LEU GLN ASN PRO ALA ALA ILE

THR ASN ALA SER LEU ILE ASP SER GLY ILE TYR ARG LEU VAL VAL THR TYR SER ASN GLY CYS VAL SER ALA ASP THR THR VAL ARG VAL GLY VAL ASN SER ASN PRO PRO VAL PRO ASN ILE VAL SER ASN GLY PRO ILE CYS PHE GLY ASP THR LEU VAL LEU SER SER SER THR SER

CYS GLY GLN SER GLN TRP ILE GLY PRO ASN GLY ASN SER GLN SER THR LEU GLY THR PRO GLY GLY SER ASN VAL LEU TRP THR ILE GLY SER THR THR SER ILE PRO MET ASN ASN ALA ASN TYR LEU PRO GLY ASN TRP TYR MET ILE CYS ILE ASP THR VAL THR GLY CYS ARG SER

GLU SER ASN THR ILE ASN VAL ILE ILE ASN ALA ASN PRO ASP THR PRO ALA VAL PHE ASN ASP GLY PRO VAL CYS GLU GLY GLY ASN SER ASN LEU SER THR ALA THR VAL SER GLY ALA SER TYR ALA TRP TYR SER ASP SER SER LEU THR SER LEU VAL SER THR ALA GLN ASN PRO

MET ILE VAL ASN ILE SER THR ASP THR THR TRP TYR LEU VAL VAL THR VAL ASN GLY CYS SER SER VAL ALA GLY SER THR THR VAL ILE VAL HIS PRO THR PRO VAL THR PRO ASN VAL PRO ALA ASN PHE ALA VAL CYS GLU GLY ASP ASN ILE THR LEU SER THR SER THR VAL ALA

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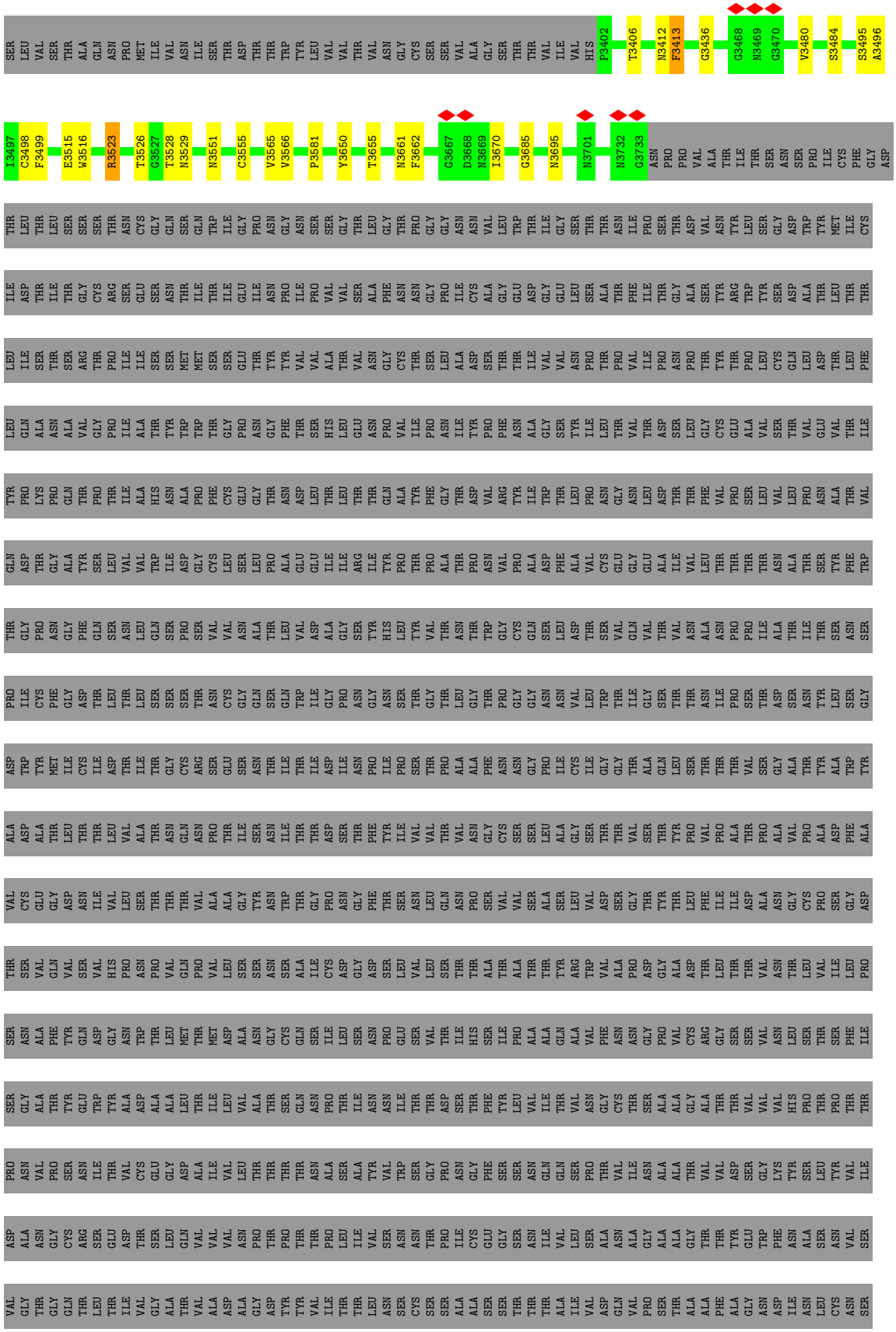
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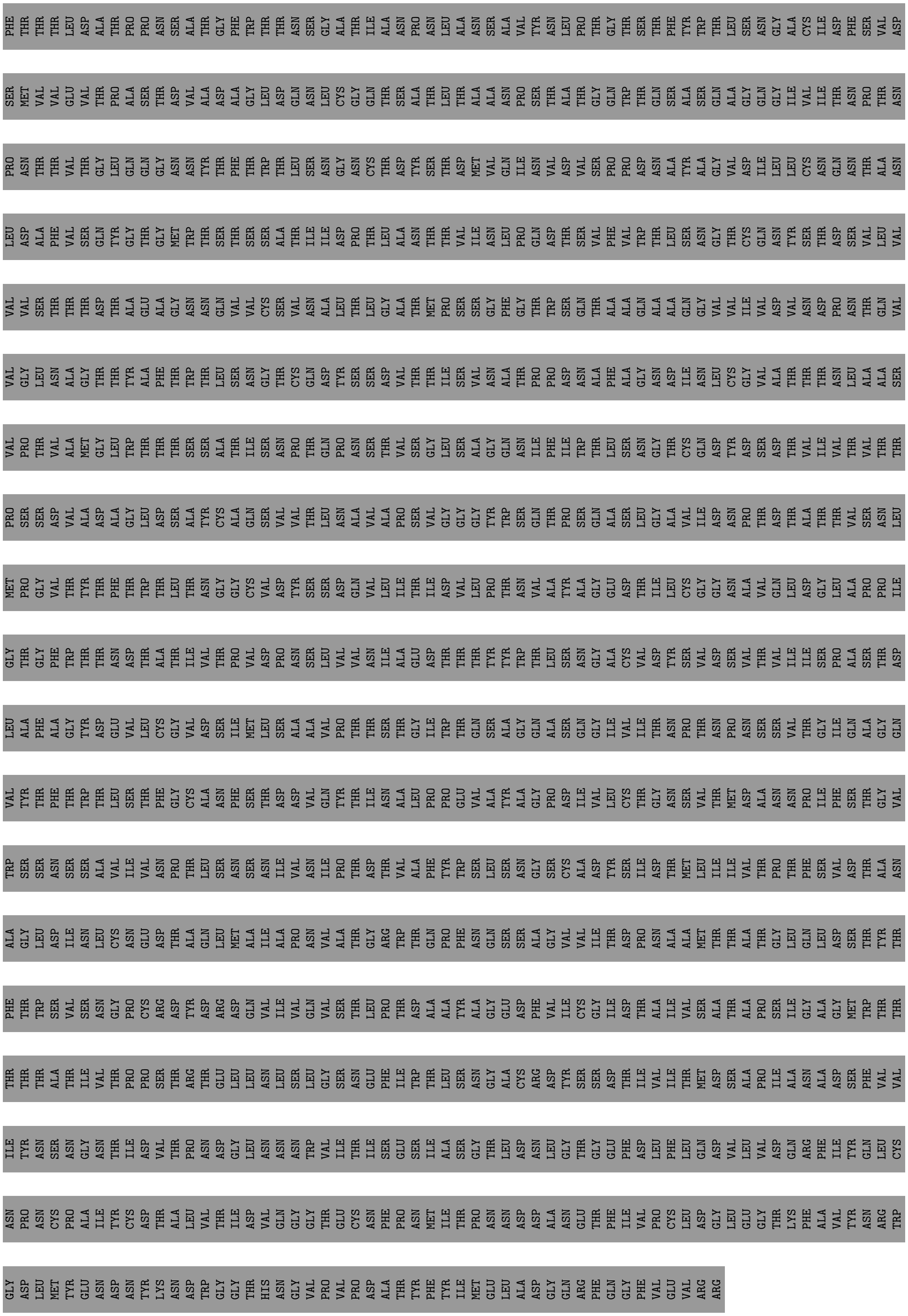

• Molecule 1: The grappling hook protein A (GhpA) in the bacterium Aureispira sp. CCB-QB1

Chain C: 5% 94%

MET GLN ILE GLN ARG HIS SER PHE LYS TRP ILE LEU TYR GLY PHE LEU CYS TRP MET THR SER PHE VAL GLN ALA GLN THR PRO THR LEU THR ASN ALA THR PRO ALA GLU GLY PHE ILE GLY GLU GLN VAL CYS PHE PRO VAL THR PHE VAL ASN THR GLY ALA PRO GLY TYR GLY PRO

TYR VAL ARG LEU ILE VAL PRO THR GLY PHE THR PHE ASP ASN ALA SER PHE GLY GLY SER ILE GLN THR VAL GLN ASN LEU GLY VAL ILE VAL SER GLY ALA PRO ASN ASN PHE VAL ILE ASP PRO ILE ALA GLN SER ASN ASN SER THR THR SER ASP THR ILE PHE ALA PRO VAL

GLY SER THR VAL ILE LEU LEU GLU TYR PRO VAL GLY SER MET VAL GLN GLY GLY VAL SER LEU ILE SER GLU VAL CYS MET THR VAL ASP PRO ALA ALA THR ILE GLY VAL PRO VAL ASP ILE CYS THR GLN GLY VAL TYR GLU PHE GLY ASP THR PRO THR GLY ASP ASN GLY PRO ILE

ALA GLY ALA ASN GLU CYS GLU PRO ILE ILE PRO ILE LEU PHE ARG PHE ASP LYS LYS VAL ASN GLY SER ASP GLY VAL TYR ASN GLU VAL PRO GLY GLY GLY ALA SER LEU CYS HIS ILE HIS GLN TYR GLU LEU ASN ILE ASP ILE ALA ALA ALA GLY THR LEU ASN GLY PRO ILE THR

ILE THR ASP VAL LEU PRO GLY GLU LEU ALA TYR PHE GLY ASN ILE SER LEU PRO ALA GLY CYS SER ALA VAL GLU PRO THR VAL GLY LEU GLY GLY THR LEU THR VAL THR CYS ASN GLY SER TYR PRO GLY SER THR ALA ASN ILE ASP MET GLN VAL THR PHE ASP ALA ALA VAL

SER ASP THR LEU ASP GLU THR ILE CYS ASP ASP THR ASP ILE ASN ASN GLY ALA THR VAL ASN VAL PRO GLY ASN PRO SER GLN SER ASP THR VAL VAL THR HIS VAL GLU HIS VAL LEU LEU GLY HIS THR ASN ASN THR VAL SER PRO VAL THR ILE GLY GLN THR VAL LEU TYR THR

ILE GLY ALA GLU ILE THR GLU TYR THR ALA GLY LEU THR ALA ALA SER ILE THR PHE ILE VAL PRO ASP GLY MET ILE TYR ASN PRO ALA SER LEU THR TRP ALA GLY THR PRO VAL ALA ALA GLY ASN VAL VAL ILE VAL PRO GLY PRO GLY THR GLY SER THR VAL THR VAL ASP VAL

HIS THR GLN ASN GLY ALA ASN ILE LEU PRO CYS ALA SER PRO SER LEU GLN TYR THR ALA ASP VAL ASN GLN THR TYR ALA ASN GLY ASP PRO VAL LEU SER ARG ASP ARG LEU THR HIS SER SER THR LEU THR TYR ASP LEU VAL GLU GLY ALA THR GLY CYS THR THR SER ALA GLY

THR PRO ILE ASP VAL ILE ASP ILE PHE PHE GLN LYS THR VAL ASN ASN SER PRO PRO THR GLY PRO GLY ARG ASN GLY GLN TRP TRP PRO GLY ASP VAL VAL GLN TYR ARG LEU GLU LEU GLN ILE PRO SER LEU ASP LEU ASP ASP VAL VAL ILE THR ASP PHE PHE PRO LEU PRO ILE

HIS ASP VAL ALA SER LEU ALA ALA THR PHE GLY THR ASP VAL ARG PHE ASP PRO ALA THR CYS TRP ASN THR ALA PRO VAL THR TYR THR ARG ASP ILE PRO THR ASN SER LEU ILE LEU ASP PHE GLY ASP VAL SER ASP LEU VAL THR GLY GLY CYS VAL ASP ILE VAL LEU LEU ILE

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THR ILE SER PRO THR VAL VAL PRO PRO ASP GLY ASN ALA THR ASP VAL SER ALA GLY ASP GLN LEU PHE PHE ASP ILE THR ILE GLU ASN VAL GLY GLY ALA PRO GLY TYR ASP VAL GLN VAL ARG ASP VAL ALA PRO PRO GLU LEU THR ASN CYS ALA LEU VAL ALA PRO ASN PRO VAL

VAL ASP GLY SER ASN ASN ALA LEU LEU ALA PHE SER GLY GLY PHE VAL GLY ASN THR LEU THR ILE ASP LEU VAL ALA PRO ASN ASP SER ILE ALA PHE ALA THR ALA PRO ASN ASN ASN ASP LEU ILE THR VAL SER TYR VAL CYS GLU ALA VAL ALA GLY ILE GLN ALA GLY THR ARG PHE

ASP ASN THR ALA GLU VAL ASP TRP SER SER THR ARG GLY GLY VAL LYS PHE PRO PRO VAL GLU ASP ASP ALA ASN GLY ARG ILE ALA ASP PRO THR MET ASN LYS VAL VAL ASP TYR ILE PHE PRO ASN TYR SER ASN THR ASN THR GLN ALA SER ILE GLY GLU VAL VAL ALA TYR GLU

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ASP ASN PRO ASN THR PRO GLY ASP ARG SER SER ILE ASN ASP ARG ALA PRO PHE VAL THR ILE VAL GLU PRO GLN LEU GLU ILE SER LYS SER PHE THR PRO ASP GLU VAL LEU PRO GLY ASN ASN SER PHE VAL THR LEU THR VAL ARG ASN PRO GLY THR SER SER ALA PRO ALA PHE

ASP VAL SER LEU THR ASP ILE LEU PRO THR GLY MET THR PHE VAL SER GLY PHE SER ALA GLY GLY THR ALA SER ILE THR THR PRO PRO THR ASN GLY GLY THR ILE THR ALA HIS TRP ASP THR ILE ASN VAL GLY GLU VAL TYR SER ILE THR PHE GLU VAL GLN ALA SER SER

SER ILE THR PRO CYS PHE THR LEU THR ASN CYS ALA ASN LEU VAL TRP GLU SER ILE ALA GLU ALA ASP GLU PRO ASN MET PRO THR ALA PHE SER SER ASN LEU GLY VAL GLN ARG THR GLY ASN PRO GLY ASN LEU GLY GLY ALA ALA ASN THR TYR THR GLN ASP SER CYS ALA ASP

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LEU SER VAL VAL ASN ALA ALA GLY CYS VAL SER PRO ALA SER ILE ALA SER ALA VAL GLU ILE ASN SER ILE PRO SER THR ALA SER ALA GLY ASN ASN GLY PRO VAL CYS THR GLY THR ASP ALA SER LEU SER ALA GLY THR VAL SER GLY ALA SER TYR ALA TRP TYR THR ASP ALA

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VAL GLN VAL THR VAL ASN ALA ALA PRO ALA GLN PRO SER MET THR THR ASN SER PRO ILE CYS ASN GLY ALA ASP LEU VAL MET SER THR SER ALA THR GLY ASN SER TYR ILE TRP ARG ALA PRO ASN GLY ALA ASP THR THR THR ALA SER SER THR LEU THR ILE VAL PRO THR SER

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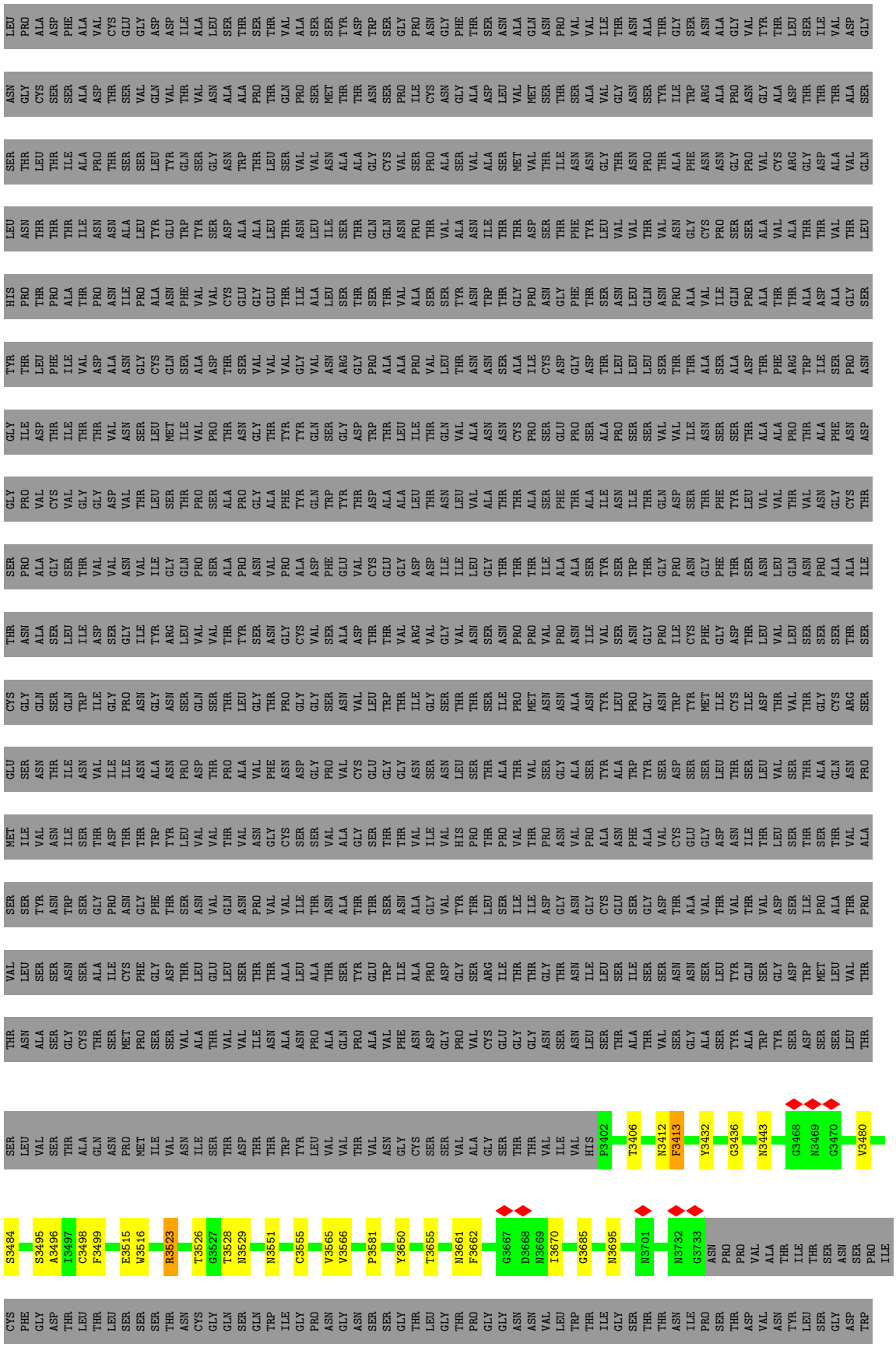
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GLU VAL THR ILE TYR PRO LYS PRO GLN THR PRO THR ILE ALA HIS ASN ALA PRO PHE CYS GLU GLY THR ASN ASP LEU THR LEU THR THR GLN ALA TYR PHE GLY THR ASP VAL ARG TYR ILE TRP THR LEU PRO ASN GLY ASN LEU ASP THR THR PHE VAL PRO SER LEU VAL LEU PRO

ASN ALA THR VAL GLN ASP THR GLY ALA TYR SER LEU VAL VAL TRP ILE ASP GLY CYS LEU SER LEU PRO ALA GLU GLU ILE ILE ARG ILE TYR PRO THR PRO ALA THR PRO ASN VAL PRO ALA ASP PHE ALA VAL CYS GLU GLY GLU ALA ILE VAL LEU THR THR THR ASN ALA THR

SER TYR PHE TRP THR GLY PRO ASN GLY PHE GLN SER ASN LEU GLN SER PRO SER VAL VAL ASN ALA THR LEU VAL ASP ALA GLY SER TYR HIS LEU TYR VAL THR ASN THR TRP GLY CYS GLN SER LEU ASP THR SER VAL GLN VAL THR VAL ASN ALA ASN PRO PRO ILE ALA THR ILE

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ALA ASP PHE ALA VAL CYS GLU GLY ASP ASN ILE VAL LEU SER THR THR THR VAL ALA ALA GLY TYR ASN TRP THR GLY PRO ASN GLY PHE THR SER ASN LEU GLN ASN PRO SER VAL VAL SER ALA SER LEU VAL ASP SER GLY THR TYR THR LEU PHE ILE ILE ASP ALA ASN GLY CYS

PRO SER GLY ASP THR SER VAL GLN VAL SER VAL HIS PRO ASN PRO VAL GLN PRO VAL LEU SER SER ASN SER ALA ILE CYS ASP GLY ASP SER LEU VAL LEU SER THR THR ALA THR ALA THR THR TYR ARG TRP VAL ALA PRO ASP GLY ALA ASP THR LEU THR THR VAL ASN THR LEU

VAL ILE LEU PRO SER ASN ALA PHE TYR GLN ASP GLY ASN TRP THR LEU MET THR MET ASP ALA ASN GLY CYS GLN SER ILE LEU SER ASN PRO GLU SER VAL THR ILE HIS SER ILE PRO ALA ALA GLN ALA VAL PHE ASN ASN GLY PRO VAL CYS ARG GLY SER SER VAL ASN LEU SER

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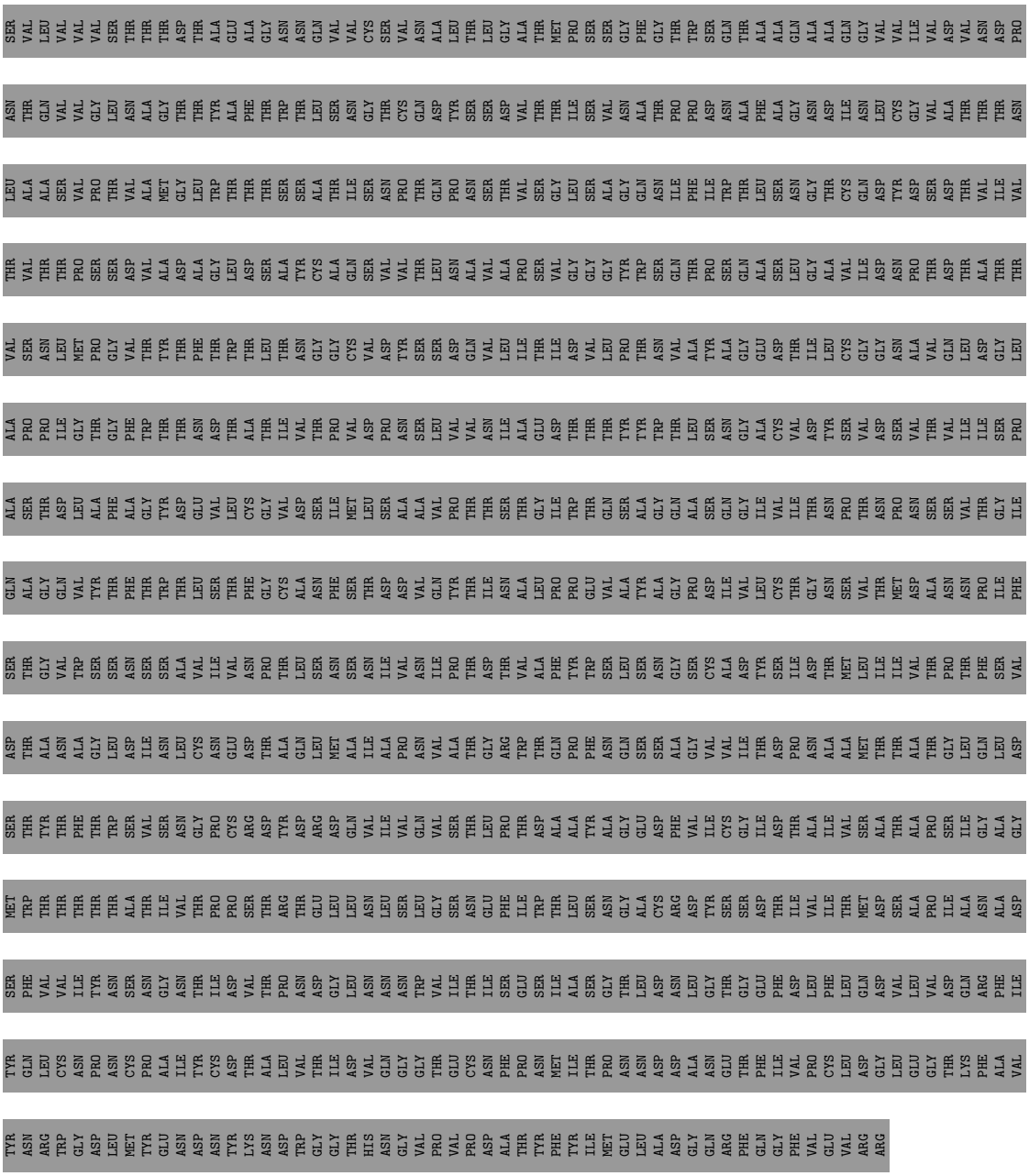
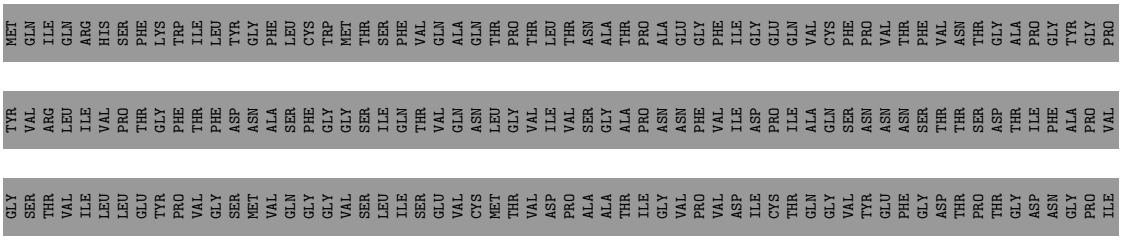
ASN THR ALA ASN LEU ASP ALA PHE VAL SER GLN TYR GLY THR GLY MET TRP THR SER THR SER SER ALA THR ILE ILE ASP PRO THR LEU ALA ASN THR THR VAL ILE ASN LEU PRO GLN ASP THR SER VAL PHE VAL TRP THR LEU SER ASN GLY THR CYS GLN ASN TYR SER THR ASP



• Molecule 1: The grappling hook protein A (GhpA) in the bacterium Aureispira sp. CCB-QB1

Chain D: 5% 94%



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ILE GLY ALA GLU ILE THR GLU TYR THR ALA GLY LEU THR ALA ALA SER ILE THR PHE ILE VAL PRO ASP GLY MET ILE TYR ASN PRO ALA SER LEU THR TRP ALA GLY THR PRO VAL ALA ALA GLY ASN VAL VAL ILE VAL PRO GLY PRO GLY THR GLY SER THR VAL THR VAL ASP VAL

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ASP VAL SER LEU THR ASP ILE LEU PRO THR GLY MET THR PHE VAL SER GLY PHE SER ALA GLY GLY THR ALA SER ILE THR THR PRO PRO THR ASN GLY GLY GLY THR ILE THR ALA HIS TRP ASP THR ILE ASN VAL GLY GLU VAL TYR SER ILE THR PHE GLU VAL GLN ALA SER SER

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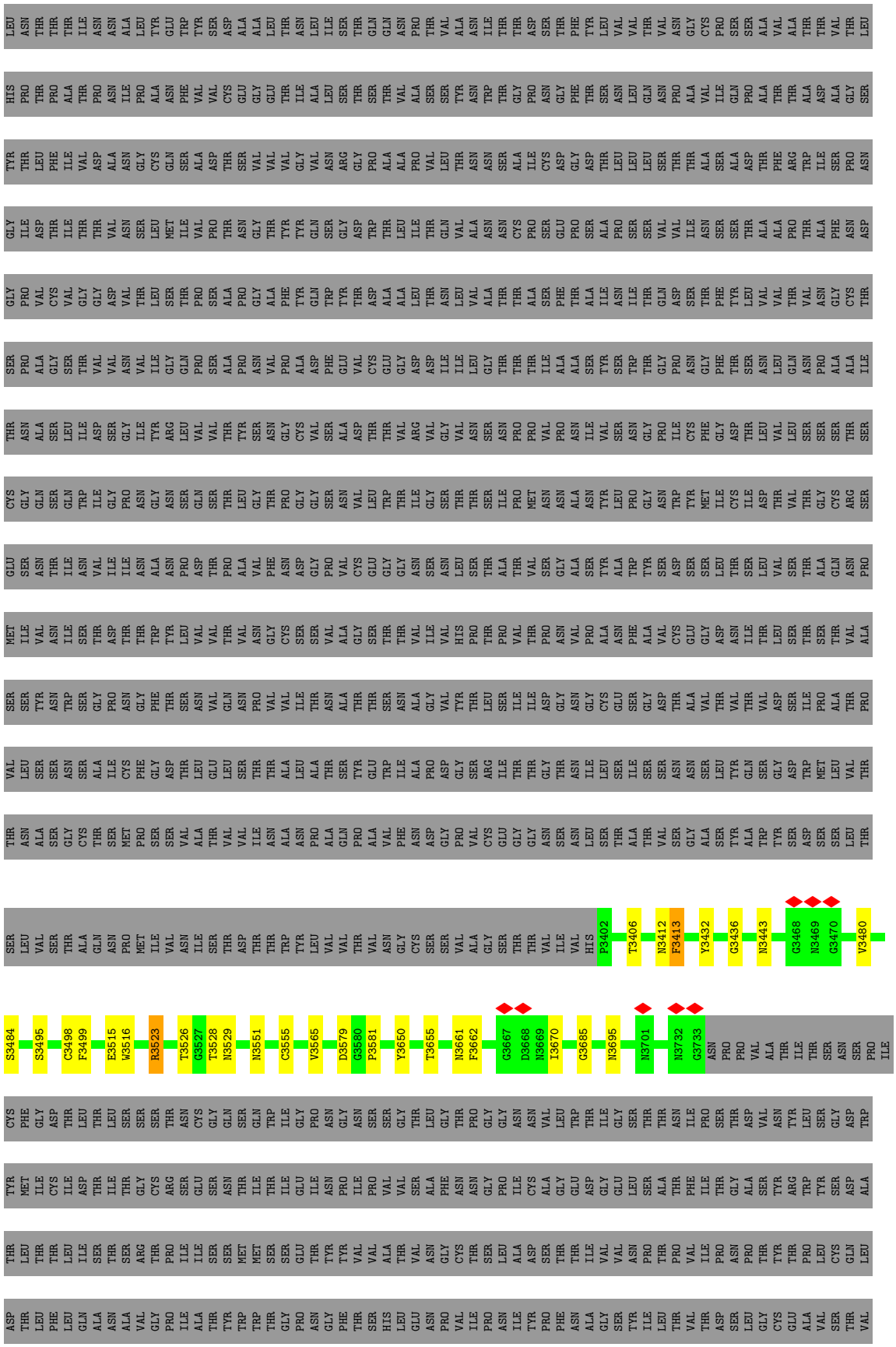
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GLU VAL THR ILE TYR PRO LYS PRO GLN THR PRO THR ILE ALA HIS ASN ALA PRO PHE CYS GLU GLY THR ASN ASP LEU THR LEU THR THR GLN ALA TYR PHE GLY THR ASP VAL ARG TYR ILE TRP THR LEU PRO ASN GLY ASN LEU ASP THR THR PHE VAL PRO SER LEU VAL LEU PRO

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THR SER PHE ILE SER GLY ALA THR TYR GLU TRP TYR ALA ASP ALA ALA LEU THR ILE LEU VAL ALA THR SER GLN ASN PRO THR ILE ASN ASN ILE THR THR ASP SER THR PHE TYR LEU VAL ILE THR VAL ASN GLY CYS THR SER ALA ALA GLY ALA THR THR VAL VAL HIS PRO

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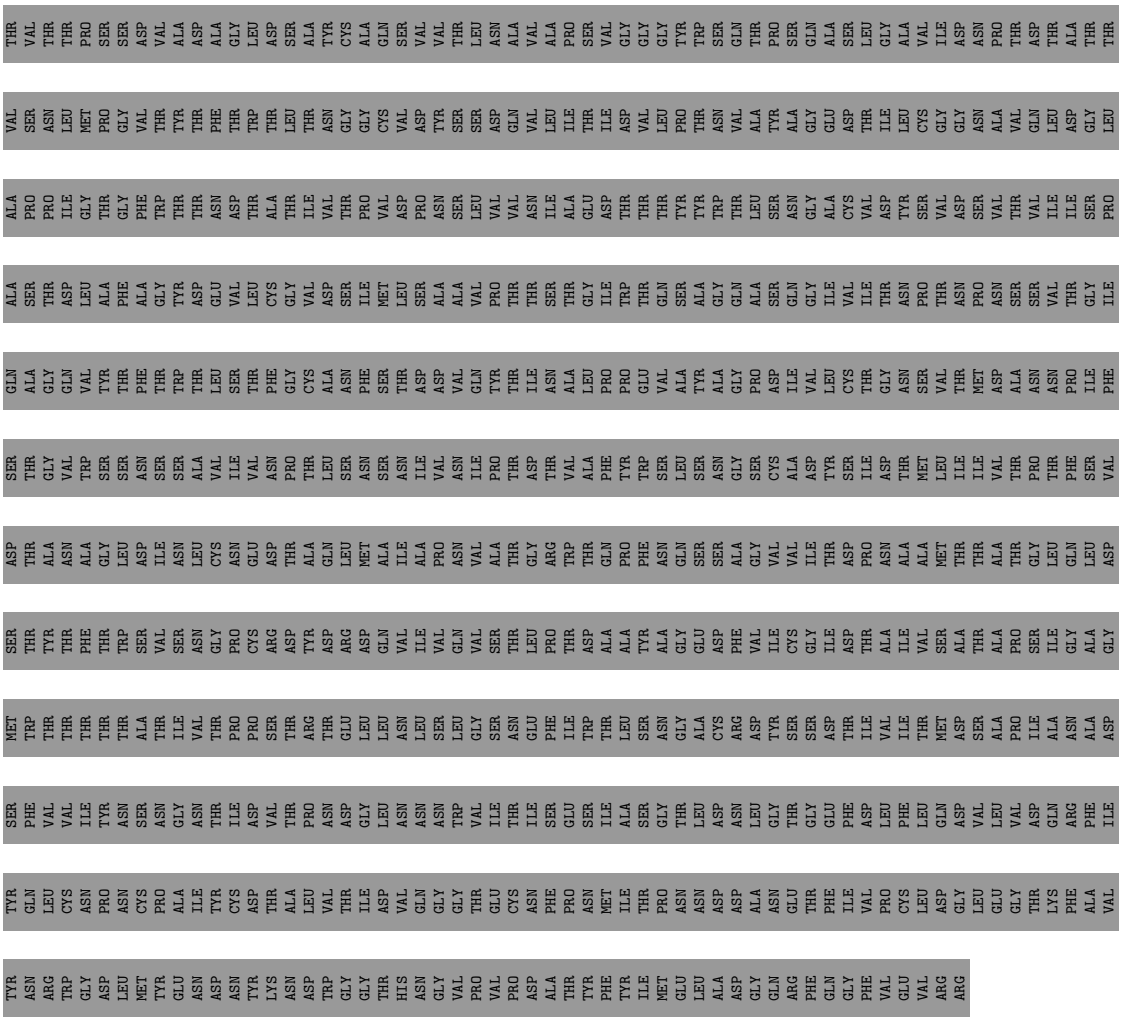
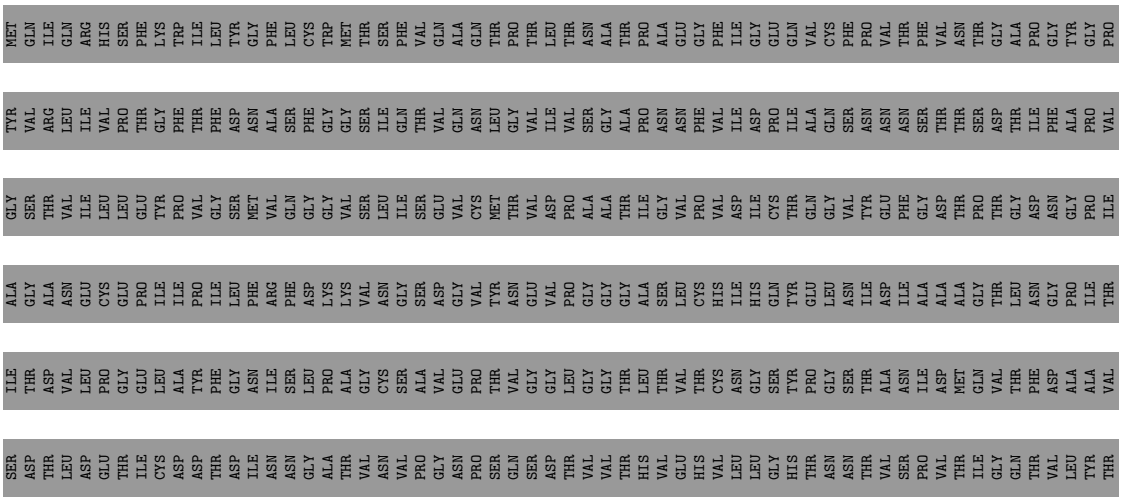


• Molecule 1: The grappling hook protein A (GhpA) in the bacterium Aureispira sp. CCB-QB1

Chain E: 5% 94%



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THR GLN PRO SER MET THR THR ASN SER PRO ILE CYS ASN GLY ALA ASP LEU VAL MET SER THR SER ALA VAL GLY ASN SER TYR ILE TRP ARG ALA PRO ASN GLY ALA ASP THR THR THR ALA SER SER THR LEU THR ILE VAL PRO THR SER SER LEU TYR GLN SER GLY ASN TRP THR

LEU SER VAL VAL ASN ALA ALA GLY CYS VAL SER PRO ALA SER ILE ALA SER ALA VAL GLU ILE ASN SER ILE PRO SER THR ALA SER ALA GLY ASN ASN GLY PRO VAL CYS THR GLY THR ASP ALA SER LEU SER ALA GLY THR VAL SER GLY ALA SER TYR ALA TRP TYR THR ASP ALA

GLY THR SER ASN GLN PHE SER THR LEU GLN ASN PRO THR VAL ASN ASN LEU THR ASN ASP SER THR PHE TYR LEU LEU VAL THR VAL ASN GLY CYS PRO SER ALA LEU ASP SER THR THR VAL VAL VAL TYR PRO LEU THR PRO SER PRO SER LEU PRO ALA ASP PHE ALA VAL CYS GLU

GLY ASP ASP ILE ALA LEU SER THR SER THR VAL ALA SER SER TYR ASP TRP SER GLY PRO ASN GLY PHE THR SER ASN ALA GLN ASN PRO VAL VAL ILE THR ASN ALA THR GLY SER ASN ALA GLY VAL TYR THR LEU SER ILE VAL ASP GLY ASN GLY CYS SER SER ALA ASP THR SER

VAL GLN VAL THR VAL ASN ALA ALA PRO ALA GLN PRO SER MET THR THR ASN SER PRO ILE CYS ASN GLY ALA ASP LEU VAL MET SER THR SER ALA THR GLY ASN SER TYR ILE TRP ARG ALA PRO ASN GLY ALA ASP THR THR THR ALA SER SER THR LEU THR ILE VAL PRO THR SER

SER LEU TYR GLN SER GLY ASN TRP THR LEU SER VAL VAL ASN ALA ALA GLY CYS VAL SER PRO ALA SER ILE ALA SER ALA VAL GLU ILE ASN SER ILE PRO SER THR ALA SER ALA GLY ASN ASN GLY PRO VAL CYS THR GLY THR ASP ALA SER LEU SER ALA GLY THR VAL SER GLY

ALA SER TYR ALA TRP TYR THR ASP ALA GLY THR SER ASN GLN PHE SER THR LEU GLN ASN PRO THR VAL ASN ASN LEU THR ASN ASP SER THR PHE TYR LEU LEU VAL THR VAL ASN GLY CYS PRO SER ALA LEU ASP SER THR THR VAL VAL VAL TYR PRO LEU THR PRO SER PRO SER

LEU PRO ALA ASP PHE ALA VAL CYS GLU GLY ASP ASP ILE ALA LEU SER THR SER THR VAL ALA SER SER TYR ASP TRP SER GLY PRO ASN GLY PHE THR SER ASN ALA GLN ASN PRO VAL VAL ILE THR ASN ALA THR GLY SER ASN ALA GLY VAL TYR THR LEU SER ILE VAL ASP GLY

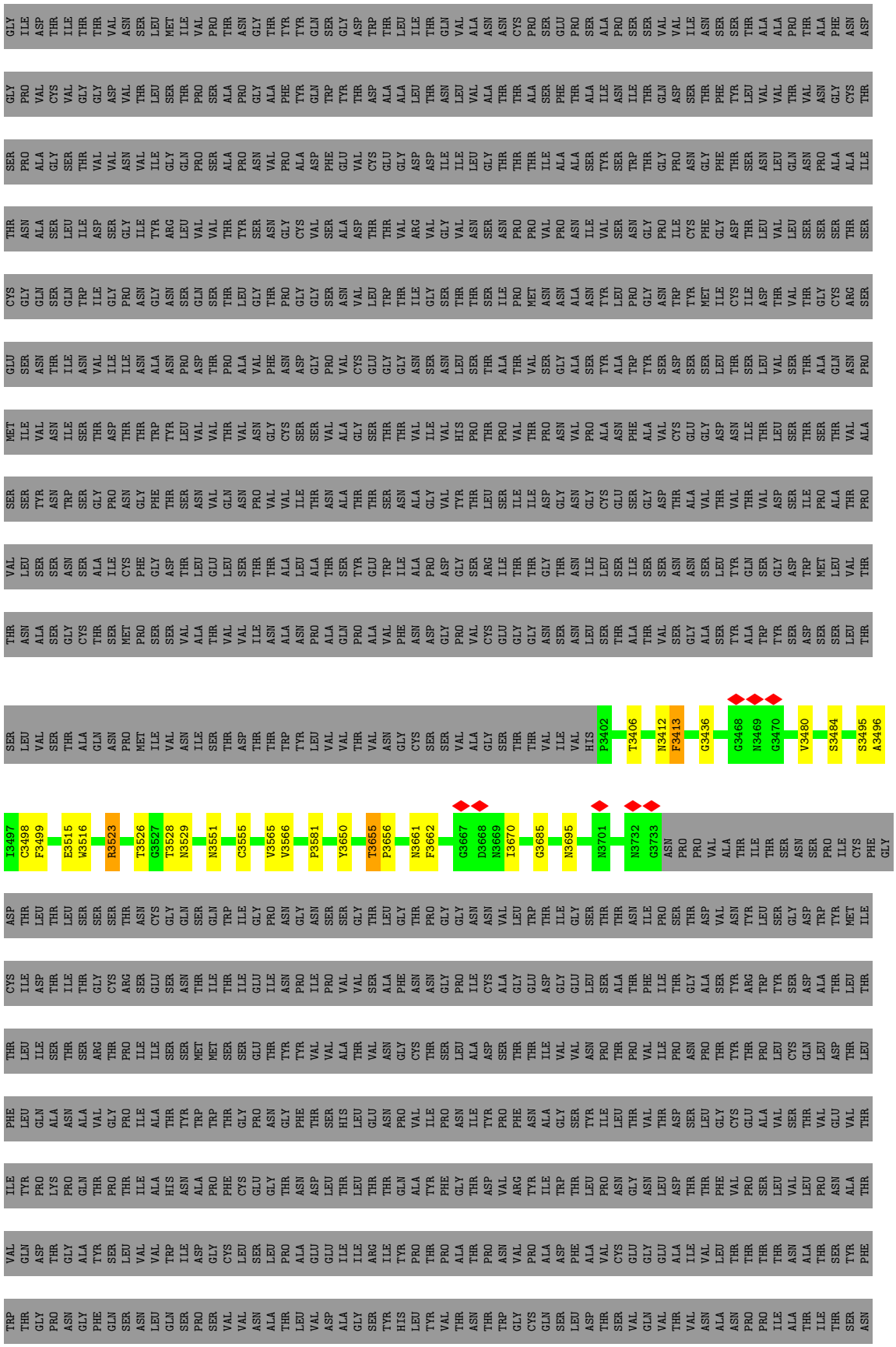
ASN GLY CYS SER SER ALA ASP THR SER VAL GLN VAL THR VAL ASN ALA ALA PRO THR GLN PRO SER MET THR THR ASN SER PRO ILE CYS ASN GLY ALA ASP LEU VAL MET SER THR SER ALA VAL GLY ASN SER TYR ILE TRP ARG ALA PRO ASN GLY ALA ASP THR THR THR ALA SER

SER THR LEU THR ILE ALA PRO THR SER SER LEU TYR GLN SER GLY ASN TRP THR LEU SER VAL VAL ASN ALA ALA GLY CYS VAL SER PRO ALA SER VAL ALA SER MET VAL THR ILE ASN ASN GLY THR ASN PRO THR ALA PHE ASN ASN GLY PRO VAL CYS ARG GLY ASP ALA VAL GLN

LEU ASN THR THR THR ILE ASN ASN ALA LEU TYR GLU TRP TYR SER ASP ALA ALA LEU THR ASN LEU ILE SER THR GLN GLN ASN PRO THR THR VAL ALA ASN ILE THR THR ASP SER THR PHE TYR LEU VAL VAL THR VAL ASN GLY CYS PRO SER SER ALA VAL ALA THR THR VAL THR LEU

HIS PRO THR PRO ALA THR PRO ASN ILE PRO ALA ASN PHE VAL VAL CYS GLU GLY GLU THR ILE ALA LEU SER THR SER THR VAL ALA SER SER TYR ASN TRP THR GLY PRO ASN GLY PHE THR SER ASN LEU GLN ASN PRO ALA VAL ILE GLN PRO ALA THR THR ALA ASP ALA GLY SER

TYR THR LEU PHE ILE VAL ASP ALA ASN GLY CYS GLN SER ALA ASP THR SER VAL VAL VAL GLY VAL ASN ARG GLY PRO ALA ALA PRO VAL LEU THR ASN ASN SER ALA ILE CYS ASP GLY ASP THR LEU LEU LEU SER THR THR ALA SER ALA ASP THR PHE ARG TRP ILE SER PRO ASN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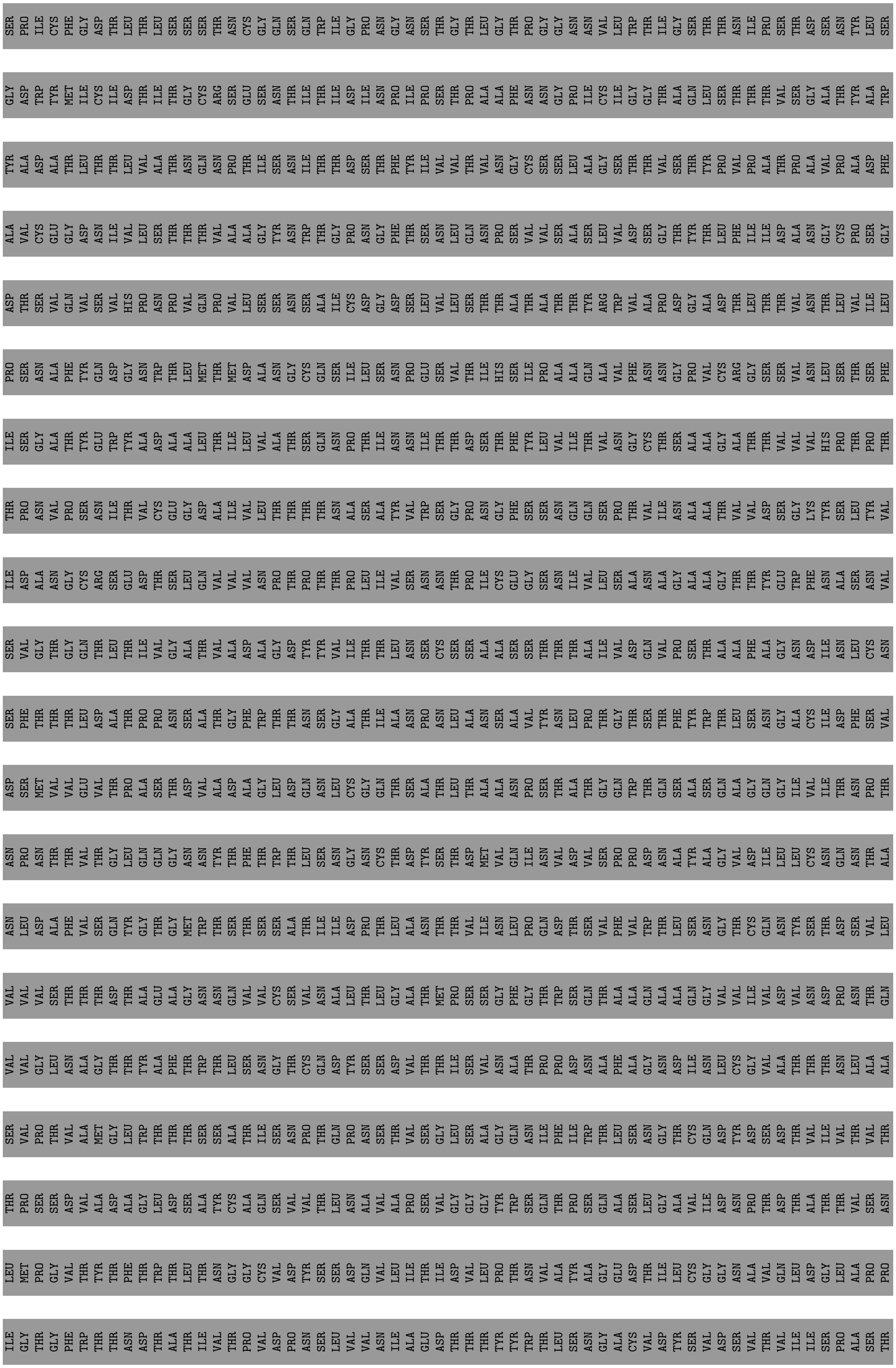

SER PRO ILE CYS PHE GLY ASP THR LEU THR LEU SER SER SER THR ASN CYS GLY GLN SER GLN TRP ILE GLY PRO ASN GLY ASN SER THR GLY THR LEU GLY THR PRO GLY GLY ASN ASN VAL LEU TRP THR ILE GLY SER THR THR ASN ILE PRO SER THR ASP SER ASN TYR LEU SER
GLY ASP TRP TYR MET ILE CYS ILE ASP THR ILE THR GLY CYS ARG SER GLU SER ASN THR ILE THR ILE ASP ILE ASN PRO ILE PRO SER THR PRO ALA ALA PHE ASN ASN GLY PRO ILE CYS ILE GLY GLY THR ALA GLN LEU SER THR THR THR VAL SER GLY ALA THR TYR ALA TRP
TYR ALA ASP ALA THR LEU THR THR LEU VAL ALA THR ASN GLN ASN PRO THR ILE SER ASN ILE THR THR ASP SER THR PHE TYR ILE VAL VAL THR VAL ASN GLY CYS SER SER LEU ALA GLY SER THR THR VAL SER THR TYR PRO VAL PRO ALA THR PRO ALA VAL PRO ALA ASP PHE
ALA VAL CYS GLU GLY ASP ASN ILE VAL LEU SER THR THR THR VAL ALA ALA GLY TYR ASN TRP THR GLY PRO ASN GLY PHE THR SER ASN LEU GLN ASN PRO SER VAL VAL SER ALA SER LEU VAL ASP SER GLY THR TYR THR LEU PHE ILE ILE ASP ALA ASN GLY CYS PRO SER GLY
ASP THR SER VAL GLN VAL SER VAL HIS PRO ASN PRO VAL GLN PRO VAL LEU SER SER ASN SER ALA ILE CYS ASP GLY ASP SER LEU VAL LEU SER THR THR ALA THR ALA THR THR TYR ARG TRP VAL ALA PRO ASP GLY ALA ASP THR LEU THR THR VAL ASN THR LEU VAL ILE LEU
PRO SER ASN ALA PHE TYR GLN ASP GLY ASN TRP THR LEU MET THR MET ASP ALA ASN GLY CYS GLN SER ILE LEU SER ASN PRO GLU SER VAL THR ILE HIS SER ILE PRO ALA ALA GLN ALA VAL PHE ASN ASN GLY PRO VAL CYS ARG GLY SER SER VAL ASN LEU SER THR SER PHE
ILE SER GLY ALA THR TYR GLU TRP TYR ALA ASP ALA ALA LEU THR ILE LEU VAL ALA THR SER GLN ASN PRO THR ILE ASN ASN ILE THR THR ASP SER THR PHE TYR LEU VAL ILE THR VAL ASN GLY CYS THR SER ALA ALA GLY ALA THR THR VAL VAL HIS PRO THR PRO THR
THR PRO ASN VAL PRO SER ASN ILE THR VAL CYS GLU GLY ASP ALA ILE VAL LEU THR THR THR ASN ALA SER ALA TYR VAL TRP SER GLY PRO ASN GLY PHE SER SER ASN GLN GLN SER PRO THR VAL ILE ASN ALA ALA THR VAL VAL ASP SER GLY LYS TYR SER LEU TYR VAL
ILE ASP ALA ASN GLY CYS ARG SER GLU ASP THR SER LEU GLN VAL VAL VAL ASN PRO THR PRO THR THR PRO LEU ILE VAL SER ASN ASN THR PRO ILE CYS GLU GLY SER ASN ILE VAL LEU SER ALA ASN ALA GLY ALA ALA GLY THR THR TYR GLU TRP PHE ASN ALA SER ASN VAL
SER VAL GLY THR GLY GLN THR LEU THR ILE VAL GLY ALA THR VAL ALA ASP ALA GLY ASP TYR TYR VAL ILE THR THR LEU ASN SER CYS SER SER ALA ALA SER SER THR THR THR ALA ILE VAL ASP GLN VAL PRO SER THR ALA ALA PHE ALA GLY ASN ASP ILE ASN LEU CYS ASN
SER PHE THR THR THR LEU ASP ALA THR PRO PRO ASN SER ALA THR GLY PHE TRP THR THR ASN SER GLY ALA THR ILE ALA ASN PRO ASN LEU ALA ASN SER ALA VAL TYR ASN LEU PRO THR GLY THR SER THR PHE TYR TRP THR LEU SER ASN GLY ALA CYS ILE ASP PHE SER VAL
ASP SER MET VAL VAL GLU VAL THR PRO ALA SER THR ASP VAL ALA ASP ALA GLY LEU ASP GLN ASN LEU CYS GLY GLN THR SER ALA THR LEU THR ALA ALA ASN PRO SER THR ALA THR GLY GLN TRP THR GLN SER ALA SER GLN ALA GLY GLN GLY ILE VAL ILE THR ASN PRO THR
ASN PRO ASN THR THR VAL THR GLY LEU GLN GLN GLY ASN ASN TYR THR PHE THR TRP THR LEU SER ASN GLY ASN CYS THR ASP TYR SER THR ASP MET VAL GLN ILE ASN VAL ASP VAL SER PRO PRO ASP ASN ALA TYR ALA GLY VAL ASP ILE LEU LEU CYS ASN GLN ASN THR ALA
ASN LEU ASP ALA PHE VAL SER GLN TYR GLY THR GLY MET TRP THR SER THR SER SER ALA THR ILE ILE ASP PRO THR LEU ALA ASN THR THR VAL ILE ASN LEU PRO GLN ASP THR SER VAL PHE VAL TRP THR LEU SER ASN GLY THR CYS GLN ASN TYR SER THR ASP SER VAL LEU
VAL VAL VAL SER THR THR THR ASP THR ALA GLU ALA GLY ASN ASN GLN VAL VAL CYS SER VAL ASN ALA LEU THR LEU GLY ALA THR MET PRO SER SER GLY PHE GLY THR TRP SER GLN THR ALA ALA GLN ALA ALA GLN GLY VAL VAL ILE VAL ASP VAL ASN ASP PRO ASN THR GLN
VAL VAL GLY LEU ASN ALA GLY THR THR TYR ALA PHE THR TRP THR LEU SER ASN GLY THR CYS GLN ASP TYR SER SER ASP VAL THR THR ILE SER VAL ASN ALA THR PRO PRO ASP ASN ALA PHE ALA GLY ASN ASP ILE ASN LEU CYS GLY VAL ALA THR THR THR ASN LEU ALA ALA
SER VAL PRO THR VAL ALA MET GLY LEU TRP THR THR THR SER SER ALA THR ILE SER ASN PRO THR GLN PRO ASN SER THR VAL SER GLY LEU SER ALA GLY GLN ASN ILE PHE ILE TRP THR LEU SER ASN GLY THR CYS GLN ASP TYR ASP SER ASP THR VAL ILE VAL THR VAL THR
THR PRO SER SER ASP VAL ALA ASP ALA GLY LEU ASP SER ALA TYR CYS ALA GLN SER VAL VAL THR LEU ASN ALA VAL ALA PRO SER VAL GLY GLY TYR TRP SER GLN THR PRO SER GLN ALA SER LEU GLY ALA VAL ILE ASP ASN PRO THR ASP THR ALA THR THR VAL SER ASN
LEU MET PRO GLY VAL THR TYR THR PHE THR TRP THR LEU THR ASN GLY GLY CYS VAL ASP TYR SER SER ASP GLN VAL LEU ILE THR ILE ASP VAL LEU PRO THR ASN VAL ALA TYR ALA GLY GLU ASP THR ILE LEU CYS GLY GLY ASN ALA VAL GLN LEU ASP GLY LEU ALA PRO PRO
ILE GLY THR GLY PHE TRP THR THR ASN ASP THR ALA THR ILE VAL THR PRO VAL ASP PRO ASN SER LEU VAL VAL ASN ILE ALA GLU ASP THR THR THR TYR TYR TRP THR LEU SER ASN GLY ALA CYS VAL ASP TYR SER VAL ASP SER VAL THR VAL ILE ILE SER PRO ALA SER THR

ASP LEU ALA PHE ALA GLY TYR ASP GLU VAL LEU CYS GLY VAL ASP SER ILE MET LEU SER ALA ALA VAL PRO THR THR SER THR GLY ILE TRP THR GLN SER ALA GLY GLN ALA SER GLN GLY ILE VAL ILE THR ASN PRO THR ASN PRO ASN SER SER VAL THR GLY ILE GLN ALA GLY

GLN VAL TYR THR PHE THR TRP THR LEU SER THR PHE GLY CYS ALA ASN PHE SER THR ASP ASP VAL GLN TYR THR ILE ASN ALA LEU PRO PRO GLU VAL ALA TYR ALA GLY PRO ASP ILE VAL LEU CYS THR GLY ASN SER VAL THR MET ASP ALA ASN ASN PRO ILE PHE SER THR GLY

VAL TRP SER SER ASN SER SER ALA VAL ILE VAL ASN PRO THR LEU SER ASN SER ASN ILE VAL ASN ILE PRO THR ASP THR VAL ALA PHE TYR TRP SER LEU SER ASN GLY SER CYS ALA ASP TYR SER ILE ASP THR MET LEU ILE ILE VAL THR PRO THR PHE SER VAL ASP THR ALA

ASN ALA GLY LEU ASP ILE ASN LEU CYS ASN GLU ASP THR ALA GLN LEU MET ALA ILE ALA PRO ASN VAL ALA THR GLY ARG TRP THR GLN PRO PHE ASN GLN SER SER ALA GLY VAL VAL ILE THR ASP PRO ASN ALA ALA MET THR THR ALA THR GLY LEU GLN LEU ASP SER THR TYR

THR PHE THR TRP SER VAL SER ASN GLY PRO CYS ARG ASP TYR ASP ARG ASP GLN VAL ILE VAL GLN VAL SER THR LEU PRO THR ASP ALA ALA TYR ALA GLY GLU ASP PHE VAL ILE CYS GLY ILE ASP THR ALA ILE VAL SER ALA THR ALA PRO SER ILE GLY ALA GLY MET TRP THR

THR THR THR THR ALA THR ILE VAL THR PRO PRO SER THR ARG THR GLU LEU LEU ASN LEU SER LEU GLY SER ASN GLU PHE ILE TRP THR LEU SER ASN GLY ALA CYS ARG ASP TYR SER SER ASP THR ILE VAL ILE THR MET ASP SER ALA PRO ILE ALA ASN ALA ASP SER PHE VAL

VAL ILE TYR ASN SER ASN GLY ASN THR ILE ASP VAL THR PRO ASN ASP GLY LEU ASN ASN ASN TRP VAL ILE THR ILE SER GLU SER ILE ALA SER GLY THR LEU ASP ASN LEU GLY THR GLY GLU PHE ASP LEU PHE LEU GLN ASP VAL LEU VAL ASP GLN ARG PHE ILE TYR GLN LEU

CYS ASN PRO ASN CYS PRO ALA ILE TYR CYS ASP THR ALA LEU VAL THR ILE ASP VAL GLN GLY GLY THR GLU CYS ASN PHE PRO ASN MET ILE THR PRO ASN ASN ASP ALA ASN GLU THR PHE ILE VAL PRO CYS LEU ASP GLY LEU GLU GLY THR LYS PHE ALA VAL TYR ASN ARG

TRP GLY ASP LEU MET TYR GLU ASN ASP ASN TYR LYS ASN ASP TRP GLY GLY THR HIS ASN GLY VAL PRO VAL PRO ASP ALA THR TYR PHE TYR ILE MET GLU LEU ALA ASP GLY GLN ARG PHE GLN GLY PHE VAL GLU VAL ARG ARG

• Molecule 1: The grappling hook protein A (GhpA) in the bacterium Aureispira sp. CCB-QB1

Chain F: 5% 94%

MET GLN ILE GLN ARG HIS SER PHE LYS TRP ILE LEU TYR GLY PHE LEU CYS TRP MET THR SER PHE VAL GLN ALA GLN THR PRO THR LEU THR ASN ALA THR PRO ALA GLU GLY PHE ILE GLY GLU GLN VAL CYS PHE PRO VAL THR PHE VAL ASN THR GLY ALA PRO GLY TYR GLY PRO

TYR VAL ARG LEU ILE VAL PRO THR GLY PHE THR PHE ASP ASN ALA SER PHE GLY GLY SER ILE GLN THR VAL GLN ASN LEU GLY VAL ILE VAL SER GLY ALA PRO ASN ASN PHE VAL ILE ASP PRO ILE ALA GLN SER ASN ASN ASN SER THR THR SER ASP THR ILE PHE ALA PRO VAL

GLY SER THR VAL ILE LEU LEU GLU TYR PRO VAL GLY SER MET VAL GLN GLY GLY VAL SER LEU ILE SER GLU VAL CYS MET THR VAL ASP PRO ALA ALA THR ILE GLY VAL PRO VAL ASP ILE CYS THR GLN GLY VAL TYR GLU PHE GLY ASP THR PRO THR GLY ASP ASN GLY PRO ILE

ALA GLY ALA ASN GLU CYS GLU PRO ILE ILE PRO ILE LEU PHE ARG PHE ASP LYS LYS VAL ASN GLY SER ASP GLY VAL TYR ASN GLU VAL PRO GLY GLY GLY ALA SER LEU CYS HIS ILE HIS GLN TYR GLU LEU ASN ILE ASP ILE ALA ALA ALA GLY THR LEU ASN GLY PRO ILE THR

ILE THR ASP VAL LEU PRO GLY GLU LEU ALA TYR PHE GLY ASN ILE SER LEU PRO ALA GLY CYS SER ALA VAL GLU PRO THR VAL GLY GLY LEU GLY GLY THR LEU THR VAL THR CYS ASN GLY SER TYR PRO GLY SER THR ALA ASN ILE ASP MET GLN VAL THR PHE ASP ALA ALA VAL

SER ASP THR LEU ASP GLU THR ILE CYS ASP ASP THR ASP ILE ASN ASN GLY ALA THR VAL ASN VAL PRO GLY ASN PRO SER GLN SER ASP THR VAL VAL THR HIS VAL GLU HIS VAL LEU LEU GLY HIS THR ASN ASN THR VAL SER PRO VAL THR ILE GLY GLN THR VAL LEU TYR THR

ILE GLY ALA GLU ILE THR GLU TYR THR ALA GLY LEU THR ALA ALA SER ILE THR PHE ILE VAL PRO ASP GLY MET ILE TYR ASN PRO ALA SER LEU THR TRP ALA GLY THR PRO VAL ALA ALA GLY ASN VAL VAL ILE VAL PRO GLY PRO GLY THR GLY SER THR VAL THR VAL ASP VAL

HIS THR GLN ASN GLY ALA ASN ILE LEU PRO CYS ALA SER PRO SER LEU GLN TYR THR ALA ASP VAL ASN GLN THR TYR ALA ASN GLY ASP PRO VAL LEU SER ARG ASP ARG LEU THR HIS SER SER THR LEU THR TYR ASP LEU VAL GLU GLY ALA THR GLY CYS THR THR SER ALA GLY

THR PRO ILE ASP VAL ILE ASP ILE PHE PHE GLN LYS THR VAL ASN ASN SER PRO PRO THR GLY PRO GLY ARG ASN GLY GLN TRP TRP PRO GLY ASP VAL VAL GLN TYR ARG LEU GLU LEU GLN ILE PRO SER LEU ASP LEU ASP ASP VAL VAL ILE THR ASP PHE PHE PRO LEU PRO ILE

HIS ASP VAL ALA SER LEU ALA ALA THR PHE GLY THR ASP VAL ARG PHE ASP PRO ALA THR CYS TRP ASN THR ALA PRO VAL THR TYR THR ARG ASP ILE PRO THR ASN SER LEU ILE LEU ASP PHE GLY ASP VAL SER ASP LEU VAL THR GLY GLY CYS VAL ASP ILE VAL LEU LEU ILE

ASP ILE PRO ILE THR THR LEU PRO PHE ALA ASP GLY LEU PHE HIS SER ASN PHE MET GLN VAL ASN SER ASP ASN SER THR ALA ASP ASN ILE THR ASN SER ALA LEU THR LEU ILE GLN VAL GLY ALA PRO ASP LEU GLU LEU THR LYS GLY ILE VAL SER SER ASP ASN PRO ASN VAL

THR ILE SER PRO THR VAL VAL PRO PRO ASP GLY ASN ALA THR ASP VAL SER ALA GLY ASP GLN LEU PHE PHE ASP ILE THR ILE GLU ASN VAL GLY GLY ALA PRO GLY TYR ASP VAL GLN VAL ARG ASP VAL ALA PRO PRO GLU LEU THR ASN CYS ALA LEU VAL ALA PRO ASN PRO VAL

VAL ASP GLY SER ASN ASN ALA LEU ALA PHE SER GLY GLY PHE VAL GLY ASN THR LEU THR ILE ASP LEU VAL ALA PRO ASN ASP SER ILE ALA PHE ALA THR ALA PRO ASN ASN ASN ASP LEU ILE THR VAL SER TYR VAL CYS GLU ALA VAL ALA GLY ILE GLN ALA GLY THR ARG PHE

ASP ASN THR ALA GLU VAL ASP TRP SER SER THR ARG GLY GLY VAL LYS PHE PRO PRO VAL GLU ASP ASP ALA ASN GLY ARG ILE ALA ASP PRO THR MET ASN LYS VAL VAL ASP TYR ILE PHE PRO ASN TYR SER ASN THR ASN THR GLN ALA SER ILE GLY GLU VAL VAL ALA TYR GLU

LEU GLN LEU ASN ILE PRO GLU GLY ASN MET ASN ASN VAL THR LEU VAL ASP GLN VAL ASP GLU GLY LEU ALA PHE VAL ALA VAL ASP SER ILE VAL ILE CYS ASN SER SER GLY SER THR ASN ILE ILE THR SER ILE GLY GLY GLY PHE PRO ALA VAL GLN SER GLY ALA THR ILE THR

ASN LEU GLY ALA ASN PRO GLN GLN GLN ASP ARG VAL LEU THR LEU ASP PHE GLY ASN LEU GLN ASN LEU ASP THR ASP ASN ILE GLU ASP THR ILE LYS VAL TYR TYR ARG THR ILE VAL ILE ASN HIS VAL THR ASN PHE ASP GLY GLU ARG VAL ARG ASN ARG ALA VAL LEU SER TRP

ASP ASN PRO ASN THR PRO GLY ASP ARG SER SER ILE ASN ASP ARG ALA PRO PHE VAL THR ILE VAL GLU PRO GLN LEU GLU ILE SER LYS SER PHE THR PRO ASP GLU VAL LEU PRO GLY ASN ASN SER PHE VAL THR LEU THR VAL ARG ASN PRO GLY THR SER SER ALA PRO ALA PHE

ASP VAL SER LEU THR ASP ILE LEU PRO THR GLY MET THR PHE VAL SER GLY PHE SER ALA GLY GLY THR ALA SER ILE THR THR PRO PRO THR ASN GLY GLY GLY THR ILE THR ALA HIS TRP ASP THR ILE ASN VAL GLY GLU VAL TYR SER ILE THR PHE GLU VAL GLN ALA SER SER

SER ILE THR PRO CYS PHE THR LEU THR ASN CYS ALA ASN LEU VAL TRP GLU SER ILE ALA GLU ALA ASP GLU PRO ASN MET PRO THR ALA PHE SER SER ASN LEU GLY VAL GLN ARG THR GLY ASN PRO GLY ASN LEU GLY GLY ALA ALA ASN THR TYR THR GLN ASP SER CYS ALA ASP

LEU ASP VAL VAL ILE ASP ASN THR PHE ASP PRO PHE ILE THR ALA ASN THR PRO LEU CYS GLU GLY ASP ARG VAL VAL LEU THR VAL GLN GLN TYR GLN GLY ASN VAL VAL ARG TYR ASN TRP THR GLY PRO GLY VAL PRO ALA GLY PHE ASN ASN TYR GLU LEU VAL LEU ASP PRO VAL

THR THR ALA ASP THR GLY THR TYR PHE VAL TYR VAL GLU LEU ASP GLY CYS ILE THR ASP THR SER ASN PHE PHE SER LEU GLN LEU ARG PRO LYS PRO VAL THR PRO ASN ILE ASN PRO GLY ASP THR THR ILE CYS GLU GLY THR SER ILE GLN PHE SER THR SER THR ILE ALA ASN

ASP TYR THR TRP THR GLY PRO ASN GLY PHE THR ALA ASN SER ALA THR THR PRO LEU ILE SER PRO VAL THR LEU ALA ASP ALA GLY ARG TYR THR LEU PHE THR THR ASN ALA GLN GLY CYS ASN SER ASP PRO ILE SER SER ASN LEU THR VAL THR PRO ARG PRO ALA GLN PRO SER

ILE ALA SER ASN THR PRO ILE CYS SER ASN GLU ASN ILE ILE LEU THR SER SER THR SER ALA ILE THR TYR GLN TRP MET ALA PRO ASN GLY GLN ASP THR ILE THR ASN ASN THR LEU THR LEU GLU PRO ASN ASN PRO LEU TYR THR ALA GLY ASN TRP THR LEU VAL VAL PHE

ASP ALA ASN GLY CYS ALA SER GLN PRO SER THR ALA ALA ASN VAL ILE ILE ASN GLY THR PRO ILE ALA PRO MET THR SER ASN SER GLY PRO ILE CYS GLU GLY GLU ASP VAL THR LEU MET VAL ASN THR VAL SER SER GLY THR TYR ALA TRP TYR SER ASP ALA ASN LEU THR ASN

LEU VAL ALA SER THR GLN ASN PRO VAL ILE SER GLY LEU LEU ALA SER ASN SER PRO ASP THR PHE TYR VAL GLN VAL SER SER ASN GLY CYS LEU SER ASP THR GLY PHE THR VAL VAL GLN VAL ASN PRO ASN PRO ALA ALA VAL SER PRO GLY TYR THR PRO LEU CYS SER GLY ASP

THR ILE PHE LEU PHE ALA ASN ALA THR ALA ASN ILE TYR ASN TRP THR GLY PRO ASN GLY PHE VAL SER ASN LEU GLU ASN PRO PHE ILE ALA ASN SER ALA ALA LEU ASN ALA GLY SER TYR THR VAL SER ILE THR ASP ALA ASN GLY CYS SER ASN SER GLY ILE VAL GLN VAL ALA

VAL ASP GLU ARG PRO VAL THR PRO THR ILE THR GLY ASN GLY PRO VAL CYS GLU GLY ASP ASN ILE GLN LEU ASN ILE GLY SER TYR THR GLY THR THR VAL GLN TYR THR TRP SER THR PRO THR GLY VAL VAL THR THR GLY VAL PRO SER LEU ASN ILE ASN ASN THR THR VAL ALA

ASP SER GLY LEU TYR SER VAL VAL VAL ALA VAL ASP GLY CYS THR SER LEU ALA ASP SER ILE ASN ILE VAL VAL ARG PRO ASN PRO ILE ALA PRO ASN VAL PRO SER ASN PHE SER VAL CYS GLU GLY ASP GLY ILE ALA LEU THR THR THR THR ASN ALA ASN ILE TYR ASN TRP THR

GLY PRO ASN GLY PHE SER SER ASN SER PRO ASN PRO THR VAL ILE SER PRO ALA SER SER ALA ASN ALA GLY THR TYR THR LEU VAL VAL GLN ASP PHE ASN GLY CYS THR SER PRO ALA ALA SER THR VAL VAL THR VAL ASN ALA ALA PRO ALA GLN PRO SER MET THR THR ASN SER

PRO ILE CYS ASN GLY ALA ASP LEU VAL MET SER THR SER ALA ALA GLY ASN SER TYR ILE TRP ARG ALA PRO ASN GLY ALA ASP THR THR THR ALA SER SER THR LEU THR ILE VAL PRO THR SER SER LEU TYR GLN SER GLY ASN TRP THR LEU SER VAL VAL ASN ALA ALA GLY CYS

VAL SER PRO ALA SER ILE ALA SER ALA VAL GLU ILE ASN SER ILE PRO SER THR ALA SER ALA GLY ASN ASN GLY PRO VAL CYS THR GLY THR ASP ALA SER LEU SER ALA GLY THR VAL SER GLY ALA SER TYR ALA TRP TYR THR ASP ALA GLY THR SER ASN GLN PHE SER THR LEU

GLN ASN PRO THR VAL ASN ASN LEU THR ASN ASP SER THR PHE TYR LEU LEU VAL THR VAL ASN GLY CYS PRO SER ALA LEU ASP SER THR THR VAL VAL VAL TYR PRO LEU THR PRO SER PRO SER LEU PRO ALA ASN PHE ALA VAL CYS GLU GLY ASP ASP ILE ALA LEU SER THR SER

THR VAL ALA SER SER TYR ASP TRP SER GLY PRO ASN GLY PHE THR SER ASN ALA GLN ASN PRO VAL VAL ILE THR ASN ALA THR GLY SER ASN ALA GLY VAL TYR THR LEU SER ILE VAL ASP GLY ASN GLY CYS SER SER ALA ASP THR SER VAL GLN VAL THR VAL ASN ALA ALA PRO

THR GLN PRO SER MET THR THR ASN SER PRO ILE CYS ASN GLY ALA ASP LEU VAL MET SER THR SER ALA VAL GLY ASN SER TYR ILE TRP ARG ALA PRO ASN GLY ALA ASP THR THR THR ALA SER SER THR LEU THR ILE VAL PRO THR SER SER LEU TYR GLN SER GLY ASN TRP THR

LEU SER VAL VAL ASN ALA ALA GLY CYS VAL SER PRO ALA SER ILE ALA SER ALA VAL GLU ILE ASN SER ILE PRO SER THR ALA SER ALA GLY ASN ASN GLY PRO VAL CYS THR GLY THR ASP ALA SER LEU SER ALA GLY THR VAL SER GLY ALA SER TYR ALA TRP TYR THR ASP ALA

GLY THR SER ASN GLN PHE SER THR LEU GLN ASN PRO THR VAL ASN ASN LEU THR ASN ASP SER THR PHE TYR LEU LEU VAL THR VAL ASN GLY CYS PRO SER ALA LEU ASP SER THR THR VAL VAL VAL TYR PRO LEU THR PRO SER PRO SER LEU PRO ALA ASP PHE ALA VAL CYS GLU

GLY ASP ASP ILE ALA LEU SER THR SER THR VAL ALA SER SER TYR ASP TRP SER GLY PRO ASN GLY PHE THR SER ASN ALA GLN ASN PRO VAL VAL ILE THR ASN ALA THR GLY SER ASN ALA GLY VAL TYR THR LEU SER ILE VAL ASP GLY ASN GLY CYS SER SER ALA ASP THR SER

VAL GLN VAL THR VAL ASN ALA ALA PRO ALA GLN PRO SER MET THR THR ASN SER PRO ILE CYS ASN GLY ALA ASP LEU VAL MET SER THR SER ALA THR GLY ASN SER TYR ILE TRP ARG ALA PRO ASN GLY ALA ASP THR THR THR ALA SER SER THR LEU THR ILE VAL PRO THR SER

SER LEU TYR GLN SER GLY ASN TRP THR LEU SER VAL VAL ASN ALA ALA GLY CYS VAL SER PRO ALA SER ILE ALA SER ALA VAL GLU ILE ASN SER ILE PRO SER THR ALA SER ALA GLY ASN ASN GLY PRO VAL CYS THR GLY THR ASP ALA SER LEU SER ALA GLY THR VAL SER GLY

ALA SER TYR ALA TRP TYR THR ASP ALA GLY THR SER ASN GLN PHE SER THR LEU GLN ASN PRO THR VAL ASN ASN LEU THR ASN ASP SER THR PHE TYR LEU LEU VAL THR VAL ASN GLY CYS PRO SER ALA LEU ASP SER THR THR VAL VAL VAL TYR PRO LEU THR PRO SER PRO SER

LEU PRO ALA ASP PHE ALA VAL CYS GLU GLY ASP ASP ILE ALA LEU SER THR SER THR VAL ALA SER SER TYR ASP TRP SER GLY PRO ASN GLY PHE THR SER ASN ALA GLN ASN PRO VAL VAL ILE THR ASN ALA THR GLY SER ASN ALA GLY VAL TYR THR LEU SER ILE VAL ASP GLY

ASN GLY CYS SER SER ALA ASP THR SER VAL GLN VAL THR VAL ASN ALA ALA PRO THR GLN PRO SER MET THR THR ASN SER PRO ILE CYS ASN GLY ALA ASP LEU VAL MET SER THR SER ALA VAL GLY ASN SER TYR ILE TRP ARG ALA PRO ASN GLY ALA ASP THR THR ALA SER

SER THR LEU THR ILE ALA PRO THR SER SER LEU TYR GLN SER GLY ASN TRP THR LEU SER VAL VAL ASN ALA ALA GLY CYS VAL SER PRO ALA SER VAL ALA SER MET VAL THR ILE ASN ASN GLY THR ASN PRO THR ALA PHE ASN ASN GLY PRO VAL CYS ARG GLY ASP ALA VAL GLN

LEU ASN THR THR THR ILE ASN ASN ALA LEU TYR GLU TRP TYR SER ASP ALA ALA LEU THR ASN LEU ILE SER THR GLN GLN ASN PRO THR VAL ALA ASN ILE THR THR ASP SER THR PHE TYR LEU VAL VAL THR VAL ASN GLY CYS PRO SER SER ALA VAL ALA THR THR VAL THR LEU

HIS PRO THR PRO ALA THR PRO ASN ILE PRO ALA ASN PHE VAL VAL CYS GLU GLY GLU THR ILE ALA LEU SER THR SER THR VAL ALA SER SER TYR ASN TRP THR GLY PRO ASN GLY PHE THR SER ASN LEU GLN ASN PRO ALA VAL ILE GLN PRO ALA THR THR ALA ASP ALA GLY SER

TYR THR LEU PHE ILE VAL ASP ALA ASN GLY CYS GLN SER ALA ASP THR SER VAL VAL VAL GLY VAL ASN ARG GLY PRO ALA ALA PRO VAL LEU THR ASN ASN SER ALA ILE CYS ASP GLY ASP THR LEU LEU LEU SER THR THR ALA SER ALA ASP THR PHE ARG TRP ILE SER PRO ASN

GLY ILE ASP THR ILE THR THR VAL ASN SER LEU MET ILE VAL PRO THR ASN GLY THR TYR TYR GLN SER GLY ASP TRP THR LEU ILE THR GLN VAL ALA ASN ASN CYS PRO SER GLU PRO SER ALA PRO SER SER VAL VAL ILE ASN SER SER THR ALA ALA PRO THR ALA PHE ASN ASP

GLY PRO VAL CYS VAL GLY GLY ASP VAL THR LEU SER THR PRO SER ALA PRO GLY ALA PHE TYR GLN TRP TYR THR ASP ALA ALA LEU THR ASN LEU VAL ALA THR ALA SER PHE THR ALA ILE ASN ILE THR GLN ASP SER THR PHE TYR LEU VAL VAL THR VAL ASN GLY CYS THR

SER PRO ALA GLY SER THR VAL ASN VAL ILE GLY GLN PRO SER ALA PRO ASN VAL PRO ALA ASP PHE GLU VAL CYS GLU GLY ASP ASP ILE ILE LEU GLY THR THR THR ILE ALA ALA SER TYR SER TRP THR GLY PRO ASN GLY PHE THR SER ASN LEU GLN ASN PRO ALA ALA ILE

S3484
S3495
A3496
I3497
C3498
F3499
E3515
W3516
R3523
T3526
G3527
T3528
N3529
N3551
C3555
V3565
V3566
P3581
Y3650
T3655
N3661
F3662
G3667
D3668
N3669
I3670
G3685
N3695
N3701
N3732
G3733
P3402
T3406
P3407
N3412
F3413
Y3432
G3436
N3443
G3468
N3469
G3470
V3480

PRO ALA ASP PHE ALA VAL CYS GLU GLY ASP ASN ILE VAL LEU SER THR THR THR VAL ALA ALA GLY TYR ASN TRP THR GLY PRO ASN GLY PHE THR SER ASN LEU GLN ASN PRO SER VAL VAL SER ALA SER LEU VAL ASP SER GLY THR TYR THR LEU PHE ILE ILE ASP ALA ASN GLY

CYS PRO SER GLY ASP THR SER VAL GLN VAL SER VAL HIS PRO ASN PRO VAL GLN PRO VAL LEU SER SER ASN SER ALA ILE CYS ASP GLY ASP SER LEU VAL LEU SER THR THR ALA THR ALA THR THR TYR ARG TRP VAL ALA PRO ASP GLY ALA ASP THR LEU THR THR VAL ASN THR

LEU VAL ILE LEU PRO SER ASN ALA PHE TYR GLN ASP GLY ASN TRP THR LEU MET THR MET ASP ALA ASN GLY CYS GLN SER ILE LEU SER ASN PRO GLU SER VAL THR ILE HIS SER ILE PRO ALA ALA GLN ALA VAL PHE ASN ASN GLY PRO VAL CYS ARG GLY SER SER VAL ASN LEU

SER THR SER PHE ILE SER GLY ALA THR TYR GLU TRP TYR ALA ASP ALA ALA LEU THR ILE LEU VAL ALA THR SER GLN ASN PRO THR ILE ASN ASN ILE THR THR ASP SER THR PHE TYR LEU VAL ILE THR VAL ASN GLY CYS THR SER ALA ALA GLY ALA THR THR VAL VAL HIS

PRO THR PRO THR THR PRO ASN VAL PRO SER ASN ILE THR VAL CYS GLU GLY ASP ALA ILE VAL LEU THR THR THR THR ASN ALA SER ALA TYR VAL TRP SER GLY PRO ASN GLY PHE SER SER ASN GLN GLN SER PRO THR VAL ILE ASN ALA ALA THR VAL VAL ASP SER GLY LYS TYR

SER LEU TYR VAL ILE ASP ALA ASN GLY CYS ARG SER GLU ASP THR SER LEU GLN VAL VAL VAL ASN PRO THR PRO THR THR PRO LEU ILE VAL SER ASN ASN THR PRO ILE CYS GLU GLY SER ASN ILE VAL LEU SER ALA ASN ALA GLY ALA ALA GLY THR THR TYR GLU TRP PHE ASN

ALA SER ASN VAL SER VAL GLY THR GLY GLN THR LEU THR ILE VAL GLY ALA THR VAL ALA ASP ALA GLY ASP TYR TYR VAL ILE THR THR LEU ASN SER CYS SER SER ALA ALA SER SER THR THR ALA ILE VAL ASP GLN VAL PRO SER THR ALA ALA PHE ALA GLY ASN ASP ILE

ASN LEU CYS ASN SER PHE THR THR THR LEU ASP ALA THR PRO PRO ASN SER ALA THR GLY PHE TRP THR THR ASN SER GLY ALA THR ILE ALA ASN PRO ASN LEU ALA ASN SER ALA VAL TYR ASN LEU PRO THR GLY THR SER THR PHE TYR TRP THR LEU SER ASN GLY ALA CYS ILE

ASP PHE SER VAL ASP SER MET VAL VAL GLU VAL THR PRO ALA SER THR ASP VAL ALA ASP ALA GLY LEU ASP GLN ASN LEU CYS GLY GLN THR SER ALA THR LEU THR ALA ALA ASN PRO SER THR ALA THR GLY GLN TRP THR GLN SER ALA SER GLN ALA GLY GLN GLY ILE VAL ILE

THR ASN PRO THR ASN PRO ASN THR THR VAL THR GLY LEU GLN GLN GLY ASN ASN TYR THR PHE THR TRP THR LEU SER ASN GLY ASN CYS THR ASP TYR SER THR ASP MET VAL GLN ILE ASN VAL ASP VAL SER PRO PRO ASP ASN ALA TYR ALA GLY VAL ASP ILE LEU LEU CYS ASN

GLN ASN THR ALA ASN LEU ASP ALA PHE VAL SER GLN TYR GLY THR GLY MET TRP THR SER THR SER SER ALA THR ILE ILE ASP PRO THR LEU ALA ASN THR THR VAL ILE ASN LEU PRO GLN ASP THR SER VAL PHE VAL TRP THR LEU SER ASN GLY THR CYS GLN ASN TYR SER THR

ASP SER VAL LEU VAL VAL VAL SER THR THR THR ASP THR ALA GLU ALA GLY ASN ASN GLN VAL VAL CYS SER VAL ASN ALA LEU THR LEU GLY ALA THR MET PRO SER SER GLY PHE GLY THR TRP SER GLN THR ALA ALA GLN ALA ALA GLN GLY VAL VAL ILE VAL ASP VAL ASN ASP

PRO ASN THR GLN VAL VAL GLY LEU ASN ALA GLY THR THR TYR ALA PHE THR TRP THR LEU SER ASN GLY THR CYS GLN ASP TYR SER SER ASP VAL THR THR ILE SER VAL ASN ALA THR PRO PRO ASP ASN ALA PHE ALA GLY ASN ASP ILE ASN LEU CYS GLY VAL ALA THR THR THR

ASN LEU ALA ALA SER VAL PRO THR VAL ALA MET GLY LEU TRP THR THR THR SER SER ALA THR ILE SER ASN PRO THR GLN PRO ASN SER THR VAL SER GLY LEU SER ALA GLY GLN ASN ILE PHE ILE TRP THR LEU SER ASN GLY THR CYS GLN ASP TYR ASP SER ASP THR VAL ILE

VAL THR VAL THR THR PRO SER SER ASP VAL ALA ASP ALA GLY LEU ASP SER ALA TYR CYS ALA GLN SER VAL VAL THR LEU ASN ALA VAL ALA PRO SER VAL GLY GLY GLY TYR TRP SER GLN THR PRO SER GLN ALA SER LEU GLY ALA VAL ILE ASP ASN PRO THR ASP THR ALA THR

THR VAL SER ASN LEU MET PRO GLY VAL THR TYR THR PHE THR TRP THR LEU THR ASN GLY GLY CYS VAL ASP TYR SER SER ASP GLN VAL LEU ILE THR ILE ASP VAL LEU PRO THR ASN VAL ALA TYR ALA GLY GLU ASP THR ILE LEU CYS GLY GLY ASN ALA VAL GLN LEU ASP GLY

LEU ALA PRO PRO ILE GLY THR GLY PHE TRP THR THR ASN ASP THR ALA THR ILE VAL THR PRO VAL ASP PRO ASN SER LEU VAL VAL ASN ILE ALA GLU ASP THR THR THR TYR TYR TRP THR LEU SER ASN GLY ALA CYS VAL ASP TYR SER VAL ASP SER VAL THR VAL ILE ILE SER

PRO ALA SER THR ASP LEU ALA PHE ALA GLY TYR ASP GLU VAL LEU CYS GLY VAL ASP SER ILE MET LEU SER ALA ALA VAL PRO THR THR SER THR GLY ILE TRP THR GLN SER ALA GLY GLN ALA SER GLN GLY ILE VAL ILE THR ASN PRO THR ASN PRO ASN SER SER VAL THR GLY

ILE GLN ALA GLY GLN VAL TYR THR PHE THR TRP THR LEU SER THR PHE GLY CYS ALA ASN PHE SER THR ASP ASP VAL GLN TYR THR ILE ASN ALA LEU PRO PRO GLU VAL ALA TYR ALA GLY PRO ASP ILE VAL LEU CYS THR GLY ASN SER VAL THR MET ASP ALA ASN ASN PRO ILE

PHE SER THR GLY VAL TRP SER SER ASN SER SER ALA VAL ILE VAL ASN PRO THR LEU SER ASN SER ASN ILE VAL ASN ILE PRO THR ASP THR VAL ALA PHE TYR TRP SER LEU SER ASN GLY SER CYS ALA ASP TYR SER ILE ASP THR MET LEU ILE ILE VAL THR PRO THR PHE SER

VAL ASP THR ALA ASN ALA GLY LEU ASP ILE ASN LEU CYS ASN GLU ASP THR ALA GLN LEU MET ALA ILE ALA PRO ASN VAL ALA THR GLY ARG TRP THR GLN PRO PHE ASN GLN SER SER ALA GLY VAL VAL ILE THR ASP PRO ASN ALA ALA MET THR THR ALA THR GLY LEU GLN LEU

ASP SER THR TYR THR PHE THR TRP SER VAL SER ASN GLY PRO CYS ARG ASP TYR ASP ARG ASP GLN VAL ILE VAL GLN VAL SER THR LEU PRO THR ASP ALA ALA TYR ALA GLY GLU ASP PHE VAL ILE CYS GLY ILE ASP THR ALA ILE VAL SER ALA THR ALA PRO SER ILE GLY ALA

GLY MET TRP THR THR THR THR ALA THR ILE VAL THR PRO PRO SER THR ARG THR GLU LEU LEU ASN LEU SER LEU GLY SER ASN GLU PHE ILE TRP THR LEU SER ASN GLY ALA CYS ARG ASP TYR SER SER ASP THR ILE VAL ILE THR MET ASP SER ALA PRO ILE ALA ASN ALA

ASP SER PHE VAL VAL ILE TYR ASN SER ASN GLY ASN THR ILE ASP VAL THR PRO ASN ASP GLY LEU ASN ASN ASN TRP VAL ILE THR ILE SER GLU SER ILE ALA SER GLY THR LEU ASP ASN LEU GLY THR GLY GLU PHE ASP LEU PHE LEU GLN ASP VAL LEU VAL ASP GLN ARG PHE

ILE TYR GLN LEU CYS ASN PRO ASN CYS PRO ALA ILE TYR CYS ASP THR ALA LEU VAL THR ILE ASP VAL GLN GLY GLY THR GLU CYS ASN PHE PRO ASN MET ILE THR PRO ASN ASN ASP ASP ALA ASN GLU THR PHE ILE VAL PRO CYS LEU ASP GLY LEU GLU GLY THR LYS PHE ALA

VAL TYR ASN ARG TRP GLY ASP LEU MET TYR GLU ASN ASP ASN TYR LYS ASN ASP TRP GLY GLY THR HIS ASN GLY VAL PRO VAL PRO ASP ALA THR TYR PHE TYR ILE MET GLU LEU ALA ASP GLY GLN ARG PHE GLN GLY PHE VAL GLU VAL ARG ARG

• Molecule 1: The grappling hook protein A (GhpA) in the bacterium Aureispira sp. CCB-QB1

Chain G: 5% 94%

MET GLN ILE GLN ARG HIS SER PHE LYS TRP ILE LEU TYR GLY PHE LEU CYS TRP MET THR SER PHE VAL GLN ALA GLN THR PRO THR LEU THR ASN ALA THR PRO ALA GLU GLY PHE ILE GLY GLU GLN VAL CYS PHE PRO VAL THR PHE VAL ASN THR GLY ALA PRO GLY TYR GLY PRO

TYR VAL ARG LEU ILE VAL PRO THR GLY PHE THR PHE ASP ASN ALA SER PHE GLY GLY SER ILE GLN THR VAL GLN ASN LEU GLY VAL ILE VAL SER GLY ALA PRO ASN ASN PHE VAL ILE ASP PRO ILE ALA GLN SER ASN ASN SER THR THR SER ASP THR ILE PHE ALA PRO VAL

GLY SER THR VAL ILE LEU LEU GLU TYR PRO VAL GLY SER MET VAL GLN GLY GLY VAL SER LEU ILE SER GLU VAL CYS MET THR VAL ASP PRO ALA ALA THR ILE GLY VAL PRO VAL ASP ILE CYS THR GLN GLY VAL TYR GLU PHE GLY ASP THR PRO THR GLY ASP ASN GLY PRO ILE

ALA GLY ALA ASN GLU CYS GLU PRO ILE ILE PRO ILE LEU PHE ARG PHE ASP LYS LYS VAL ASN GLY SER ASP GLY VAL TYR ASN GLU VAL PRO GLY GLY GLY ALA SER LEU CYS HIS ILE HIS GLN TYR GLU LEU ASN ILE ASP ILE ALA ALA GLY THR LEU ASN GLY PRO ILE THR

ILE THR ASP VAL LEU PRO GLY GLU LEU ALA TYR PHE GLY ASN ILE SER LEU PRO ALA GLY CYS SER ALA VAL GLU PRO THR VAL GLY LEU GLY GLY THR LEU THR VAL THR CYS ASN GLY SER TYR PRO GLY SER THR ALA ASN ILE ASP MET GLN VAL THR PHE ASP ALA VAL

SER ASP THR LEU ASP GLU THR ILE CYS ASP THR ASP ILE ASN ASN GLY ALA THR VAL ASN VAL PRO GLY ASN PRO SER GLN SER ASP THR VAL VAL THR HIS VAL GLU HIS VAL LEU LEU GLY HIS THR ASN ASN THR VAL SER PRO VAL THR ILE GLY GLN THR VAL LEU TYR THR

ILE GLY ALA GLU ILE THR GLU TYR THR ALA GLY LEU THR ALA ALA SER ILE THR PHE ILE VAL PRO ASP GLY MET ILE TYR ASN PRO ALA SER LEU THR TRP ALA GLY THR PRO VAL ALA ALA GLY ASN VAL VAL ILE VAL PRO GLY PRO GLY THR GLY SER THR VAL THR VAL ASP VAL

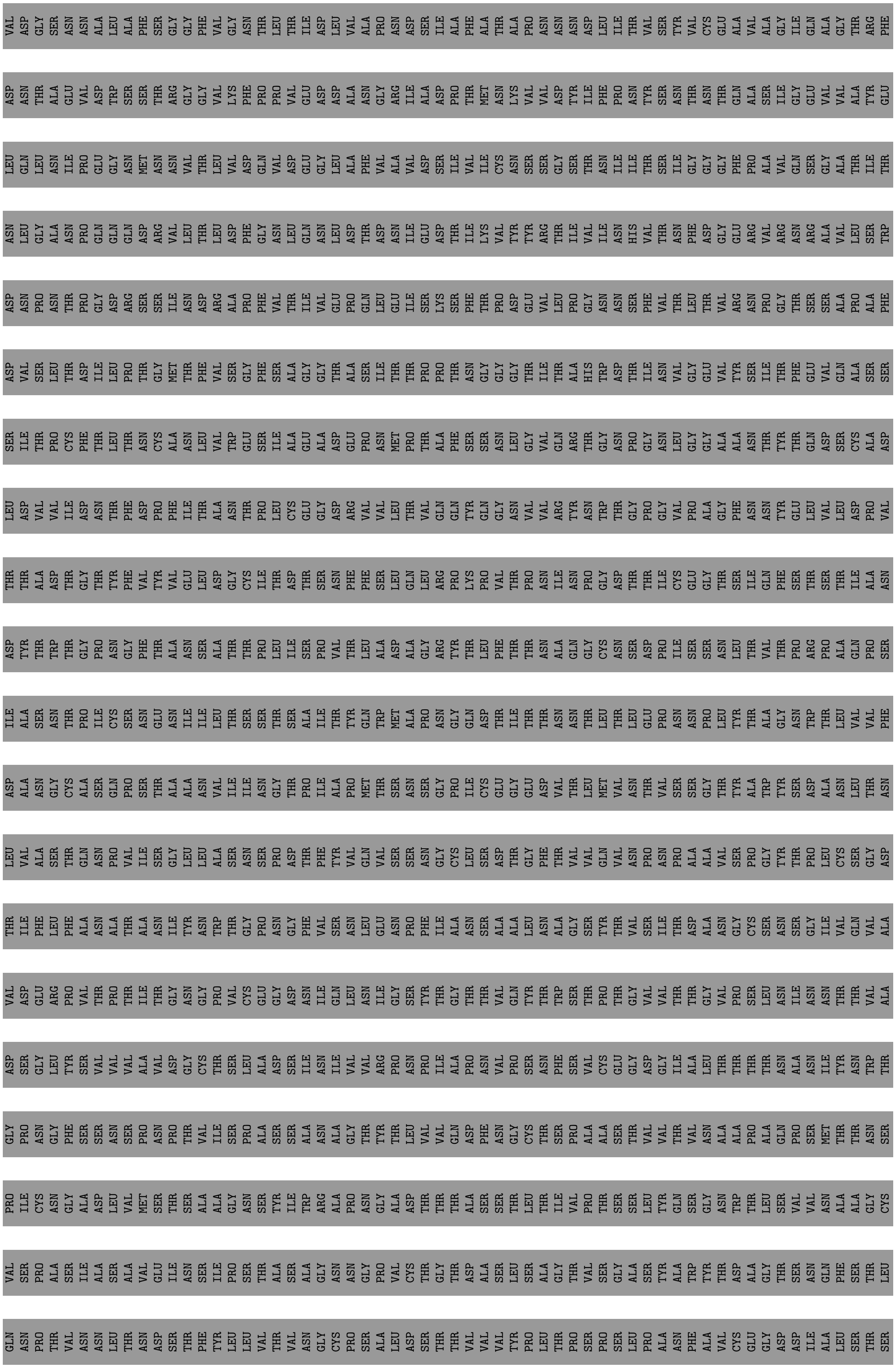
HIS THR GLN ASN GLY ALA ASN ILE LEU PRO CYS ALA SER PRO SER LEU GLN TYR THR ALA ASP VAL ASN GLN THR TYR ALA ASN GLY ASP PRO VAL LEU SER ARG ASP ARG LEU THR HIS SER SER THR LEU THR TYR ASP LEU VAL GLU GLY ALA THR GLY CYS THR THR SER ALA GLY

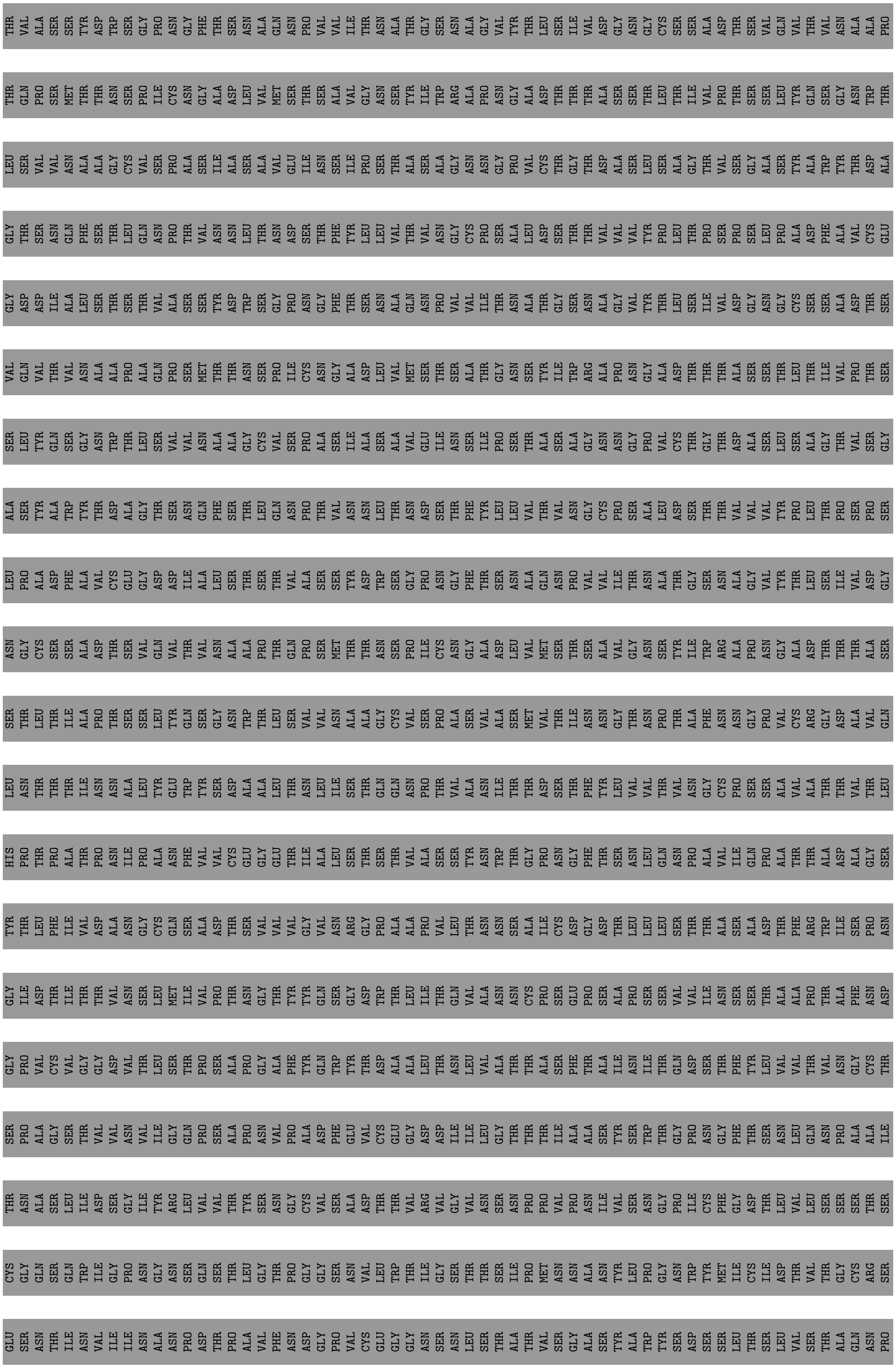
THR PRO ILE ASP VAL ILE ASP ILE PHE PHE GLN LYS THR VAL ASN ASN SER PRO PRO THR GLY PRO GLY ARG ASN GLY GLN TRP TRP PRO GLY ASP VAL VAL GLN TYR ARG LEU GLU LEU GLN ILE PRO SER LEU ASP LEU ASP ASP VAL VAL ILE THR ASP PHE PHE PRO LEU PRO ILE

HIS ASP VAL ALA SER LEU ALA ALA THR PHE GLY THR ASP VAL ARG PHE ASP PRO ALA THR CYS TRP ASN THR ALA PRO VAL THR TYR THR ARG ASP ILE PRO THR ASN SER LEU ILE LEU ASP PHE GLY ASP VAL SER ASP LEU VAL THR GLY GLY CYS VAL ASP ILE VAL LEU LEU ILE

ASP ILE PRO ILE THR THR LEU PRO PHE ALA ASP GLY LEU PHE HIS SER ASN PHE MET GLN VAL ASN SER ASP ASN SER THR ALA ASP ASN ILE THR ASN SER ALA LEU THR LEU ILE GLN VAL GLY ALA PRO ASP LEU GLU LEU THR LYS GLY ILE VAL SER SER ASP ASN PRO ASN VAL

THR ILE SER PRO THR VAL VAL PRO PRO ASP GLY ASN ALA THR ASP VAL SER ALA GLY ASP GLN LEU PHE PHE ASP ILE THR ILE GLU ASN VAL GLY GLY ALA PRO GLY TYR ASP VAL GLN VAL ARG ASP VAL ALA PRO PRO GLU LEU THR ASN CYS ALA LEU VAL ALA PRO ASN PRO VAL


VAL ASP GLY SER ASN ASN ALA LEU ALA PHE SER GLY GLY PHE VAL GLY ASN THR LEU THR ILE ASP LEU VAL ALA PRO ASN ASP SER ILE ALA PHE ALA THR ALA PRO ASN ASN ASN ASP LEU ILE THR VAL SER TYR VAL CYS GLU ALA VAL ALA GLY ILE GLN ALA GLY THR ARG PHE
ASP ASN THR ALA GLU VAL ASP TRP SER SER THR ARG GLY GLY VAL LYS PHE PRO PRO VAL GLU ASP ASP ALA ASN GLY ARG ILE ALA ASP PRO THR MET ASN LYS VAL VAL ASP TYR ILE PHE PRO ASN TYR SER ASN THR ASN THR GLN ALA SER ILE GLY GLU VAL VAL ALA TYR GLU
LEU GLN LEU ASN ILE PRO GLU GLY ASN MET ASN ASN VAL THR LEU VAL ASP GLN VAL ASP GLU GLY LEU ALA PHE VAL ALA VAL ASP SER ILE VAL ILE CYS ASN SER SER GLY SER THR ASN ILE ILE THR SER ILE GLY GLY GLY PHE PRO ALA VAL GLN SER GLY ALA THR ILE THR
ASN LEU GLY ALA ASN PRO GLN GLN GLN ASP ARG VAL LEU THR LEU ASP PHE GLY ASN LEU GLN ASN LEU ASP THR ASP ASN ILE GLU ASP THR ILE LYS VAL TYR TYR ARG THR ILE VAL ILE ASN HIS VAL THR ASN PHE ASP GLY GLU ARG VAL ARG ASN ARG ALA VAL LEU SER TRP
ASP ASN PRO ASN THR PRO GLY ASP ARG SER SER ILE ASN ASP ARG ALA PRO PHE VAL THR ILE VAL GLU PRO GLN LEU GLU ILE SER LYS SER PHE THR PRO ASP GLU VAL LEU PRO GLY ASN ASN SER PHE VAL THR LEU THR VAL ARG ASN PRO GLY THR SER SER ALA PRO ALA PHE
ASP VAL SER LEU THR ASP ILE LEU PRO THR GLY MET THR PHE VAL SER GLY PHE SER ALA GLY GLY THR ALA SER ILE THR THR PRO PRO THR ASN GLY GLY GLY THR ILE THR ALA HIS TRP ASP THR ILE ASN VAL GLY GLU VAL TYR SER ILE THR PHE GLU VAL GLN ALA SER SER
SER ILE THR PRO CYS PHE THR LEU THR ASN CYS ALA ASN LEU VAL TRP GLU SER ILE ALA GLU ALA ASP GLU PRO ASN MET PRO THR ALA PHE SER SER ASN LEU GLY VAL GLN ARG THR GLY ASN PRO GLY ASN LEU GLY GLY ALA ALA ASN THR TYR THR GLN ASP SER CYS ALA ASP
LEU ASP VAL VAL ILE ASP ASN THR PHE ASP PRO PHE ILE THR ALA ASN THR PRO LEU CYS GLU GLY ASP ARG VAL VAL LEU THR VAL GLN GLN TYR GLN GLY ASN VAL VAL ARG TYR ASN TRP THR GLY PRO GLY VAL PRO ALA GLY PHE ASN ASN TYR GLU LEU VAL LEU ASP PRO VAL
THR THR ALA ASP THR GLY THR TYR PHE VAL TYR VAL GLU LEU ASP GLY CYS ILE THR ASP THR SER ASN PHE PHE SER LEU GLN LEU ARG PRO LYS PRO VAL THR PRO ASN ILE ASN PRO GLY ASP THR THR ILE CYS GLU GLY THR SER ILE GLN PHE SER THR SER THR ILE ALA ASN
ASP TYR THR TRP THR GLY PRO ASN GLY PHE THR ALA ASN SER ALA THR THR PRO LEU ILE SER PRO VAL THR LEU ALA ASP ALA GLY ARG TYR THR LEU PHE THR THR ASN ALA GLN GLY CYS ASN SER ASP PRO ILE SER SER ASN LEU THR VAL THR PRO ARG PRO ALA GLN PRO SER
ILE ALA SER ASN THR PRO ILE CYS SER ASN GLU ASN ILE ILE LEU THR SER SER THR SER ALA ILE THR TYR GLN TRP MET ALA PRO ASN GLY GLN ASP THR ILE THR THR ASN ASN THR LEU THR LEU GLU PRO ASN ASN PRO LEU TYR THR ALA GLY ASN TRP THR LEU VAL VAL PHE
ASP ALA ASN GLY CYS ALA SER GLN PRO SER THR ALA ALA ASN VAL ILE ILE ASN GLY THR PRO ILE ALA PRO MET THR SER ASN SER GLY PRO ILE CYS GLU GLY GLU ASP VAL THR LEU MET VAL ASN THR VAL SER SER GLY THR TYR ALA TRP TYR SER ASP ALA ASN LEU THR ASN
LEU VAL ALA SER THR GLN ASN PRO VAL ILE SER GLY LEU LEU ALA SER ASN SER PRO ASP THR PHE TYR VAL GLN VAL SER SER ASN GLY CYS LEU SER ASP THR GLY PHE THR VAL VAL GLN VAL ASN PRO ASN PRO ALA ALA VAL SER PRO GLY TYR THR PRO LEU CYS SER GLY ASP
THR ILE PHE LEU PHE ALA ASN ALA THR ALA ASN ILE TYR ASN TRP THR GLY PRO ASN GLY PHE VAL SER ASN LEU GLU ASN PRO PHE ILE ALA ASN SER ALA ALA LEU ASN ALA GLY SER TYR THR VAL SER ILE THR ASP ALA ASN GLY CYS SER ASN SER GLY ILE VAL GLN VAL ALA
VAL ASP GLU ARG PRO VAL THR PRO THR ILE THR GLY ASN GLY PRO VAL CYS GLU GLY ASP ASN ILE GLN LEU ASN ILE GLY SER TYR THR GLY THR THR VAL GLN TYR THR TRP SER THR PRO THR GLY VAL VAL THR THR GLY VAL PRO SER LEU ASN ILE ASN ASN THR THR VAL ALA
ASP SER GLY LEU TYR SER VAL VAL VAL ALA VAL ASP GLY CYS THR SER LEU ALA ASP SER ILE ASN ILE VAL VAL ARG PRO ASN PRO ILE ALA PRO ASN VAL PRO SER ASN PHE SER VAL CYS GLU GLY ASP GLY ILE ALA LEU THR THR THR THR ASN ALA ASN ILE TYR ASN TRP THR
GLY PRO ASN GLY PHE SER SER ASN SER PRO ASN PRO THR VAL ILE SER PRO ALA SER SER ALA ASN ALA GLY THR TYR THR LEU VAL VAL GLN ASP PHE ASN GLY CYS THR SER PRO ALA ALA SER THR VAL VAL THR VAL ASN ALA ALA PRO ALA GLN PRO SER MET THR THR ASN SER
PRO ILE CYS ASN GLY ALA ASP LEU VAL MET SER THR SER ALA ALA GLY ASN SER TYR ILE TRP ARG ALA PRO ASN GLY ALA ASP THR THR THR ALA SER SER THR LEU THR ILE VAL PRO THR SER SER LEU TYR GLN SER GLY ASN TRP THR LEU SER VAL VAL ASN ALA ALA GLY CYS
VAL SER PRO ALA SER ILE ALA SER ALA VAL GLU ILE ASN SER ILE PRO SER THR ALA SER ALA GLY ASN ASN GLY PRO VAL CYS THR GLY THR ASP ALA SER LEU SER ALA GLY THR VAL SER GLY ALA SER TYR ALA TRP TYR THR ASP ALA GLY THR SER ASN GLN PHE SER THR LEU
GLN ASN PRO THR VAL ASN ASN LEU THR ASN ASP SER THR PHE TYR LEU LEU VAL THR VAL ASN GLY CYS PRO SER ALA LEU ASP SER THR THR VAL VAL TYR PRO LEU THR PRO SER PRO SER LEU PRO ALA ASN PHE ALA VAL CYS GLU GLY ASP ASP ILE ALA LEU SER THR SER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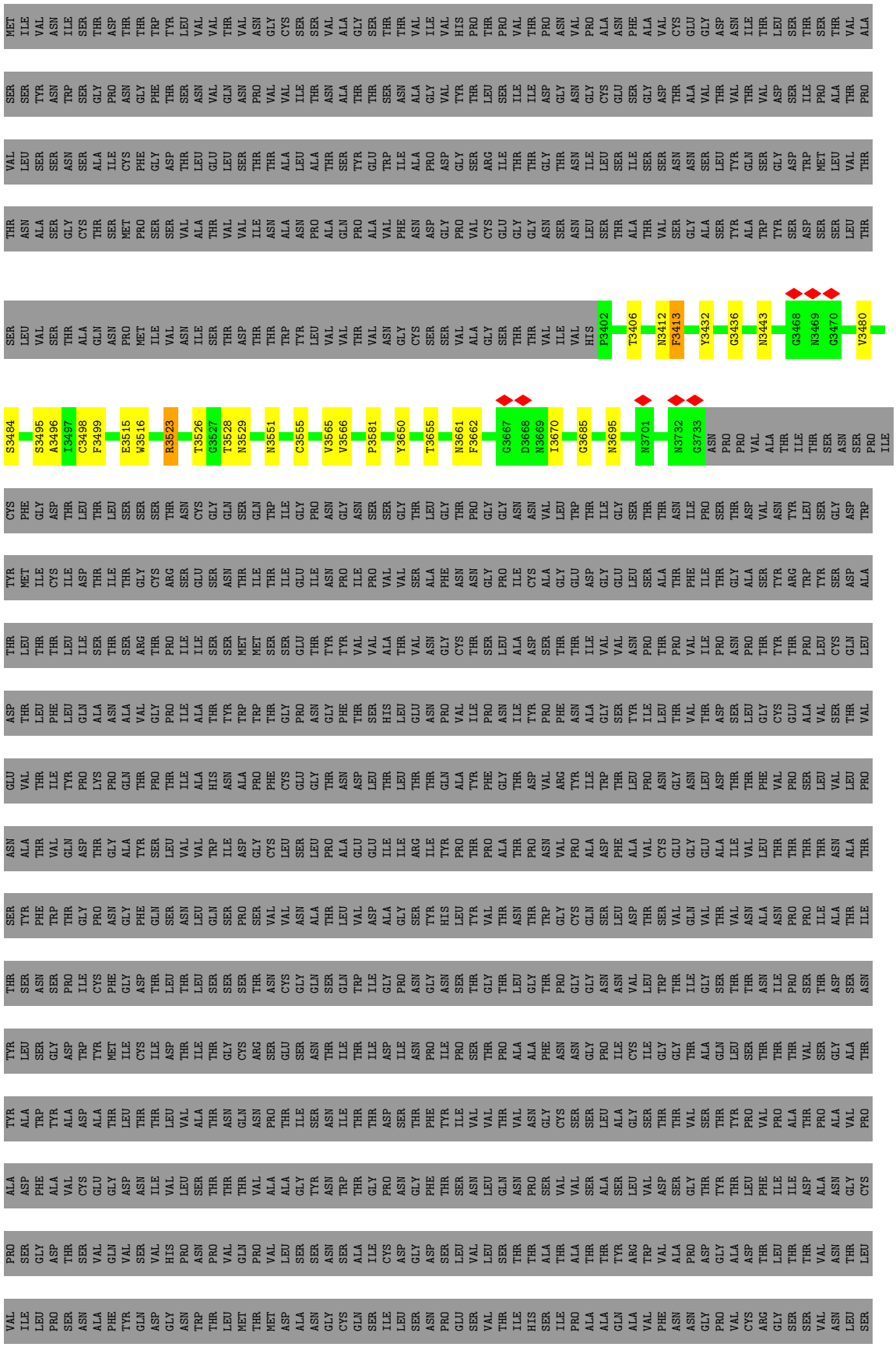
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4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	113824	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	8.025	Depositor
Minimum map value	-5.229	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.159	Depositor
Recommended contour level	1	Depositor
Map size (Å)	319.50003, 319.50003, 319.50003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.90	0/2407	1.11	15/3332 (0.5%)
1	B	0.90	0/2407	1.11	15/3332 (0.5%)
1	C	0.90	0/2407	1.11	15/3332 (0.5%)
1	D	0.90	0/2407	1.11	15/3332 (0.5%)
1	E	0.90	0/2407	1.11	15/3332 (0.5%)
1	F	0.90	0/2407	1.11	15/3332 (0.5%)
1	G	0.90	0/2407	1.11	15/3332 (0.5%)
All	All	0.90	0/16849	1.11	105/23324 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
All	All	0	7

There are no bond length outliers.

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	3413	PHE	CA-CB-CG	9.06	122.86	113.80
1	D	3413	PHE	CA-CB-CG	9.04	122.84	113.80
1	F	3413	PHE	CA-CB-CG	9.04	122.84	113.80
1	C	3413	PHE	CA-CB-CG	9.04	122.84	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3413	PHE	CA-CB-CG	9.03	122.83	113.80
1	B	3413	PHE	CA-CB-CG	9.03	122.83	113.80
1	G	3413	PHE	CA-CB-CG	9.02	122.81	113.80
1	G	3412	ASN	CA-C-N	-8.63	110.77	122.16
1	G	3412	ASN	C-N-CA	-8.63	110.77	122.16
1	A	3412	ASN	CA-C-N	-8.60	110.81	122.16
1	A	3412	ASN	C-N-CA	-8.60	110.81	122.16
1	B	3412	ASN	CA-C-N	-8.60	110.81	122.16
1	B	3412	ASN	C-N-CA	-8.60	110.81	122.16
1	E	3412	ASN	CA-C-N	-8.59	110.82	122.16
1	E	3412	ASN	C-N-CA	-8.59	110.82	122.16
1	F	3412	ASN	CA-C-N	-8.59	110.82	122.16
1	F	3412	ASN	C-N-CA	-8.59	110.82	122.16
1	C	3412	ASN	CA-C-N	-8.59	110.83	122.16
1	C	3412	ASN	C-N-CA	-8.59	110.83	122.16
1	D	3412	ASN	CA-C-N	-8.58	110.83	122.16
1	D	3412	ASN	C-N-CA	-8.58	110.83	122.16
1	F	3695	ASN	CA-C-N	6.76	127.15	119.92
1	F	3695	ASN	C-N-CA	6.76	127.15	119.92
1	B	3695	ASN	CA-C-N	6.76	127.15	119.92
1	B	3695	ASN	C-N-CA	6.76	127.15	119.92
1	G	3695	ASN	CA-C-N	6.74	127.14	119.92
1	G	3695	ASN	C-N-CA	6.74	127.14	119.92
1	C	3695	ASN	CA-C-N	6.74	127.13	119.92
1	C	3695	ASN	C-N-CA	6.74	127.13	119.92
1	D	3695	ASN	CA-C-N	6.72	127.12	119.92
1	D	3695	ASN	C-N-CA	6.72	127.12	119.92
1	A	3695	ASN	CA-C-N	6.72	127.11	119.92
1	A	3695	ASN	C-N-CA	6.72	127.11	119.92
1	E	3695	ASN	CA-C-N	6.71	127.10	119.92
1	E	3695	ASN	C-N-CA	6.71	127.10	119.92
1	G	3661	ASN	CA-C-N	-5.58	110.88	121.54
1	G	3661	ASN	C-N-CA	-5.58	110.88	121.54
1	A	3661	ASN	CA-C-N	-5.58	110.88	121.54
1	A	3661	ASN	C-N-CA	-5.58	110.88	121.54
1	B	3661	ASN	CA-C-N	-5.58	110.89	121.54
1	B	3661	ASN	C-N-CA	-5.58	110.89	121.54
1	E	3661	ASN	CA-C-N	-5.58	110.89	121.54
1	E	3661	ASN	C-N-CA	-5.58	110.89	121.54
1	C	3661	ASN	CA-C-N	-5.57	110.90	121.54
1	C	3661	ASN	C-N-CA	-5.57	110.90	121.54
1	D	3661	ASN	CA-C-N	-5.56	110.92	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	3661	ASN	C-N-CA	-5.56	110.92	121.54
1	F	3661	ASN	CA-C-N	-5.55	110.93	121.54
1	F	3661	ASN	C-N-CA	-5.55	110.93	121.54
1	G	3436	GLY	CA-C-N	5.51	125.46	119.78
1	G	3436	GLY	C-N-CA	5.51	125.46	119.78
1	C	3436	GLY	CA-C-N	5.51	125.45	119.78
1	C	3436	GLY	C-N-CA	5.51	125.45	119.78
1	D	3436	GLY	CA-C-N	5.49	125.43	119.78
1	D	3436	GLY	C-N-CA	5.49	125.43	119.78
1	B	3436	GLY	CA-C-N	5.48	125.43	119.78
1	B	3436	GLY	C-N-CA	5.48	125.43	119.78
1	A	3436	GLY	CA-C-N	5.47	125.41	119.78
1	A	3436	GLY	C-N-CA	5.47	125.41	119.78
1	E	3436	GLY	CA-C-N	5.47	125.41	119.78
1	E	3436	GLY	C-N-CA	5.47	125.41	119.78
1	F	3436	GLY	CA-C-N	5.45	125.39	119.78
1	F	3436	GLY	C-N-CA	5.45	125.39	119.78
1	F	3655	THR	CA-C-N	5.42	125.36	119.78
1	F	3655	THR	C-N-CA	5.42	125.36	119.78
1	C	3655	THR	CA-C-N	5.41	125.35	119.78
1	C	3655	THR	C-N-CA	5.41	125.35	119.78
1	A	3655	THR	CA-C-N	5.38	125.32	119.78
1	A	3655	THR	C-N-CA	5.38	125.32	119.78
1	B	3655	THR	CA-C-N	5.37	125.31	119.78
1	B	3655	THR	C-N-CA	5.37	125.31	119.78
1	E	3655	THR	CA-C-N	5.36	125.30	119.78
1	E	3655	THR	C-N-CA	5.36	125.30	119.78
1	D	3655	THR	CA-C-N	5.35	125.29	119.78
1	D	3655	THR	C-N-CA	5.35	125.29	119.78
1	G	3406	THR	CA-C-N	5.33	125.28	119.78
1	G	3406	THR	C-N-CA	5.33	125.28	119.78
1	D	3406	THR	CA-C-N	5.33	125.27	119.78
1	D	3406	THR	C-N-CA	5.33	125.27	119.78
1	G	3655	THR	CA-C-N	5.33	125.27	119.78
1	G	3655	THR	C-N-CA	5.33	125.27	119.78
1	F	3406	THR	CA-C-N	5.32	125.26	119.78
1	F	3406	THR	C-N-CA	5.32	125.26	119.78
1	A	3406	THR	CA-C-N	5.32	125.26	119.78
1	A	3406	THR	C-N-CA	5.32	125.26	119.78
1	E	3406	THR	CA-C-N	5.30	125.24	119.78
1	E	3406	THR	C-N-CA	5.30	125.24	119.78
1	C	3406	THR	CA-C-N	5.29	125.23	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	3406	THR	C-N-CA	5.29	125.23	119.78
1	B	3406	THR	CA-C-N	5.29	125.23	119.78
1	B	3406	THR	C-N-CA	5.29	125.23	119.78
1	C	3685	GLY	CA-C-N	5.27	125.21	119.78
1	C	3685	GLY	C-N-CA	5.27	125.21	119.78
1	B	3685	GLY	CA-C-N	5.25	125.18	119.78
1	B	3685	GLY	C-N-CA	5.25	125.18	119.78
1	A	3685	GLY	CA-C-N	5.24	125.17	119.78
1	A	3685	GLY	C-N-CA	5.24	125.17	119.78
1	F	3685	GLY	CA-C-N	5.23	125.17	119.78
1	F	3685	GLY	C-N-CA	5.23	125.17	119.78
1	E	3685	GLY	CA-C-N	5.22	125.16	119.78
1	E	3685	GLY	C-N-CA	5.22	125.16	119.78
1	G	3685	GLY	CA-C-N	5.22	125.16	119.78
1	G	3685	GLY	C-N-CA	5.22	125.16	119.78
1	D	3685	GLY	CA-C-N	5.20	125.13	119.78
1	D	3685	GLY	C-N-CA	5.20	125.13	119.78

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3523	ARG	Sidechain
1	B	3523	ARG	Sidechain
1	C	3523	ARG	Sidechain
1	D	3523	ARG	Sidechain
1	E	3523	ARG	Sidechain
1	F	3523	ARG	Sidechain
1	G	3523	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2360	0	2237	16	0
1	B	2360	0	2237	16	0
1	C	2360	0	2237	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2360	0	2237	17	0
1	E	2360	0	2237	17	0
1	F	2360	0	2237	18	0
1	G	2360	0	2237	17	0
All	All	16520	0	15659	118	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (118) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3515:GLU:OE2	1:G:3523:ARG:HD3	1.25	1.32
1:F:3515:GLU:OE2	1:F:3523:ARG:HD3	1.25	1.32
1:C:3515:GLU:OE2	1:C:3523:ARG:HD3	1.25	1.28
1:B:3515:GLU:OE2	1:B:3523:ARG:HD3	1.25	1.27
1:D:3515:GLU:OE2	1:D:3523:ARG:HD3	1.25	1.26
1:A:3515:GLU:OE2	1:A:3523:ARG:HD3	1.25	1.25
1:E:3515:GLU:OE2	1:E:3523:ARG:HD3	1.25	1.25
1:D:3515:GLU:OE2	1:D:3523:ARG:CD	2.21	0.78
1:B:3515:GLU:OE2	1:B:3523:ARG:CD	2.21	0.77
1:C:3581:PRO:HB2	1:C:3650:TYR:CE2	2.21	0.76
1:G:3581:PRO:HB2	1:G:3650:TYR:CE2	2.21	0.76
1:D:3581:PRO:HB2	1:D:3650:TYR:CE2	2.21	0.75
1:A:3581:PRO:HB2	1:A:3650:TYR:CE2	2.21	0.75
1:E:3581:PRO:HB2	1:E:3650:TYR:CE2	2.21	0.75
1:B:3581:PRO:HB2	1:B:3650:TYR:CE2	2.21	0.75
1:F:3581:PRO:HB2	1:F:3650:TYR:CE2	2.21	0.75
1:E:3515:GLU:OE2	1:E:3523:ARG:CD	2.21	0.74
1:A:3515:GLU:OE2	1:A:3523:ARG:CD	2.21	0.73
1:C:3515:GLU:OE2	1:C:3523:ARG:CD	2.21	0.72
1:F:3515:GLU:OE2	1:F:3523:ARG:CD	2.21	0.71
1:G:3515:GLU:OE2	1:G:3523:ARG:CD	2.21	0.71
1:G:3516:TRP:HE1	1:G:3526:THR:CG2	2.08	0.67
1:C:3516:TRP:HE1	1:C:3526:THR:CG2	2.08	0.67
1:D:3516:TRP:HE1	1:D:3526:THR:CG2	2.08	0.67
1:E:3516:TRP:HE1	1:E:3526:THR:CG2	2.08	0.67
1:B:3516:TRP:HE1	1:B:3526:THR:CG2	2.08	0.66
1:A:3516:TRP:HE1	1:A:3526:THR:CG2	2.08	0.66
1:F:3516:TRP:HE1	1:F:3526:THR:CG2	2.08	0.65
1:B:3516:TRP:HE1	1:B:3526:THR:HG21	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3516:TRP:HE1	1:G:3526:THR:HG21	1.63	0.64
1:D:3516:TRP:HE1	1:D:3526:THR:HG21	1.63	0.64
1:A:3516:TRP:HE1	1:A:3526:THR:HG21	1.63	0.63
1:F:3516:TRP:HE1	1:F:3526:THR:HG21	1.63	0.63
1:C:3516:TRP:HE1	1:C:3526:THR:HG21	1.63	0.62
1:E:3516:TRP:HE1	1:E:3526:THR:HG21	1.63	0.62
1:F:3581:PRO:HB2	1:F:3650:TYR:CZ	2.37	0.60
1:E:3581:PRO:HB2	1:E:3650:TYR:CZ	2.37	0.59
1:A:3581:PRO:HB2	1:A:3650:TYR:CZ	2.37	0.59
1:D:3581:PRO:HB2	1:D:3650:TYR:CZ	2.37	0.59
1:G:3581:PRO:HB2	1:G:3650:TYR:CZ	2.37	0.59
1:C:3581:PRO:HB2	1:C:3650:TYR:CZ	2.37	0.59
1:B:3581:PRO:HB2	1:B:3650:TYR:CZ	2.37	0.58
1:E:3662:PHE:CZ	1:E:3670:ILE:HG23	2.41	0.55
1:F:3662:PHE:CZ	1:F:3670:ILE:HG23	2.41	0.55
1:F:3495:SER:HA	1:F:3565:VAL:HA	1.89	0.55
1:G:3495:SER:HA	1:G:3565:VAL:HA	1.89	0.55
1:A:3495:SER:HA	1:A:3565:VAL:HA	1.89	0.55
1:G:3662:PHE:CZ	1:G:3670:ILE:HG23	2.41	0.55
1:A:3662:PHE:CZ	1:A:3670:ILE:HG23	2.41	0.55
1:C:3662:PHE:CZ	1:C:3670:ILE:HG23	2.41	0.55
1:D:3662:PHE:CZ	1:D:3670:ILE:HG23	2.41	0.55
1:B:3662:PHE:CZ	1:B:3670:ILE:HG23	2.41	0.54
1:B:3495:SER:HA	1:B:3565:VAL:HA	1.89	0.54
1:E:3495:SER:HA	1:E:3565:VAL:HA	1.89	0.54
1:C:3495:SER:HA	1:C:3565:VAL:HA	1.89	0.53
1:D:3495:SER:HA	1:D:3565:VAL:HA	1.89	0.53
1:A:3662:PHE:HZ	1:A:3670:ILE:HG23	1.80	0.47
1:C:3484:SER:O	1:C:3555:CYS:SG	2.73	0.47
1:E:3484:SER:O	1:E:3555:CYS:SG	2.73	0.47
1:A:3551:ASN:OD1	1:A:3555:CYS:HB2	2.15	0.47
1:C:3551:ASN:OD1	1:C:3555:CYS:HB2	2.15	0.47
1:D:3484:SER:O	1:D:3555:CYS:SG	2.73	0.46
1:E:3551:ASN:OD1	1:E:3555:CYS:HB2	2.15	0.46
1:B:3484:SER:O	1:B:3555:CYS:SG	2.73	0.46
1:B:3551:ASN:OD1	1:B:3555:CYS:HB2	2.15	0.46
1:F:3551:ASN:OD1	1:F:3555:CYS:HB2	2.15	0.46
1:F:3516:TRP:HE1	1:F:3526:THR:HG22	1.80	0.46
1:D:3516:TRP:HE1	1:D:3526:THR:HG22	1.81	0.46
1:G:3484:SER:O	1:G:3555:CYS:SG	2.73	0.46
1:D:3551:ASN:OD1	1:D:3555:CYS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3484:SER:O	1:F:3555:CYS:SG	2.73	0.46
1:G:3551:ASN:OD1	1:G:3555:CYS:HB2	2.15	0.46
1:A:3484:SER:O	1:A:3555:CYS:SG	2.73	0.46
1:D:3662:PHE:HZ	1:D:3670:ILE:HG23	1.80	0.46
1:G:3516:TRP:HE1	1:G:3526:THR:HG22	1.80	0.46
1:B:3516:TRP:HE1	1:B:3526:THR:HG22	1.81	0.45
1:B:3528:THR:OG1	1:B:3529:ASN:N	2.49	0.45
1:C:3516:TRP:HE1	1:C:3526:THR:HG22	1.80	0.45
1:C:3528:THR:OG1	1:C:3529:ASN:N	2.50	0.45
1:E:3413:PHE:CE1	1:E:3480:VAL:HG22	2.52	0.45
1:D:3413:PHE:CE1	1:D:3480:VAL:HG22	2.52	0.45
1:E:3662:PHE:HZ	1:E:3670:ILE:HG23	1.80	0.45
1:B:3413:PHE:CE1	1:B:3480:VAL:HG22	2.52	0.45
1:E:3528:THR:OG1	1:E:3529:ASN:N	2.50	0.45
1:F:3413:PHE:CE1	1:F:3480:VAL:HG22	2.52	0.45
1:F:3662:PHE:HZ	1:F:3670:ILE:HG23	1.80	0.45
1:G:3662:PHE:HZ	1:G:3670:ILE:HG23	1.80	0.45
1:A:3498:CYS:O	1:A:3499:PHE:C	2.59	0.45
1:C:3413:PHE:CE1	1:C:3480:VAL:HG22	2.52	0.45
1:A:3413:PHE:CE1	1:A:3480:VAL:HG22	2.52	0.45
1:C:3662:PHE:HZ	1:C:3670:ILE:HG23	1.80	0.45
1:B:3662:PHE:HZ	1:B:3670:ILE:HG23	1.80	0.44
1:D:3528:THR:OG1	1:D:3529:ASN:N	2.50	0.44
1:F:3528:THR:OG1	1:F:3529:ASN:N	2.49	0.44
1:G:3413:PHE:CE1	1:G:3480:VAL:HG22	2.52	0.44
1:F:3498:CYS:O	1:F:3499:PHE:C	2.59	0.44
1:A:3516:TRP:HE1	1:A:3526:THR:HG22	1.80	0.44
1:E:3498:CYS:O	1:E:3499:PHE:C	2.59	0.44
1:B:3498:CYS:O	1:B:3499:PHE:C	2.59	0.44
1:G:3498:CYS:O	1:G:3499:PHE:C	2.59	0.44
1:D:3498:CYS:O	1:D:3499:PHE:C	2.59	0.44
1:D:3579:ASP:N	1:D:3579:ASP:OD1	2.48	0.43
1:E:3516:TRP:HE1	1:E:3526:THR:HG22	1.80	0.43
1:G:3528:THR:OG1	1:G:3529:ASN:N	2.50	0.43
1:A:3528:THR:OG1	1:A:3529:ASN:N	2.50	0.42
1:C:3498:CYS:O	1:C:3499:PHE:C	2.59	0.42
1:B:3496:ALA:HA	1:B:3566:VAL:HB	2.02	0.42
1:F:3496:ALA:HA	1:F:3566:VAL:HB	2.02	0.41
1:C:3496:ALA:HA	1:C:3566:VAL:HB	2.02	0.41
1:A:3496:ALA:HA	1:A:3566:VAL:HB	2.02	0.41
1:E:3496:ALA:HA	1:E:3566:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3432:TYR:O	1:D:3443:ASN:HA	2.21	0.41
1:F:3406:THR:HA	1:F:3407:PRO:HD3	1.96	0.41
1:F:3432:TYR:O	1:F:3443:ASN:HA	2.21	0.41
1:G:3496:ALA:HA	1:G:3566:VAL:HB	2.02	0.41
1:E:3655:THR:HA	1:E:3656:PRO:HD3	1.93	0.41
1:C:3432:TYR:O	1:C:3443:ASN:HA	2.21	0.40
1:G:3432:TYR:O	1:G:3443:ASN:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	330/5898 (6%)	326 (99%)	4 (1%)	0	100	100
1	B	330/5898 (6%)	326 (99%)	4 (1%)	0	100	100
1	C	330/5898 (6%)	326 (99%)	4 (1%)	0	100	100
1	D	330/5898 (6%)	326 (99%)	4 (1%)	0	100	100
1	E	330/5898 (6%)	326 (99%)	4 (1%)	0	100	100
1	F	330/5898 (6%)	326 (99%)	4 (1%)	0	100	100
1	G	330/5898 (6%)	326 (99%)	4 (1%)	0	100	100
All	All	2310/41286 (6%)	2282 (99%)	28 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/4919 (6%)	278 (100%)	0	100	100
1	B	278/4919 (6%)	278 (100%)	0	100	100
1	C	278/4919 (6%)	278 (100%)	0	100	100
1	D	278/4919 (6%)	278 (100%)	0	100	100
1	E	278/4919 (6%)	278 (100%)	0	100	100
1	F	278/4919 (6%)	278 (100%)	0	100	100
1	G	278/4919 (6%)	278 (100%)	0	100	100
All	All	1946/34433 (6%)	1946 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3433	ASN
1	A	3695	ASN
1	B	3433	ASN
1	B	3695	ASN
1	C	3433	ASN
1	C	3695	ASN
1	D	3433	ASN
1	D	3695	ASN
1	E	3433	ASN
1	E	3695	ASN
1	F	3433	ASN
1	F	3695	ASN
1	G	3433	ASN
1	G	3695	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

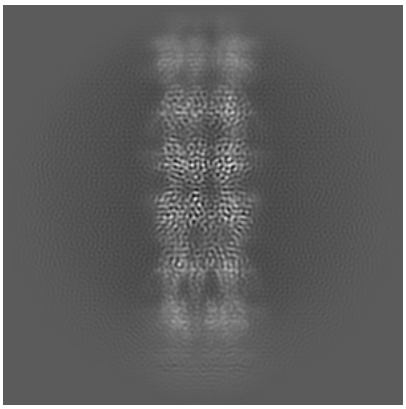
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-50539. These allow visual inspection of the internal detail of the map and identification of artifacts.

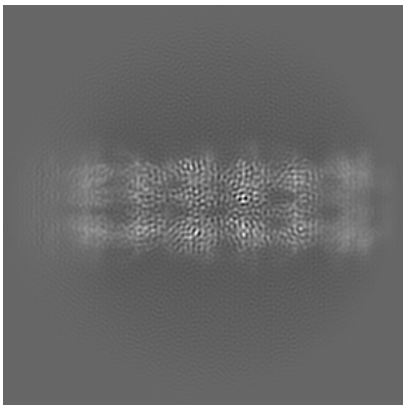
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

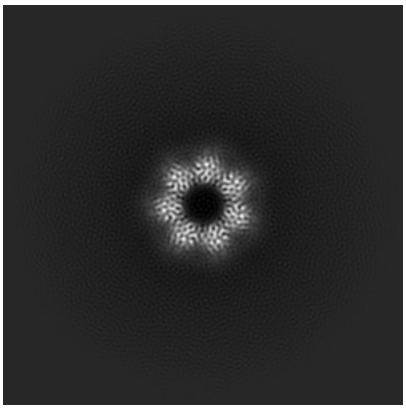
6.1.1 Primary map



X

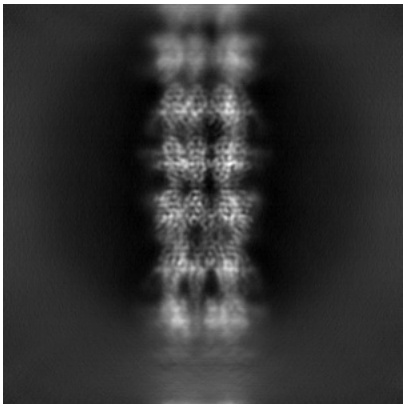


Y

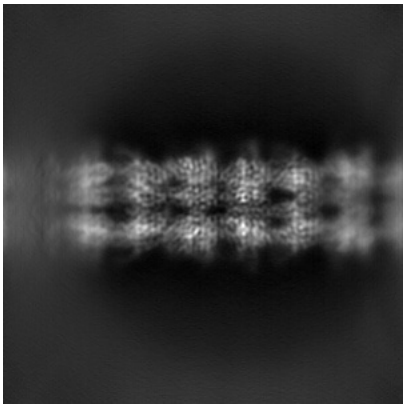


Z

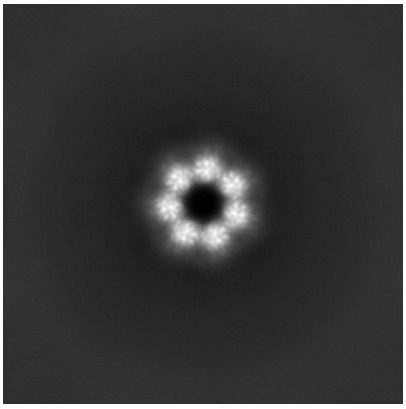
6.1.2 Raw map



X



Y

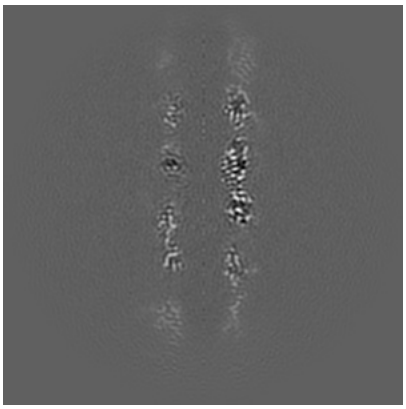


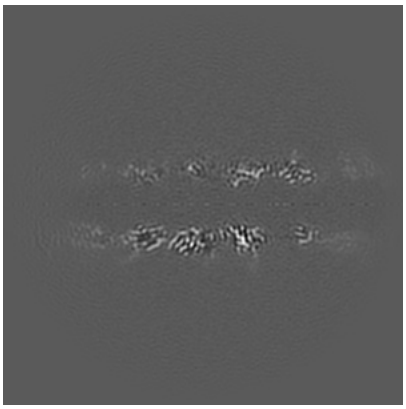
Z

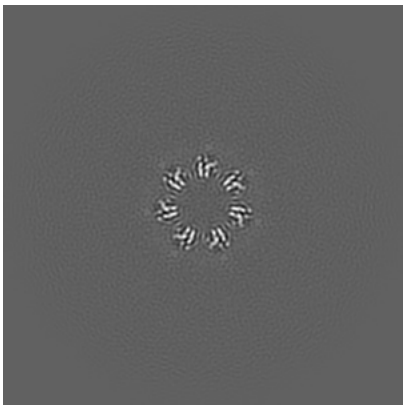
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

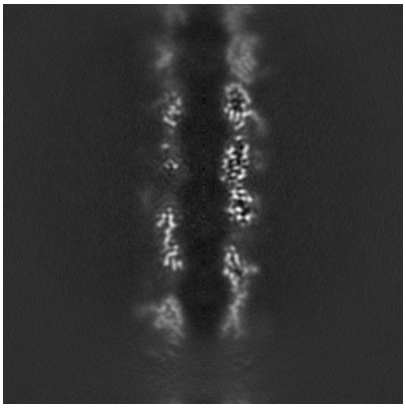
6.2.1 Primary map

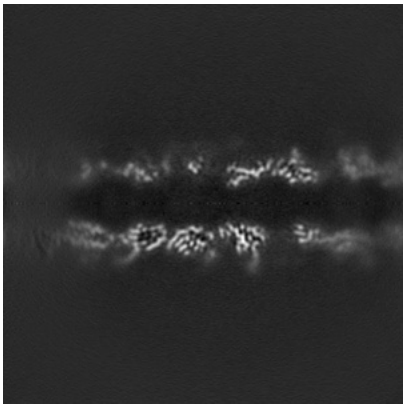

X Index: 150

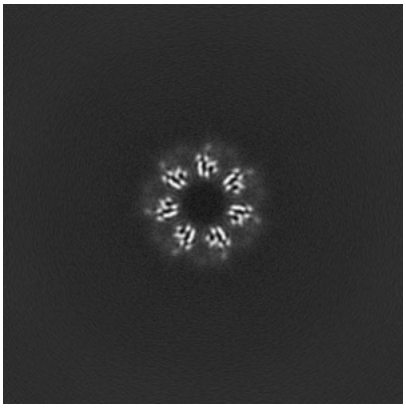

Y Index: 150


Z Index: 150

6.2.2 Raw map


X Index: 150

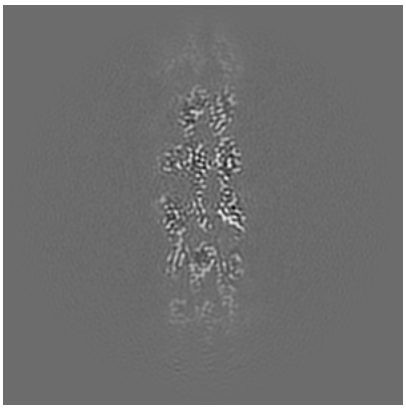

Y Index: 150

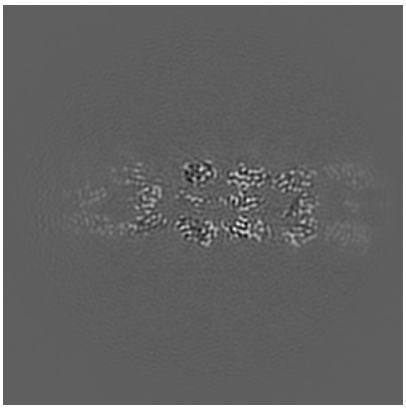

Z Index: 150

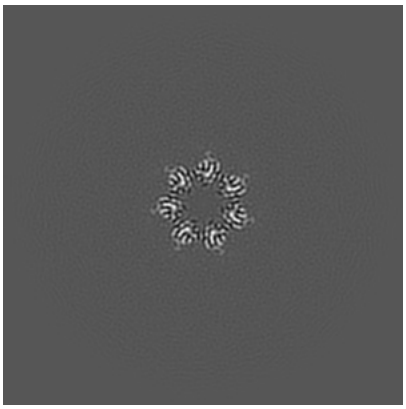
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

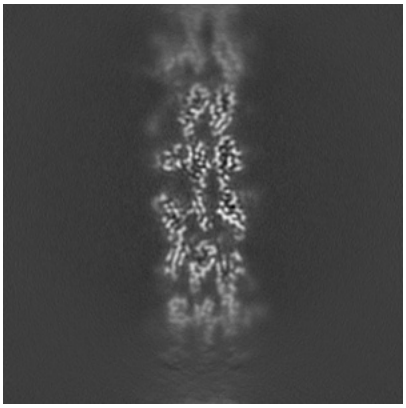
6.3.1 Primary map

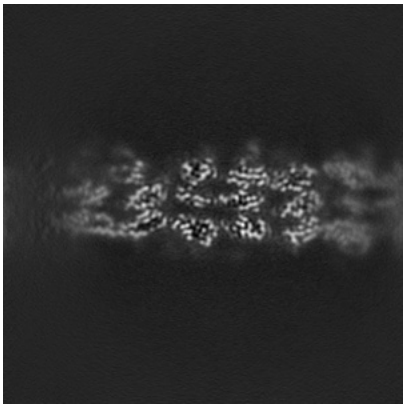

X Index: 129

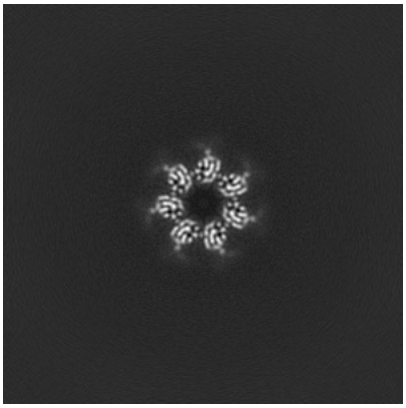

Y Index: 169


Z Index: 180

6.3.2 Raw map


X Index: 129

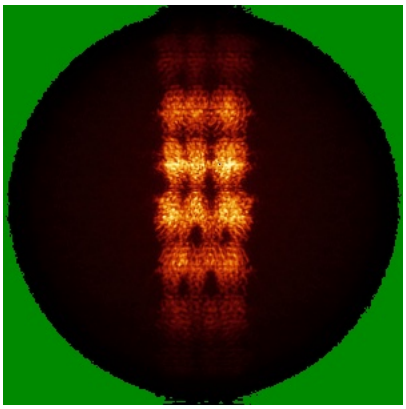

Y Index: 170

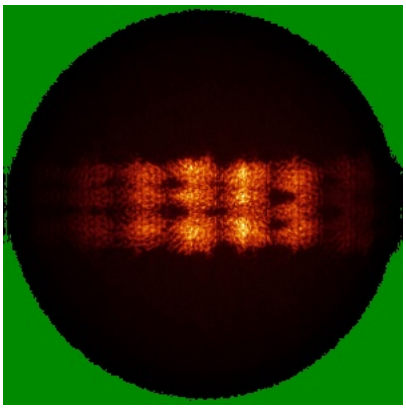

Z Index: 180

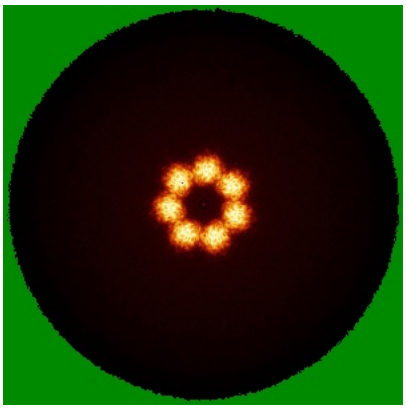
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

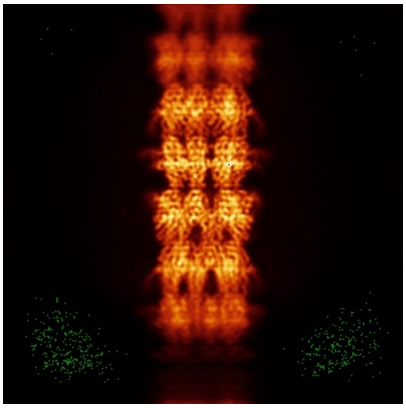
6.4.1 Primary map

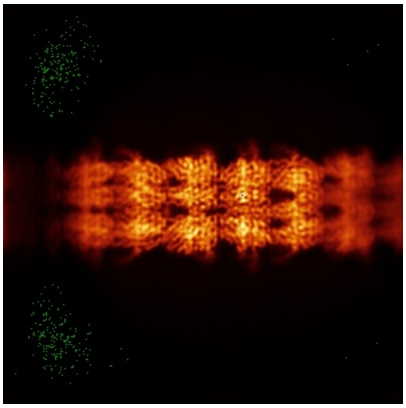

X

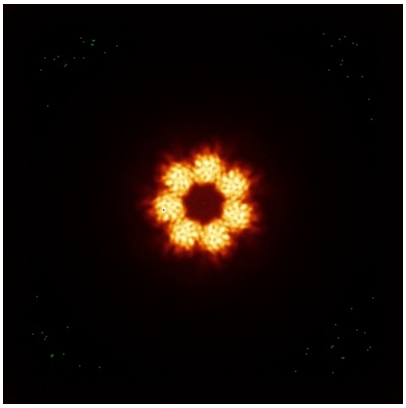

Y


Z

6.4.2 Raw map


X

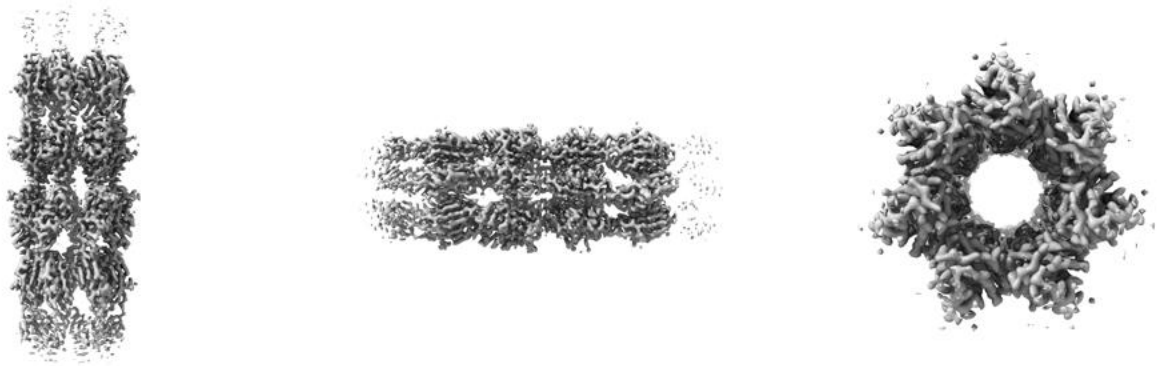

Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

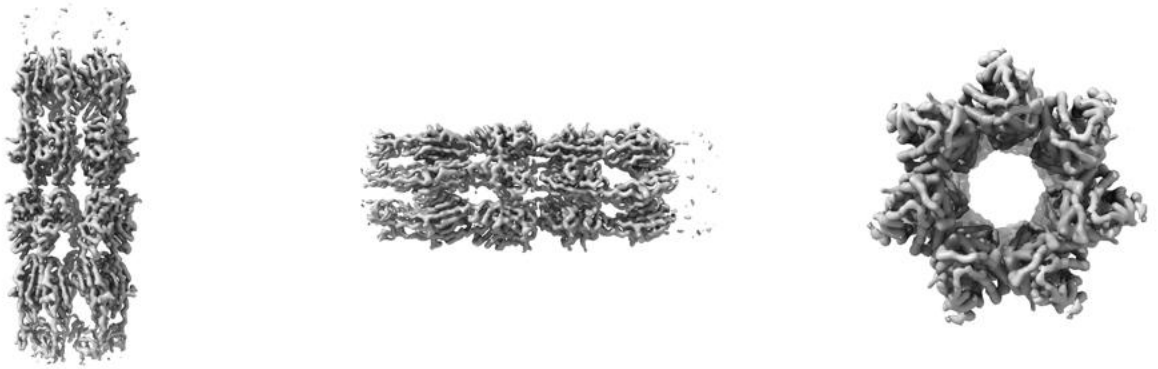
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

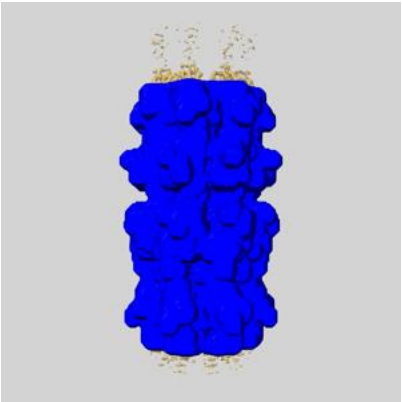
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

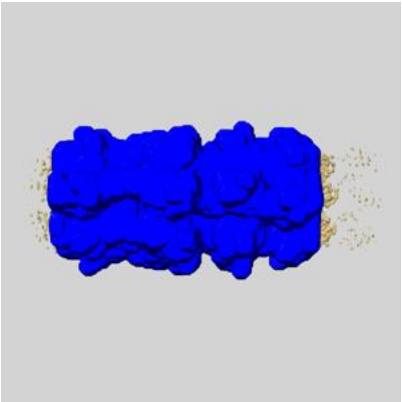
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

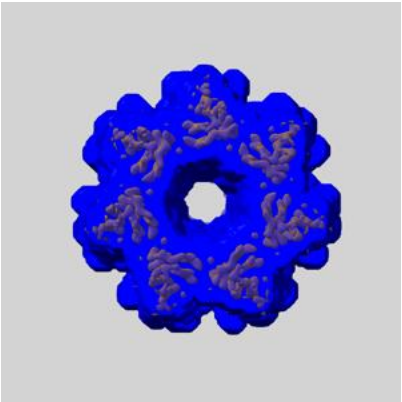
6.6.1 emd_50539_msk_1.map (i)



X



Y

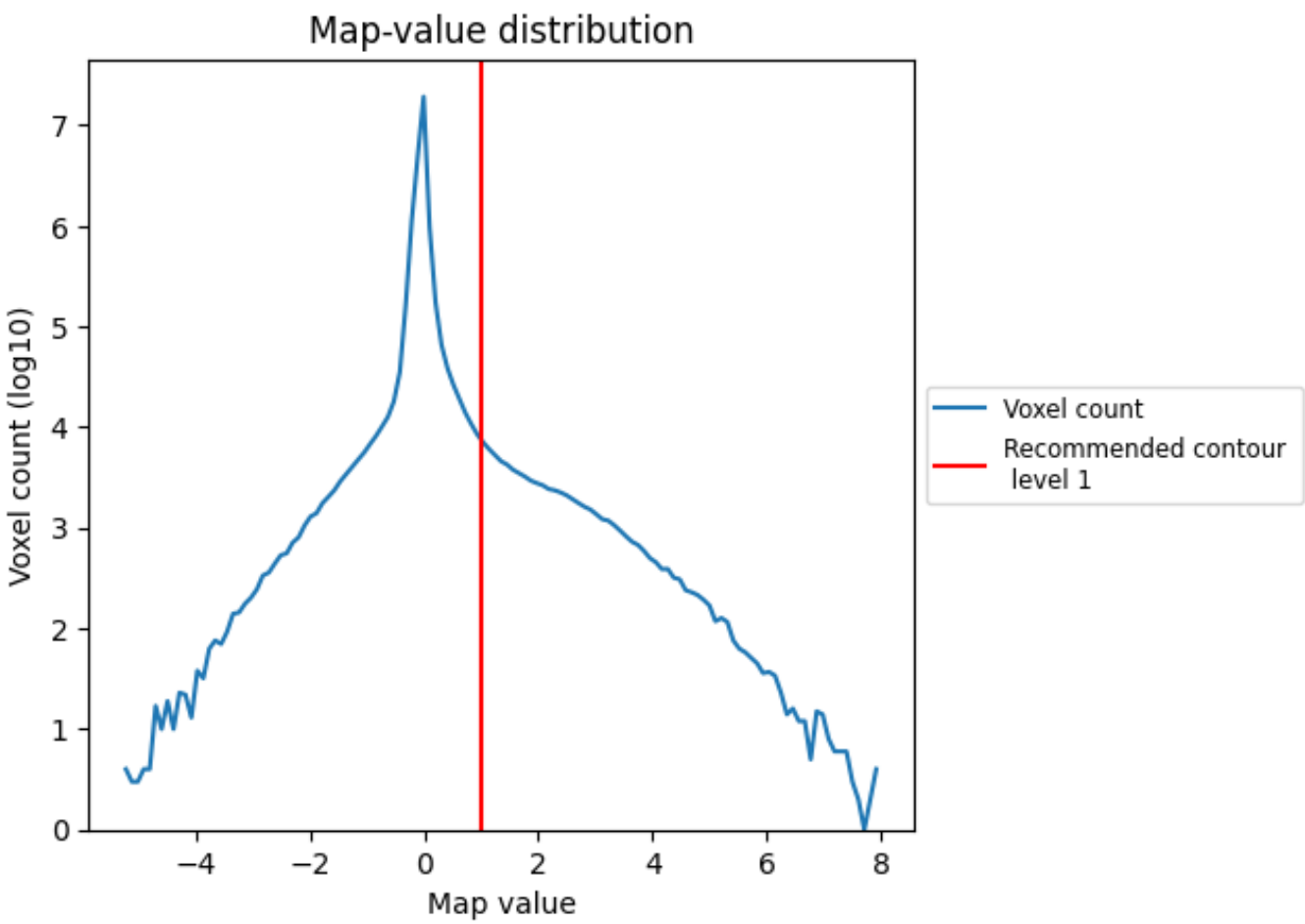


Z

7 Map analysis (i)

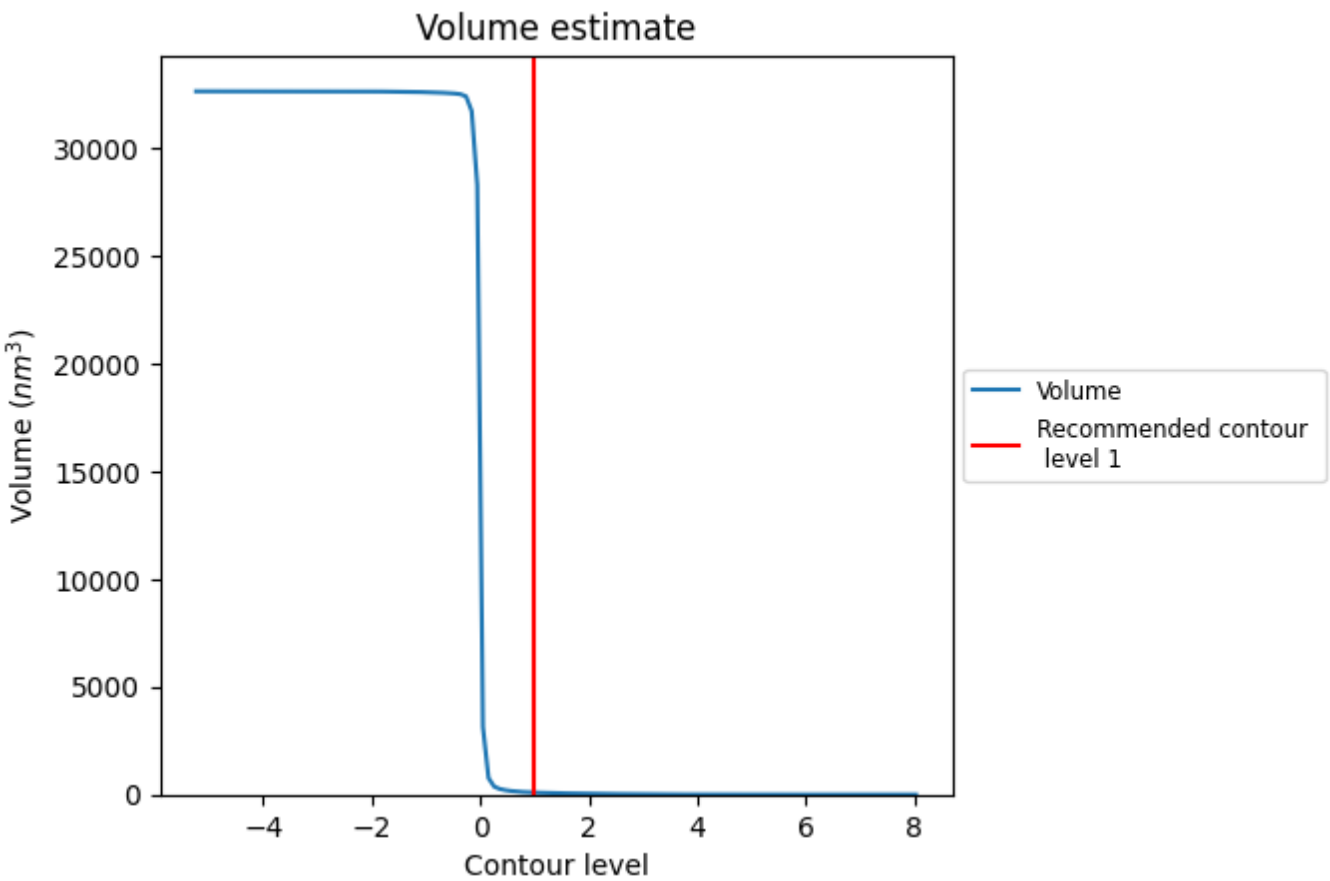
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

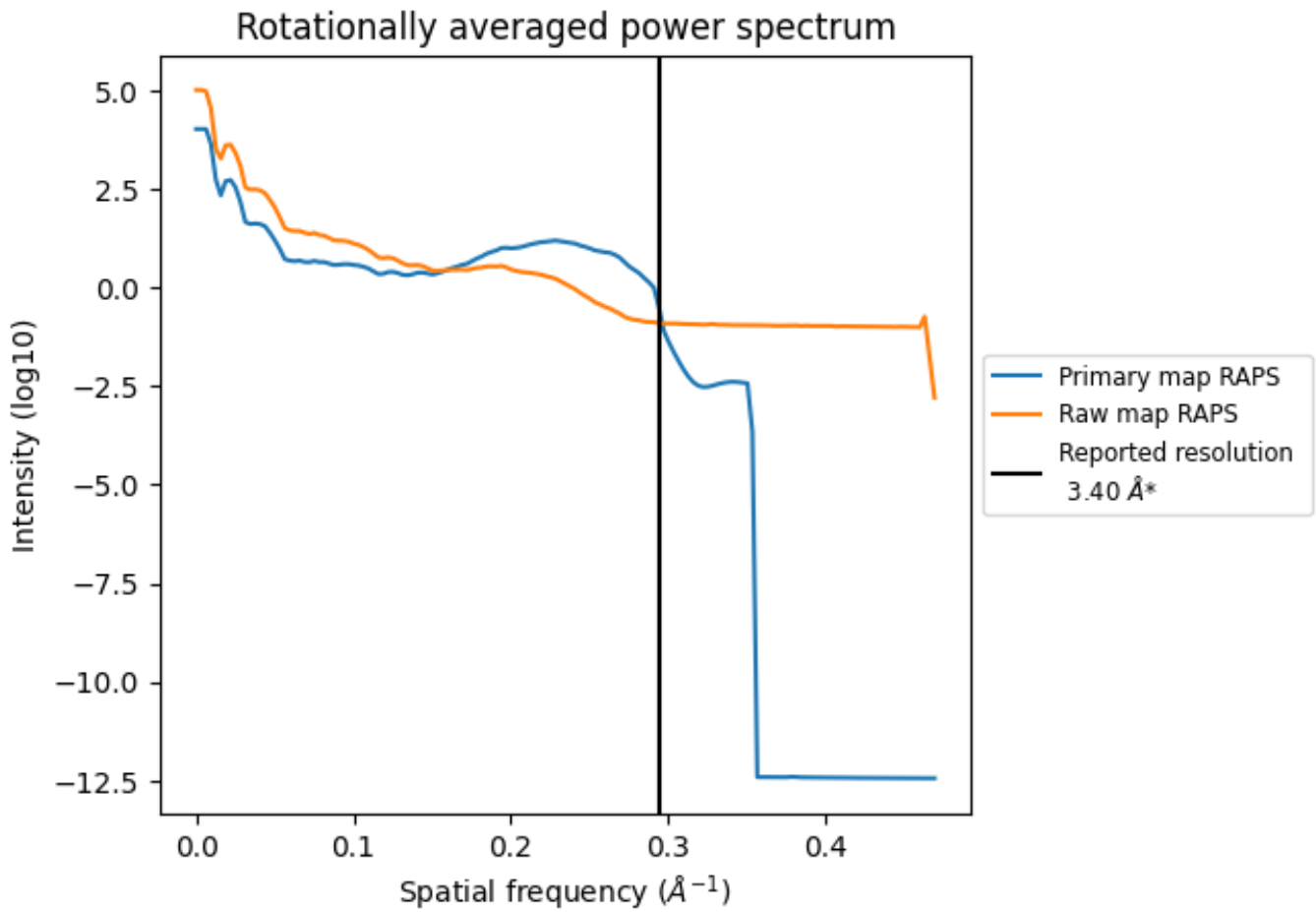
7.2 Volume estimate (i)



The volume at the recommended contour level is 94 nm^3; this corresponds to an approximate mass of 85 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

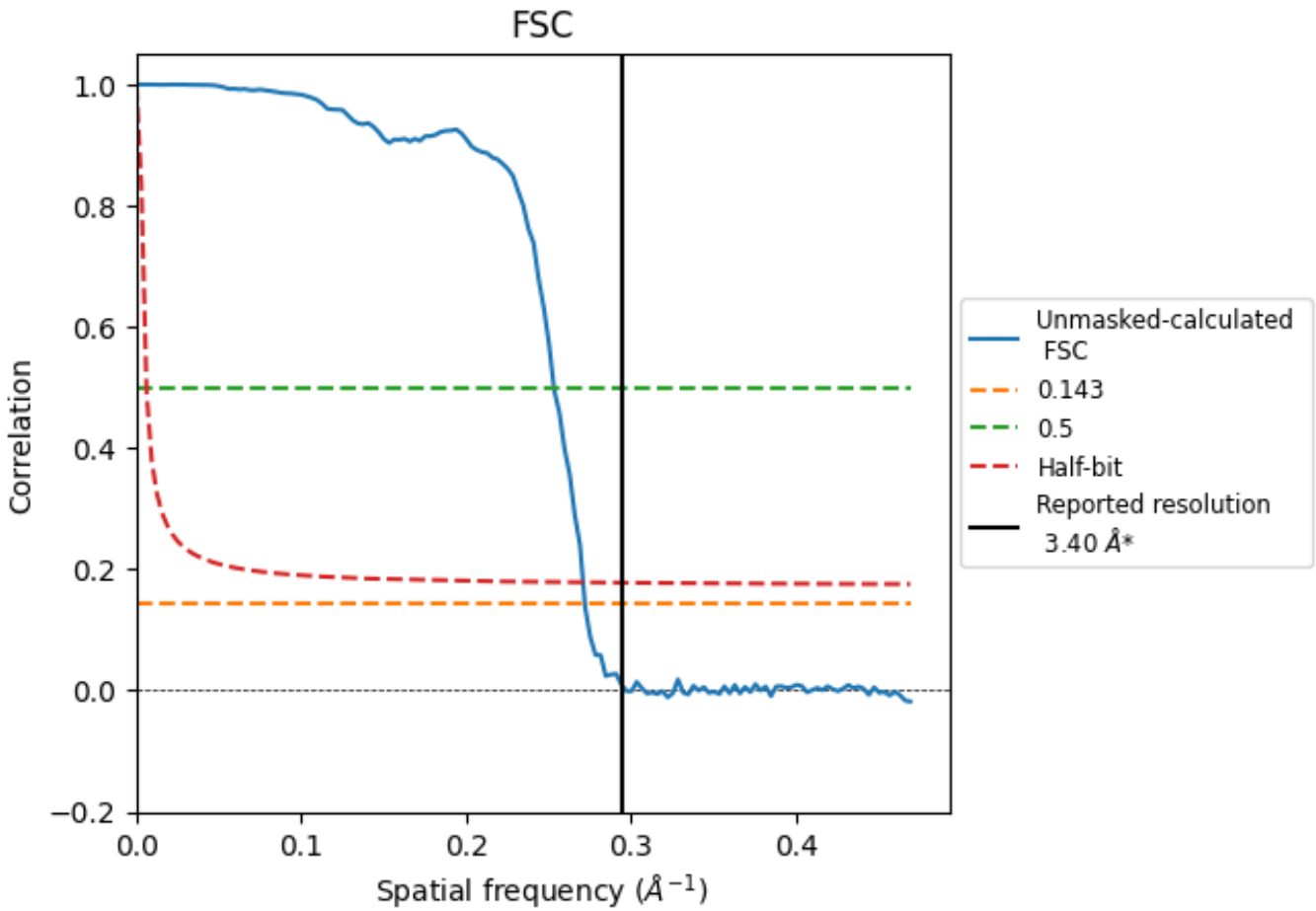


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

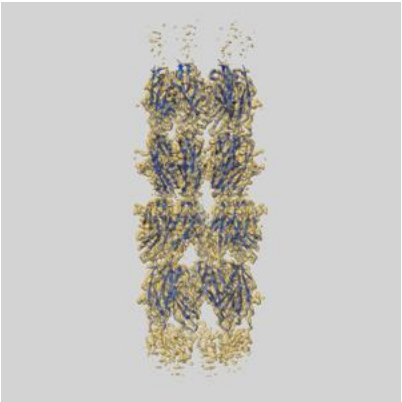
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.68	3.95	3.69

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

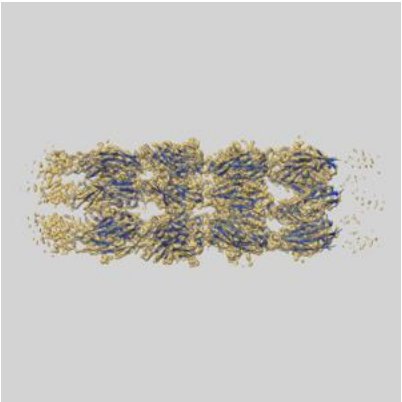
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-50539 and PDB model 9FLU. Per-residue inclusion information can be found in section 3 on page 5.

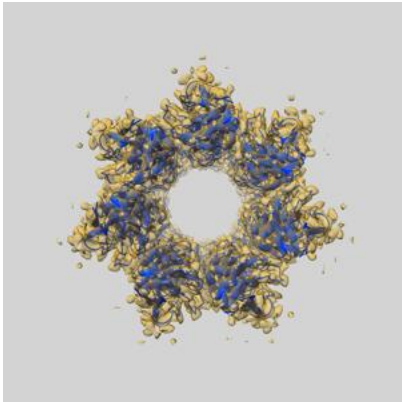
9.1 Map-model overlay (i)



X



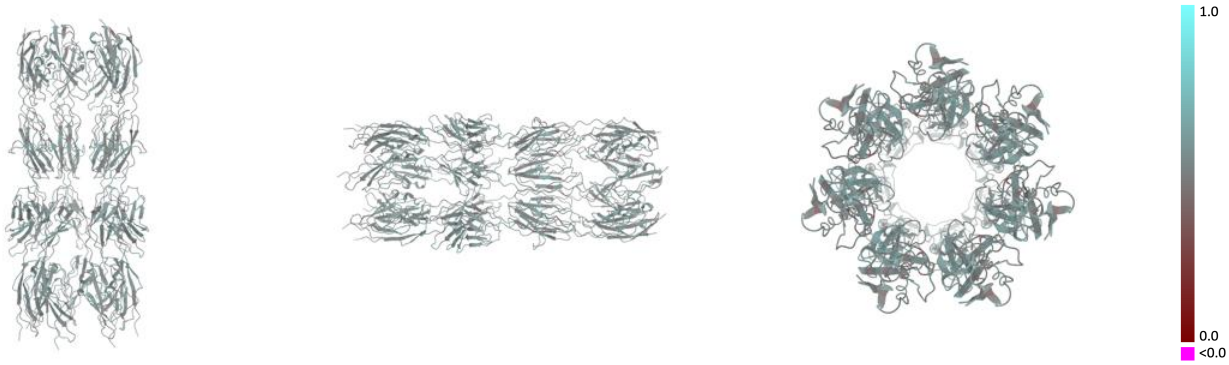
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

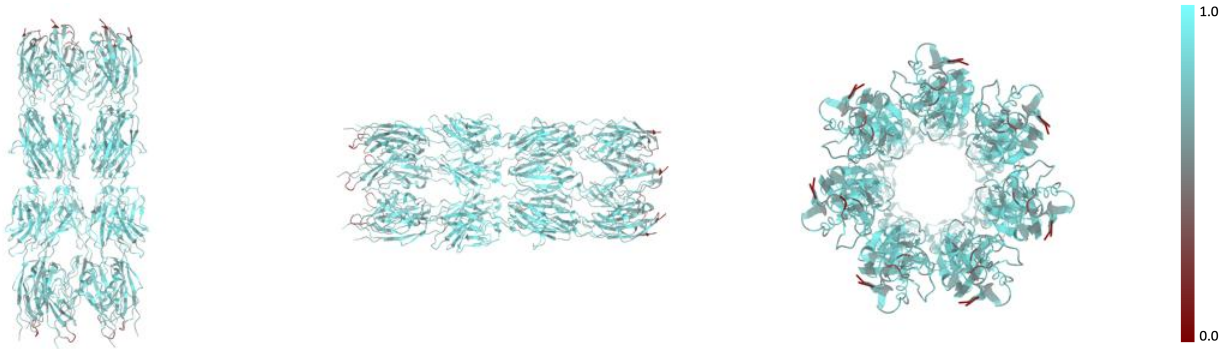
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

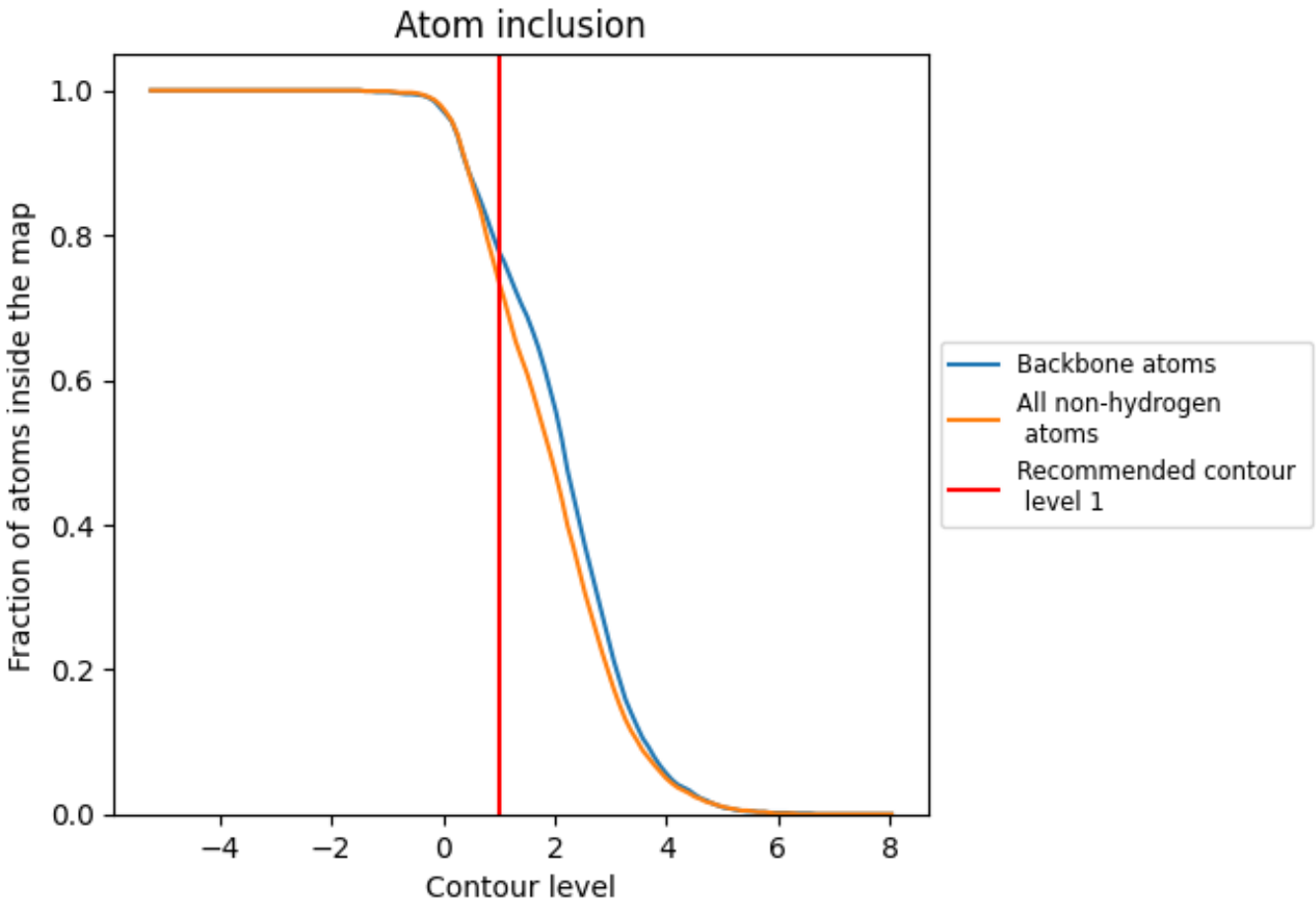
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7350	0.5250
A	0.7320	0.5250
B	0.7350	0.5250
C	0.7370	0.5260
D	0.7310	0.5260
E	0.7370	0.5260
F	0.7380	0.5260
G	0.7340	0.5250