Full wwPDB EM Validation Report (i)

Mar 24, 2026 – 08:19 AM UTC

PDB ID	:	9FLP / pdb_00009flp
EMDB ID	:	EMD-50537
Title	:	CryoEM structure of the neck (1403-2314) 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	:	3.80 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:

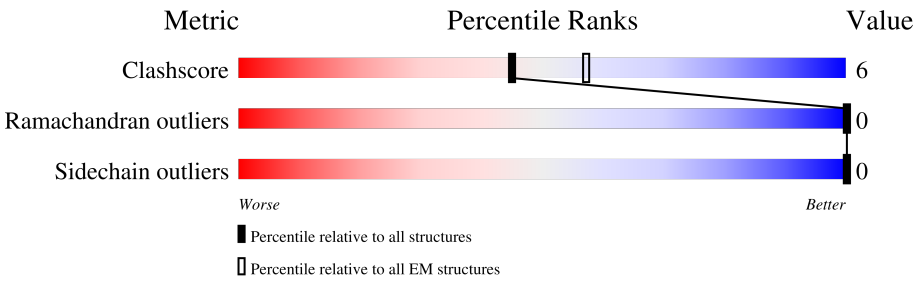
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

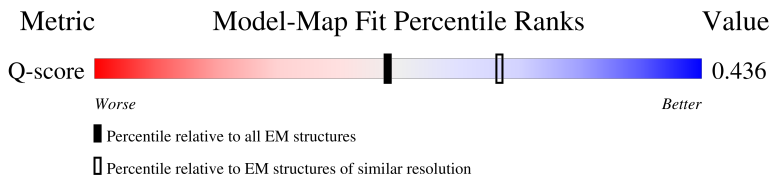
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	14% • 85%
1	B	5898	14% • 85%
1	C	5898	14% • 85%
1	D	5898	14% • 85%

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Mol	Chain	Length	Quality of chain
1	E	5898	14% · 85%
1	F	5898	14% · 85%
1	G	5898	14% · 85%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 45101 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 in the bacterium Aureispira sp. CCB-QB1.

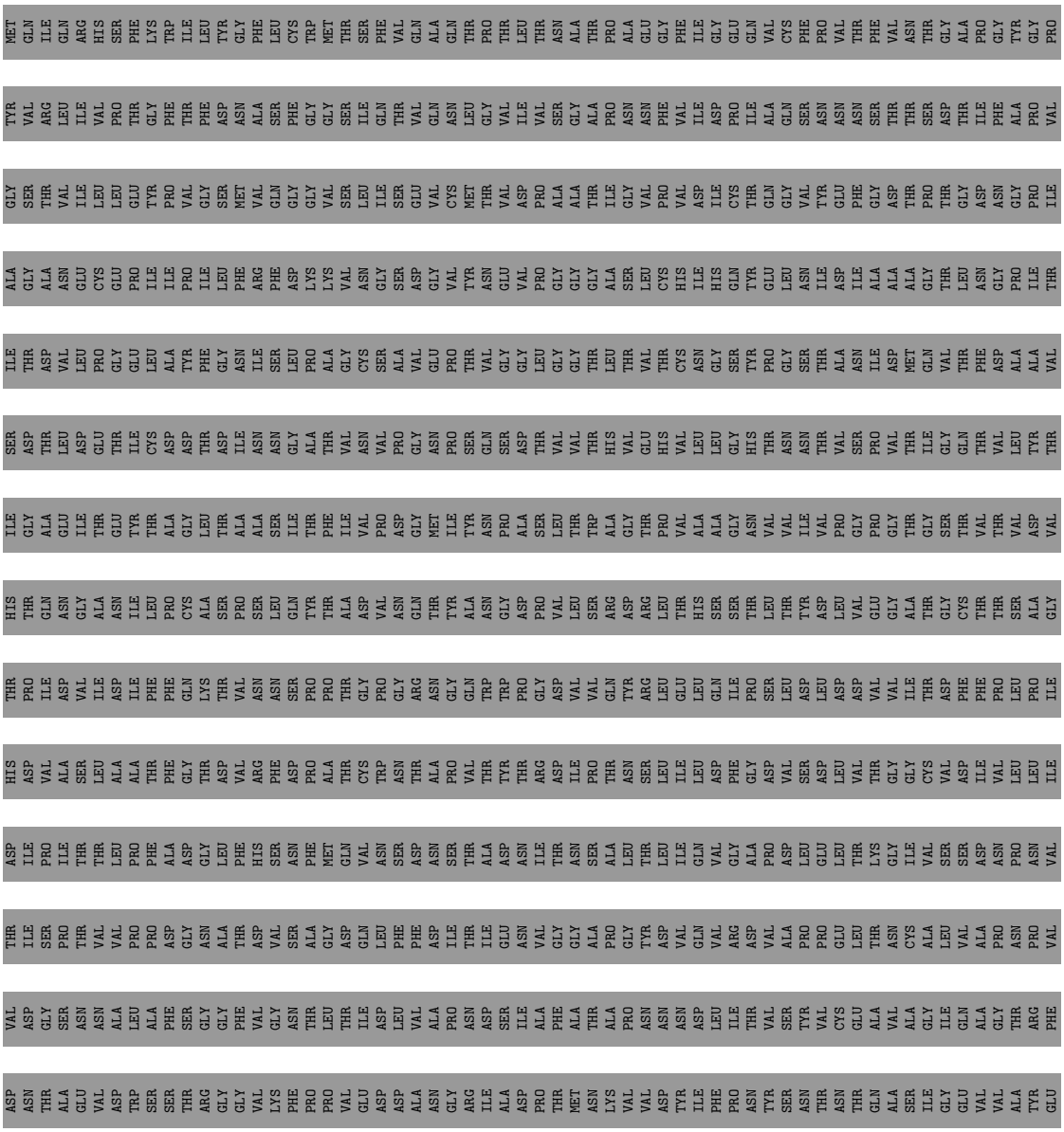
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	912	6443	3965	1052	1396	30	0	0
1	B	912	6443	3965	1052	1396	30	0	0
1	C	912	6443	3965	1052	1396	30	0	0
1	D	912	6443	3965	1052	1396	30	0	0
1	E	912	6443	3965	1052	1396	30	0	0
1	F	912	6443	3965	1052	1396	30	0	0
1	G	912	6443	3965	1052	1396	30	0	0

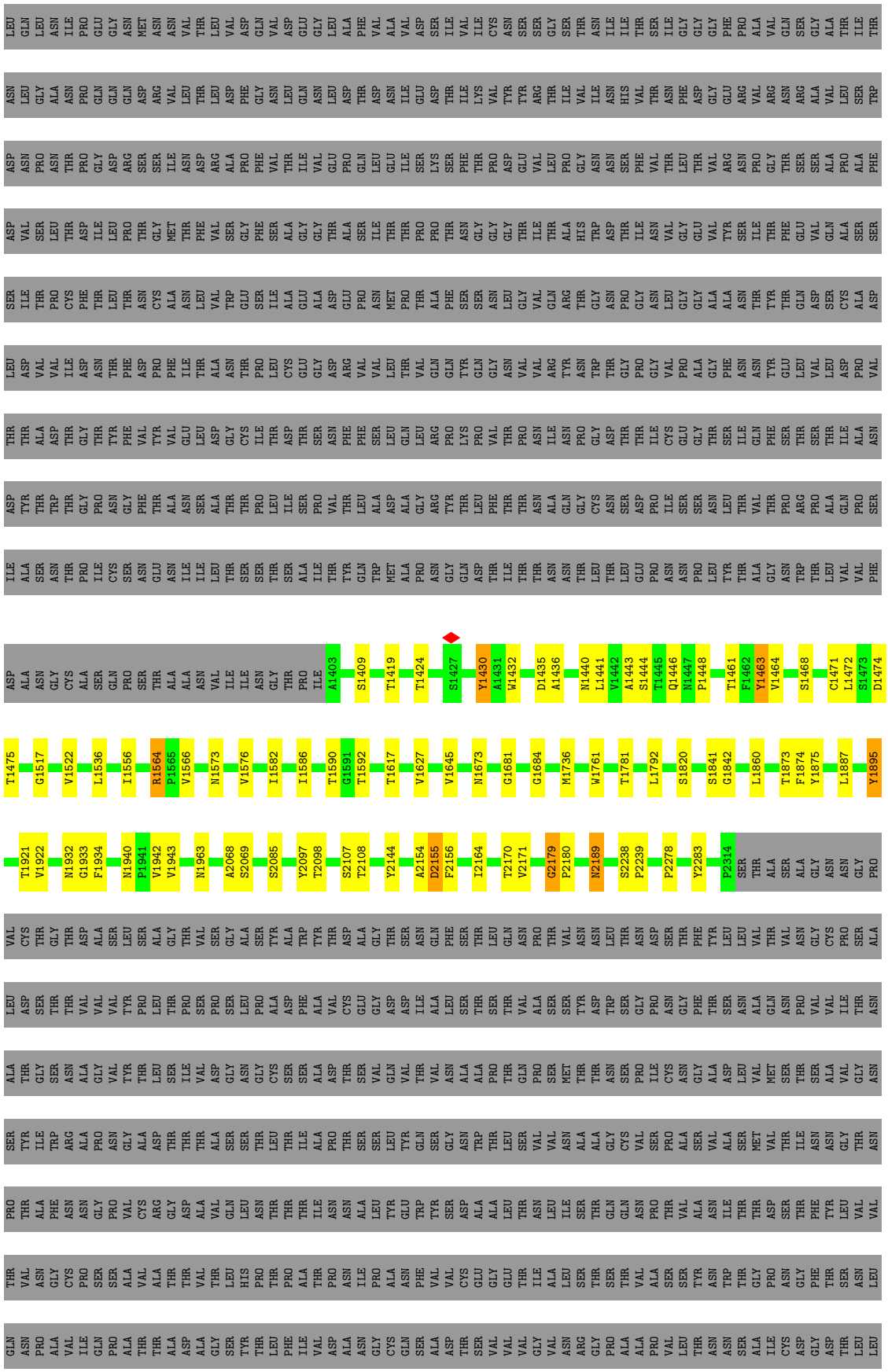
3 Residue-property plots (i)

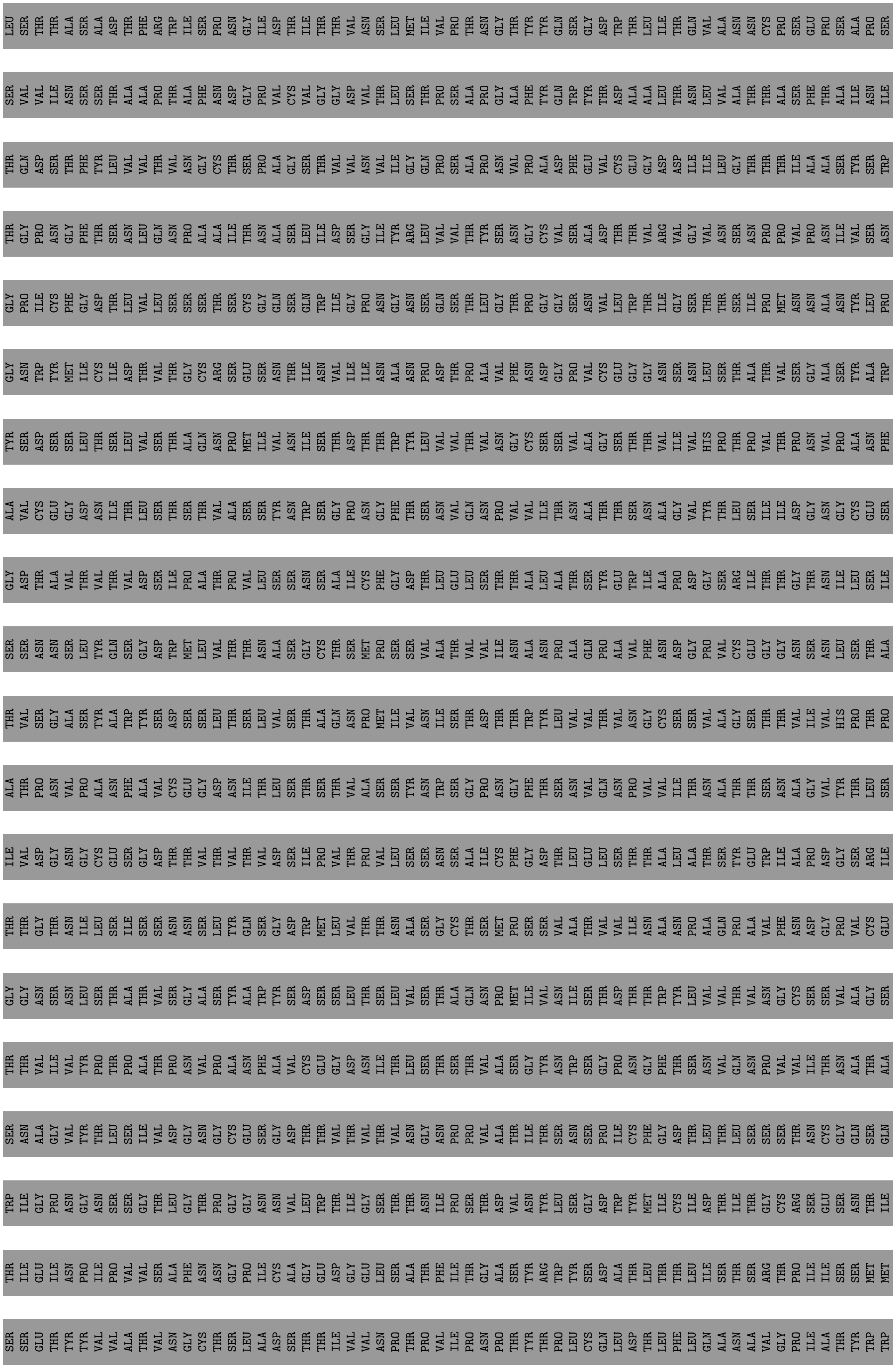
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 in the bacterium Aureispira sp. CCB-QB1

Chain A: 14% 85%




T1921 V1922 N1932 G1933 F1934 N1940 P1941 V1942 V1943 N1963 A2068 S2069 S2085 Y2097 T2098 S2107 T2108 Y2144 A2154 D2155 F2156 I2164 T2170 V2171 G2179 P2180 N2189 S2238 P2239 P2278 Y2283 P2314
T1475 G1517 V1522 L1536 I1556 R1564 P1565 V1566 N1573 V1576 I1582 I1586 T1590 G1591 T1592 T1617 V1627 V1645 N1673 G1681 G1684 M1736 W1761 T1781 L1792 S1820 S1841 G1842 L1860 T1873 F1874 Y1875 L1887 Y1895
ASP ALA ASN GLY CYS ALA SER GLN PRO SER THR ALA ALA ASN VAL ILE ILE ASN GTY THR PRO ILE A1403 S1409 T1419 T1424 S1427 Y1430 A1431 W1432 D1435 A1436 N1440 L1441 V1442 A1443 S1444 T1445 Q1446 N1447 P1448 T1461 F1462 Y1463 V1464 S1468 C1471 L1472 S1473 D1474



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

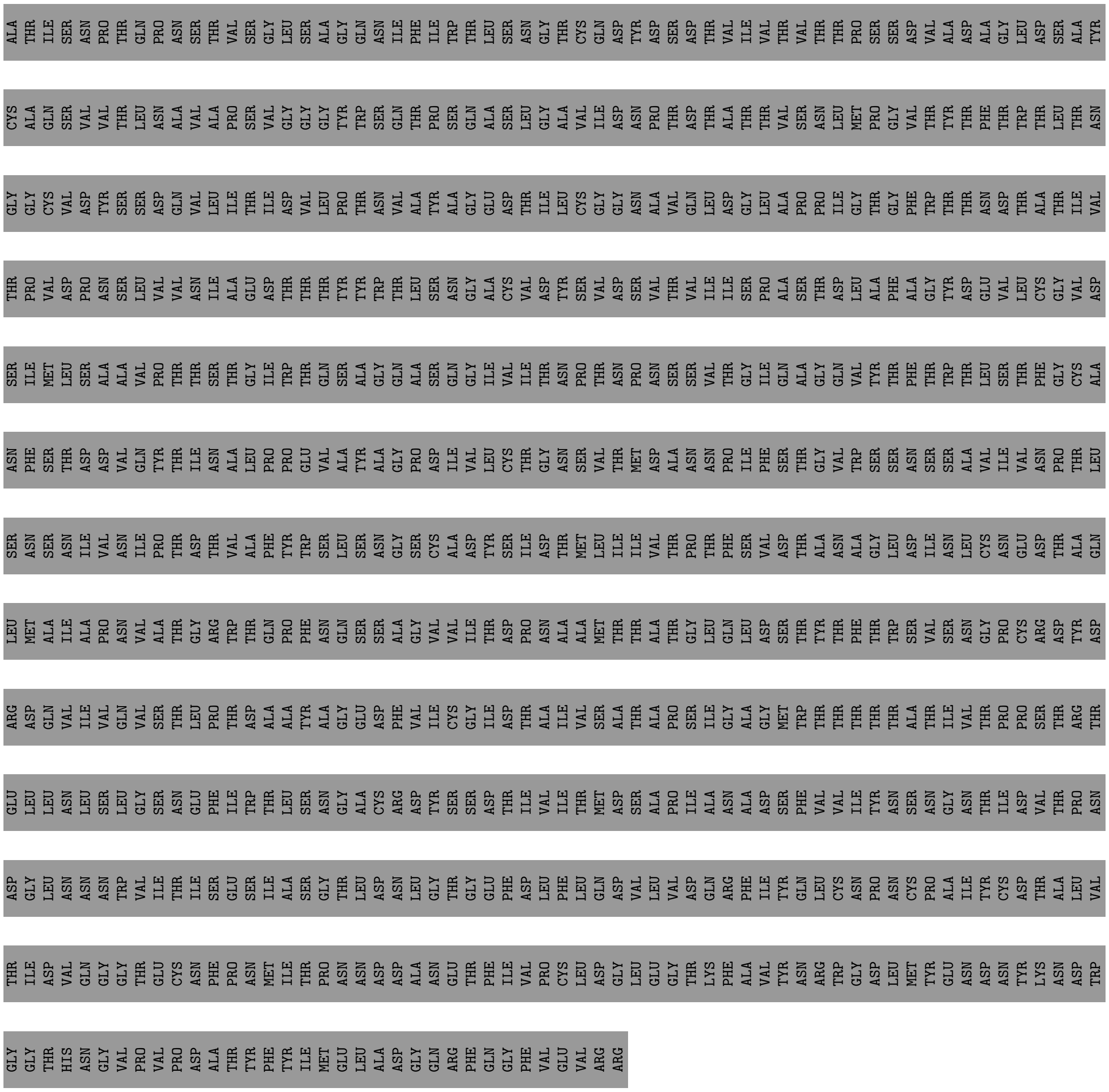
ASP ALA GLY LEU ASP GLN ASN LEU CYS GLY GLN THR SER ALA THR LEU THR ALA ALA ASN PRO SER THR ALA THR GLY GLN TRP THR GLN SER ALA SER GLN ALA GLY GLN GLY ILE VAL ILE THR ASN PRO THR ASN PRO ASN THR THR VAL THR GLY LEU GLN GLN GLY ASN ASN TYR

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 SER THR THR THR ASP THR ALA GLU ALA GLY ASN ASN

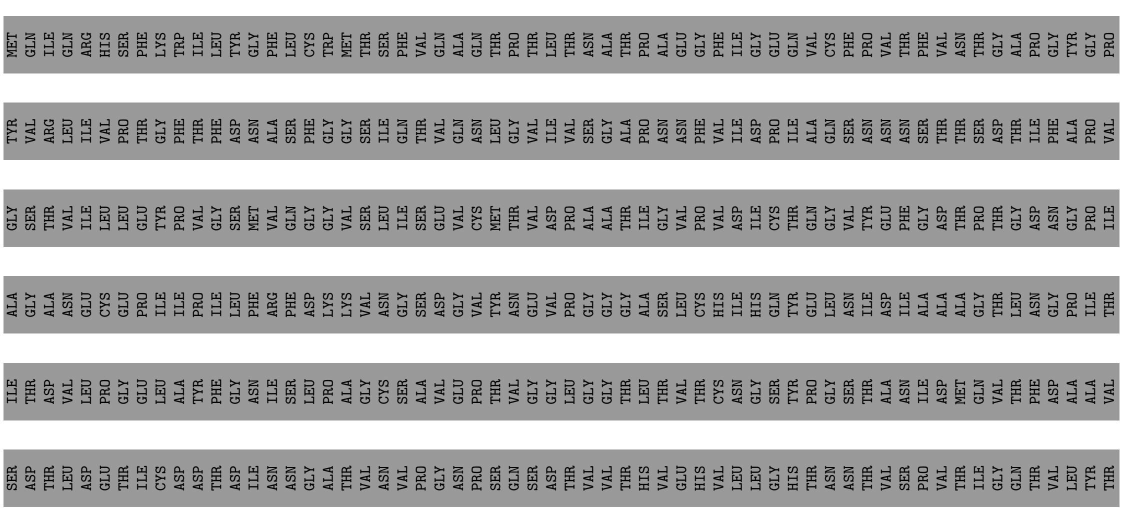
GLN VAL VAL CYS SER VAL ASN ALA LEU THR LEU GLY ALA THR MET PRO SER SER GLY PHE GLY THR TRP SER GLN THR ALA ALA GLN ALA ALA GLN GLY VAL VAL ILE VAL ASP VAL ASN ASP PRO ASN THR GLN VAL VAL GLY LEU ASN ALA GLY THR THR TYR ALA PHE THR TRP THR

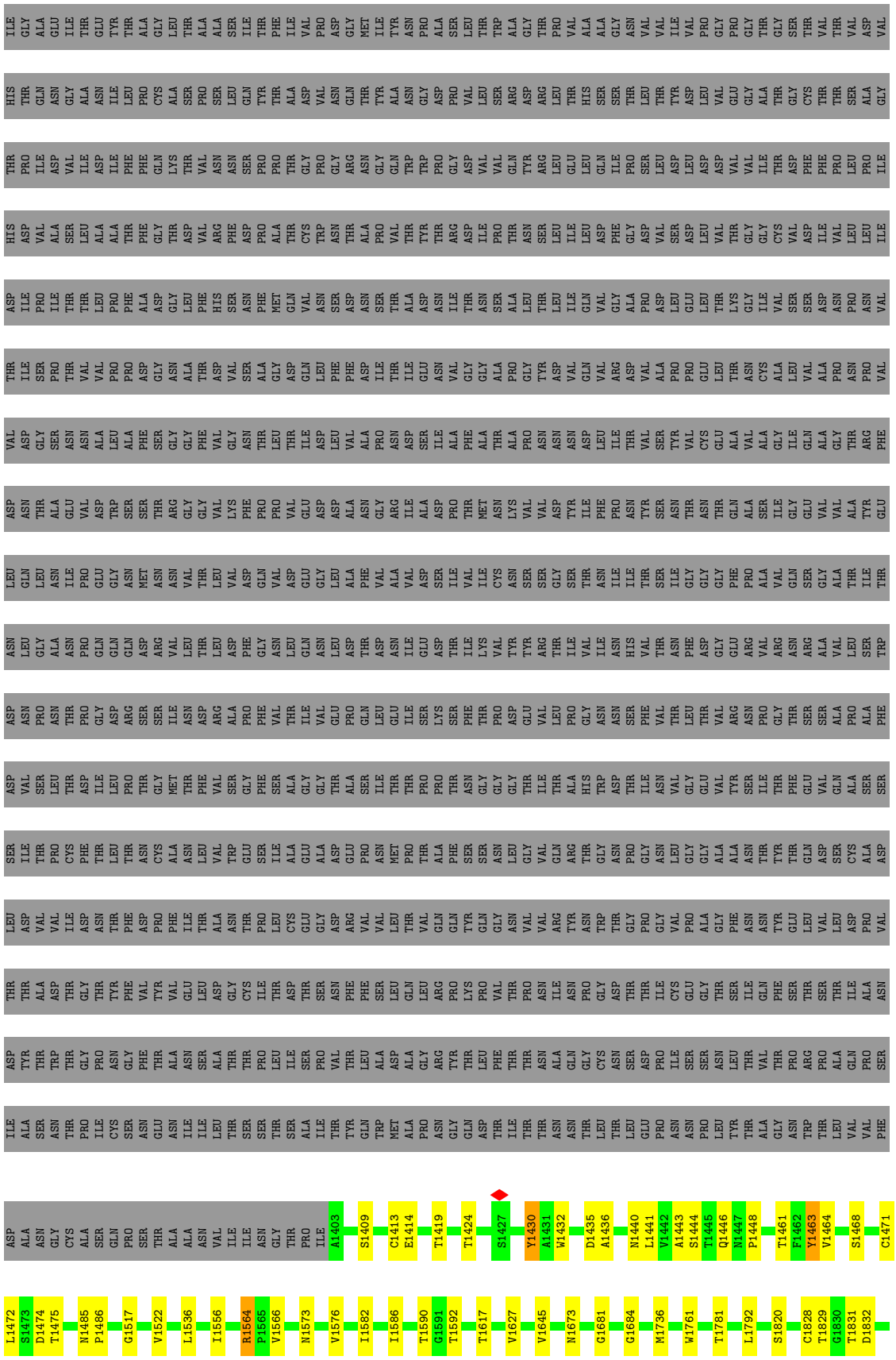
LEU SER ASN GLY THR CYS GLN ASP TYR SER SER ASP VAL THR THR ILE SER VAL ASN ALA THR PRO PRO ASP ASN ALA PHE ALA GLY ASN ASP ILE ASN LEU CYS GLY VAL ALA THR THR THR ASN LEU ALA ALA SER VAL PRO THR VAL ALA MET GLY LEU TRP THR THR THR SER SER



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

Chain B:




L1472 S1473 D1474 T1475 N1485 P1486 G1517 V1522 L1536 I1556 R1564 P1565 V1566 N1573 V1576 I1582 I1586 T1590 G1591 T1592 T1617 V1627 V1645 N1673 G1681 G1684 M1736 W1761 T1781 L1792 S1820 C1828 T1829 G1830 T1831 D1832
A1403 S1409 C1413 E1414 T1419 T1424 S1427 Y1430 A1431 W1432 D1435 A1436 N1440 L1441 V1442 A1443 S1444 T1445 Q1446 M1447 P1448 T1461 F1462 Y1463 V1464 S1468 C1471

S1841 G1842 L1860 T1873 F1874 Y1875 L1887 Y1895 T1921 V1922 N1932 G1933 F1934 V1942 V1943 N1963 A2068 S2069 S2085 Y2097 T2098 S2107 T2108 Y2144 A2154 D2155 F2156 I2164 T2170 V2171 G2179 P2180 N2189 S2238 P2239 P2278 Y2283 P2314

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

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

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

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

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

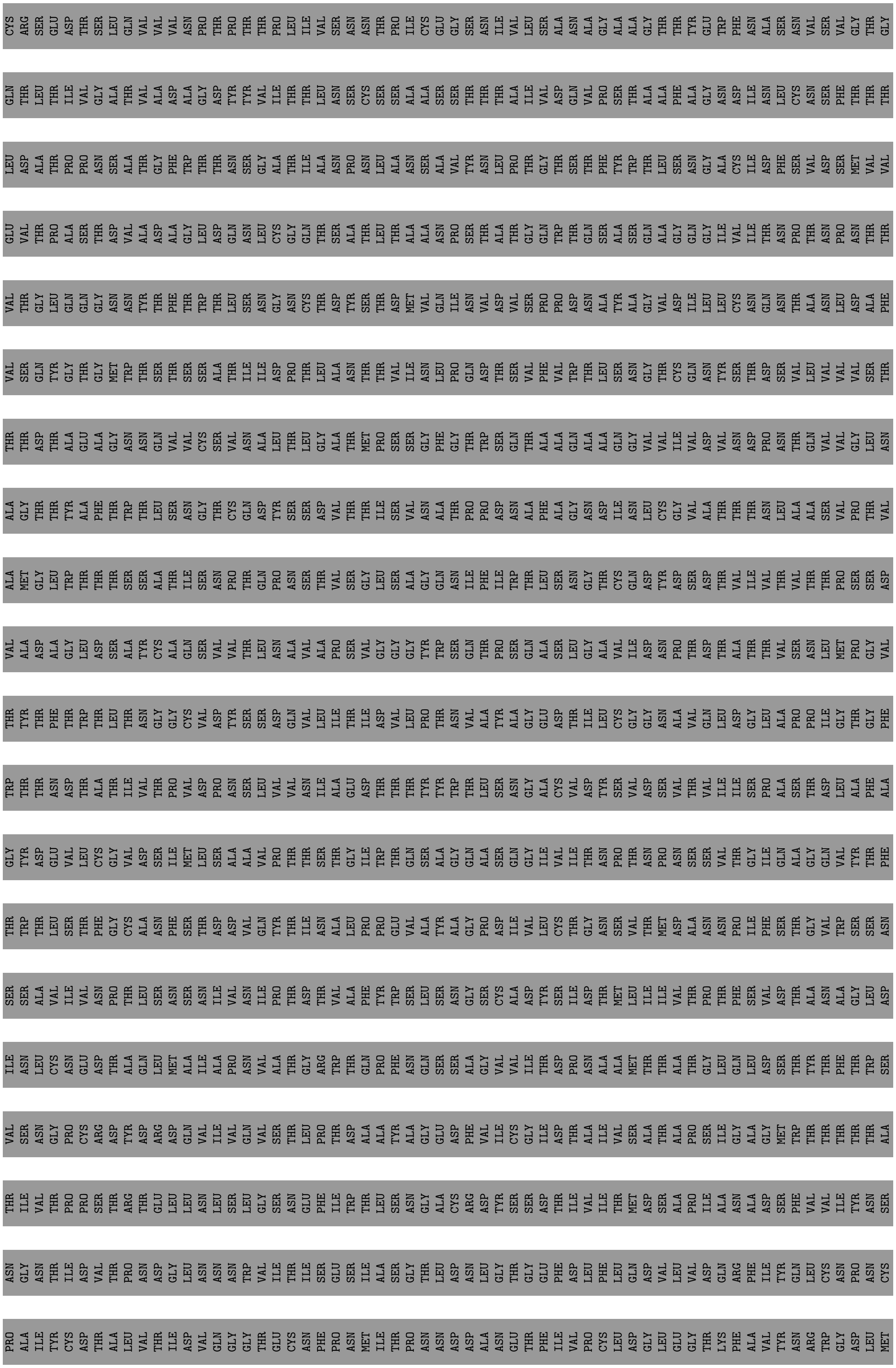
ASP ASN ILE VAL LEU SER THR THR THR VAL ALA ALA GLY TYR ASN TRP THR GLY PRO ASN GLY PHE THR SER ASN LEU GLN ASN PRO SER VAL VAL SER ALA SER LEU VAL ASP SER GLY THR TYR THR LEU PHE ILE ILE ASP ALA ASN GLY CYS PRO SER GLY ASP THR SER VAL GLN

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 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



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 in the bacterium Aureispira sp. CCB-QB1

Chain C:

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 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 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

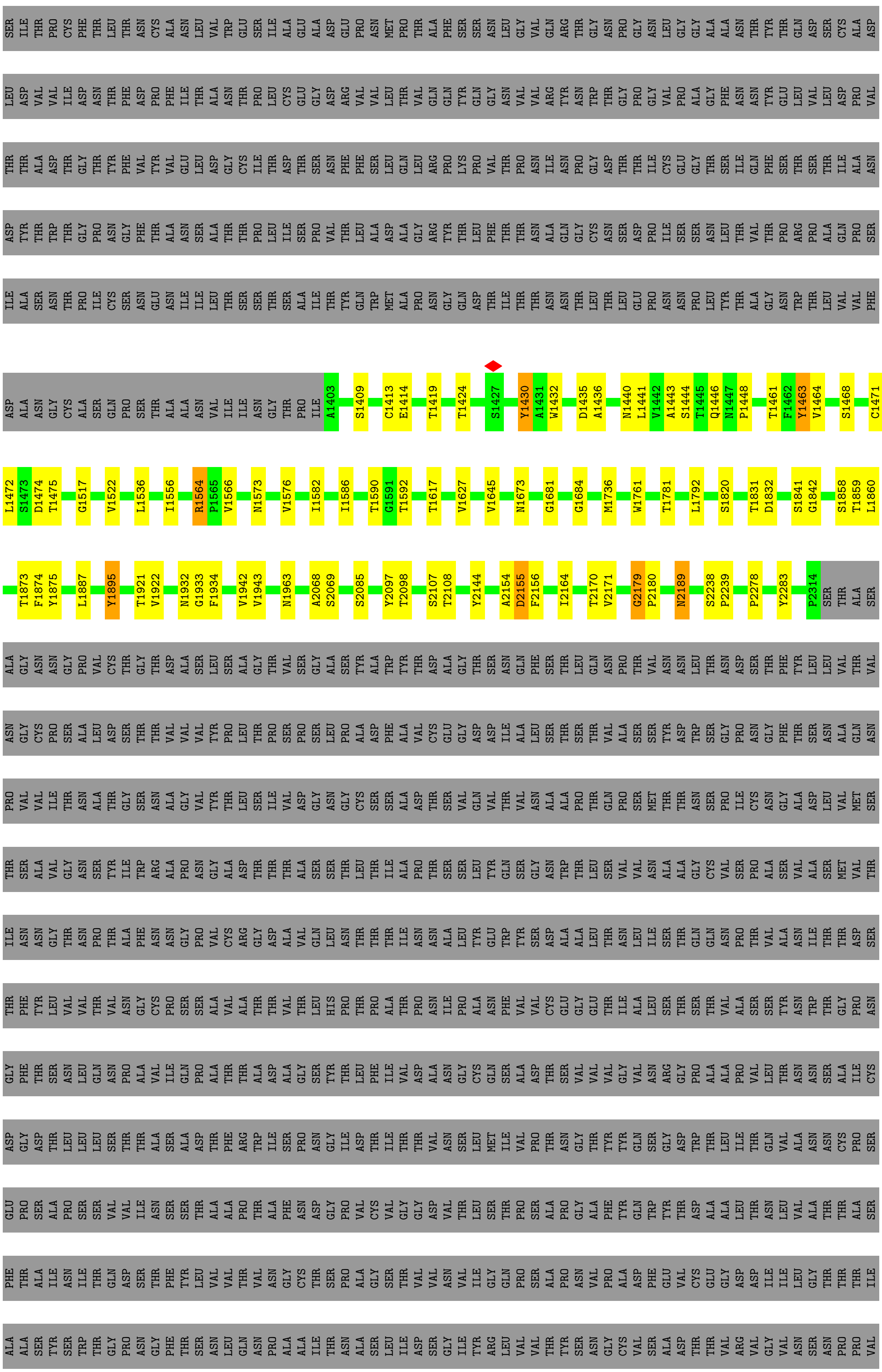
ASP ASN THR ALA GLU VAL ASP TRP SER SER THR ARG GLY GLY VAL LYS PHE PRO PRO VAL GLU ASP ASP ALA ASN GLY ARG ILE ALA ASP PRO THR MET ASN LYS VAL VAL ASP TYR ILE PHE PRO ASN TYR SER ASN THR ASN THR GLN ALA SER ILE GLY GLU VAL VAL ALA TYR GLU

LEU GLN LEU ASN ILE PRO GLU GLY 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 VAL ILE 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 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 A1403 S1409 C1413 E1414 T1419 T1424 S1427 Y1430 A1431 W1432 D1435 A1436 N1440 L1441 V1442 A1443 S1444 T1445 Q1446 N1447 P1448 T1461 F1462 Y1463 V1464 S1468 C1471
L1472 S1473 D1474 T1475 G1517 V1522 L1536 I1556 R1564 P1565 V1566 N1573 V1576 I1582 I1586 T1590 G1591 T1592 T1617 V1627 V1645 N1673 G1681 G1684 M1736 W1761 T1781 L1792 S1820 T1831 D1832 S1841 G1842 S1858 T1859 L1860
T1873 F1874 Y1875 L1887 Y1895 T1921 V1922 N1932 G1933 F1934 V1942 V1943 N1963 A2068 S2069 S2085 Y2097 T2098 S2107 T2108 Y2144 A2154 D2155 F2156 I2164 T2170 V2171 G2179 P2180 N2189 S2238 P2239 P2278 Y2283 P2314 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 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 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 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 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 SER SER TYR ASN TRP SER GLY PRO ASN GLY PHE THR SER ASN VAL GLN ASN PRO VAL VAL ILE THR ASN ALA THR THR SER ASN ALA GLY VAL TYR THR LEU SER ILE ILE ASP

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

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

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

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

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

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

ILE ALA THR TYR TRP TRP THR GLY PRO ASN GLY PHE THR SER HIS LEU GLU ASN PRO VAL ILE PRO ASN ILE TYR PRO PHE ASN ALA GLY SER TYR ILE LEU THR VAL THR ASP SER LEU GLY CYS GLU ALA VAL SER THR VAL 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 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 THR SER ASN 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 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 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 in the bacterium Aureispira sp. CCB-QB1

Chain D: 14% • 85%

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 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

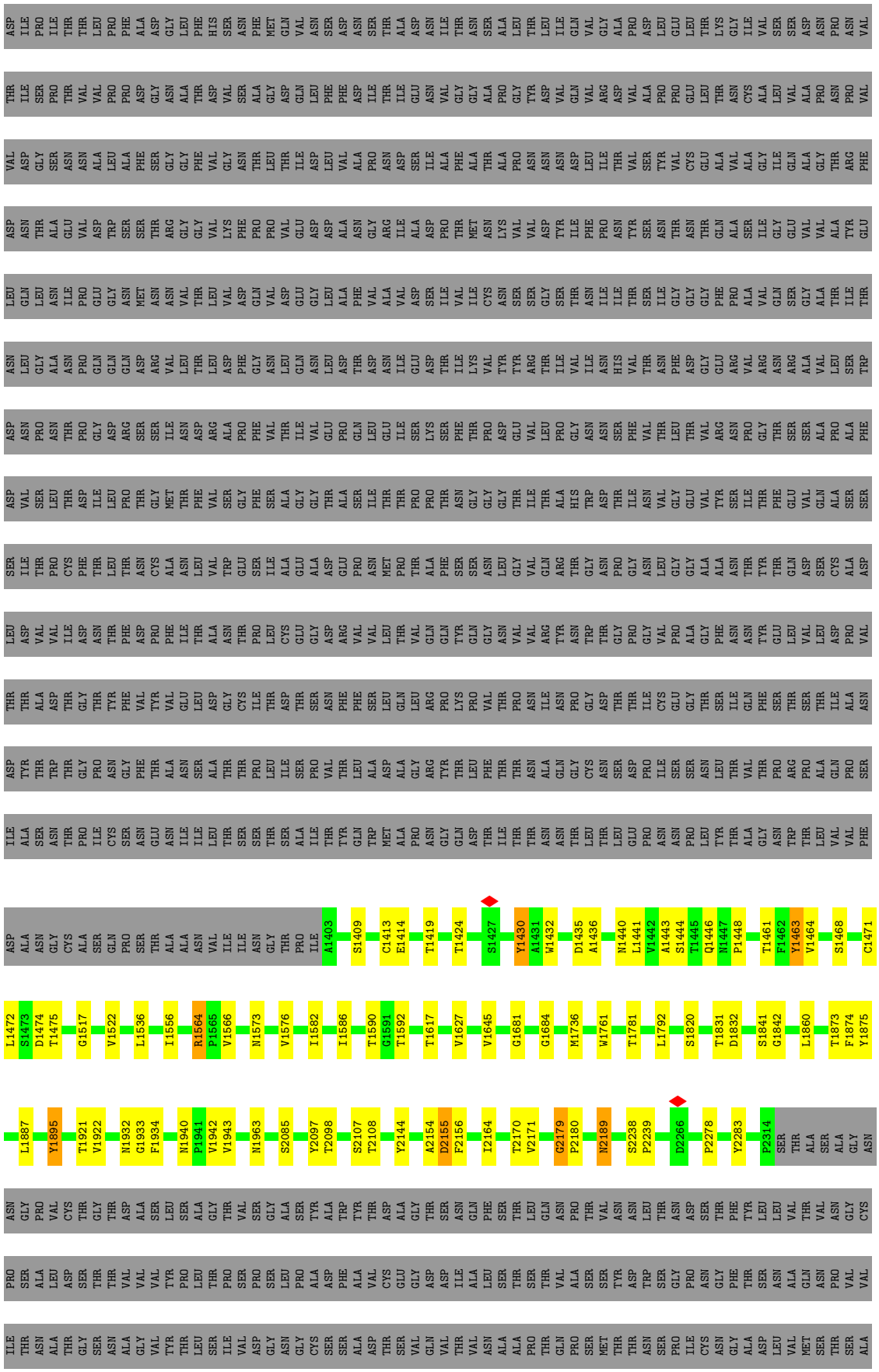
SER ASP THR LEU ASP GLU THR ILE CYS ASP THR ASP ILE ASN ASN GLY ALA THR VAL ASN VAL PRO GLY ASN PRO SER GLN SER ASP THR VAL VAL THR HIS VAL GLU HIS VAL LEU LEU GLY HIS THR ASN ASN THR VAL SER PRO VAL THR ILE GLY GLN THR VAL LEU TYR THR

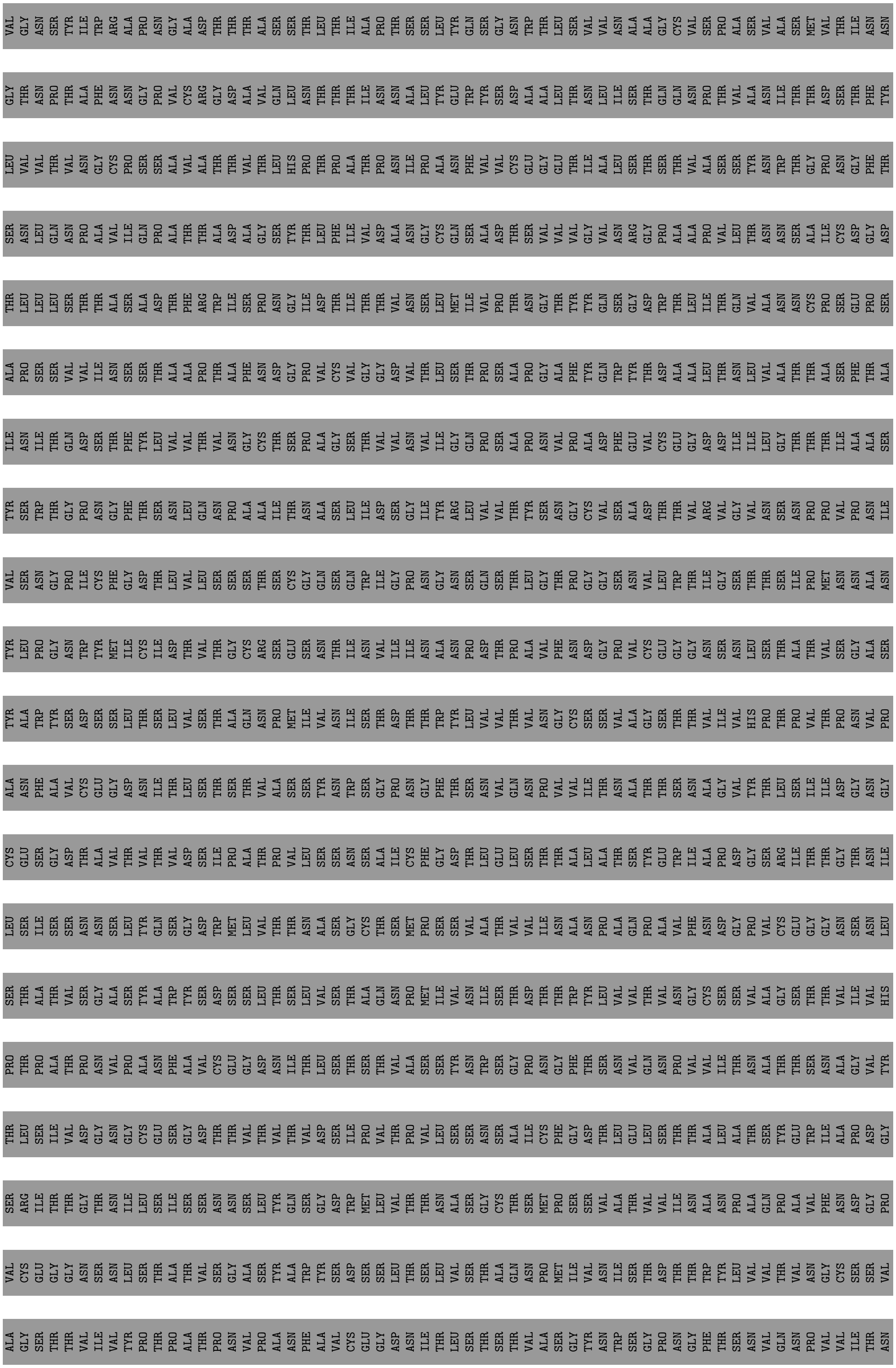
ILE GLY ALA GLU ILE THR GLU TYR THR ALA GLY LEU THR ALA ALA SER ILE THR PHE ILE VAL PRO ASP GLY MET ILE TYR ASN PRO ALA SER LEU THR TRP ALA GLY THR PRO VAL ALA ALA GLY ASN VAL VAL ILE VAL PRO GLY PRO GLY THR GLY SER THR VAL THR VAL ASP VAL

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 GLU LEU GLN ILE PRO SER LEU ASP LEU ASP ASP VAL ILE 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 CYS VAL ASP ILE VAL LEU LEU ILE


L1887 Y1895 T1921 V1922 N1932 G1933 F1934 N1940 P1941 V1942 V1943 N1963 S2085 Y2097 T2098 S2107 T2108 Y2144 A2154 D2155 F2156 I2164 T2170 V2171 G2179 P2180 N2189 S2238 P2239 D2266 P2278 Y2283 P2314
L1472 S1473 D1474 T1475 G1517 V1522 L1536 I1556 R1564 P1565 V1566 N1573 V1576 I1582 I1586 T1590 G1591 T1592 T1617 V1627 V1645 G1681 G1684 M1736 W1761 T1781 L1792 S1820 T1831 D1832 S1841 G1842 L1860 T1873 F1874 Y1875
ASP ALA ASN GLY CYS ALA SER GLN PRO SER THR ALA ASN VAL ILE SER PRO ILE A1403 S1409 C1413 E1414 T1419 T1424 S1427 Y1430 A1431 W1432 D1435 A1436 N1440 L1441 V1442 A1443 S1444 T1445 Q1446 N1447 P1448 T1461 F1462 Y1463 V1464 S1468 C1471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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 GLN ASN PRO ALA 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 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 LEU 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 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 SER SER TYR ASN TRP SER GLY PRO ASN GLY PHE THR SER ASN VAL GLN ASN PRO VAL VAL ILE THR ASN ALA THR THR SER ASN ALA GLY VAL TYR THR LEU SER ILE ILE ASP GLY ASN GLY
CYS GLU SER GLY ASP THR ALA VAL THR VAL THR VAL ASP SER ILE PRO ALA THR PRO VAL LEU SER SER ASN SER ALA ILE CYS PHE GLY ASP THR LEU GLU LEU SER THR THR ALA LEU ALA THR SER TYR GLU TRP ILE ALA PRO ASP GLY SER ARG ILE THR THR GLY THR ASN ILE
LEU SER ILE SER SER ASN ASN SER LEU TYR GLN SER GLY ASP TRP MET LEU VAL THR THR ASN ALA SER GLY CYS THR SER MET PRO SER SER VAL ALA THR VAL VAL ILE ASN ALA ASN PRO ALA GLN 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 ALA THR PRO ASN VAL PRO ALA ASN PHE ALA VAL CYS GLU GLY ASP ASN ILE THR LEU SER THR SER THR VAL ALA SER SER TYR ASN TRP SER GLY PRO ASN GLY PHE THR SER ASN VAL GLN ASN PRO VAL VAL ILE THR ASN ALA THR THR SER ASN ALA GLY VAL TYR
THR LEU SER ILE VAL ASP GLY ASN GLY CYS GLU SER GLY ASP THR THR VAL THR VAL THR VAL ASP SER ILE PRO VAL THR PRO VAL LEU SER SER ASN SER ALA ILE CYS PHE GLY ASP THR LEU GLU LEU SER THR THR ALA LEU ALA THR SER TYR GLU TRP ILE ALA PRO ASP GLY
SER ARG ILE THR THR GLY THR ASN ILE LEU SER ILE SER SER ASN ASN SER LEU TYR GLN SER GLY ASP TRP MET LEU VAL THR THR ASN ALA SER GLY CYS THR SER MET PRO SER SER VAL ALA THR VAL VAL ILE ASN ALA ASN PRO ALA GLN 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 TYR PRO THR PRO ALA THR PRO ASN VAL PRO ALA ASN PHE ALA VAL CYS GLU GLY ASP ASN ILE THR LEU SER THR SER THR VAL ALA SER GLY TYR ASN TRP SER GLY PRO ASN GLY PHE THR SER ASN VAL GLN ASN PRO VAL VAL ILE THR ASN

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

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

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

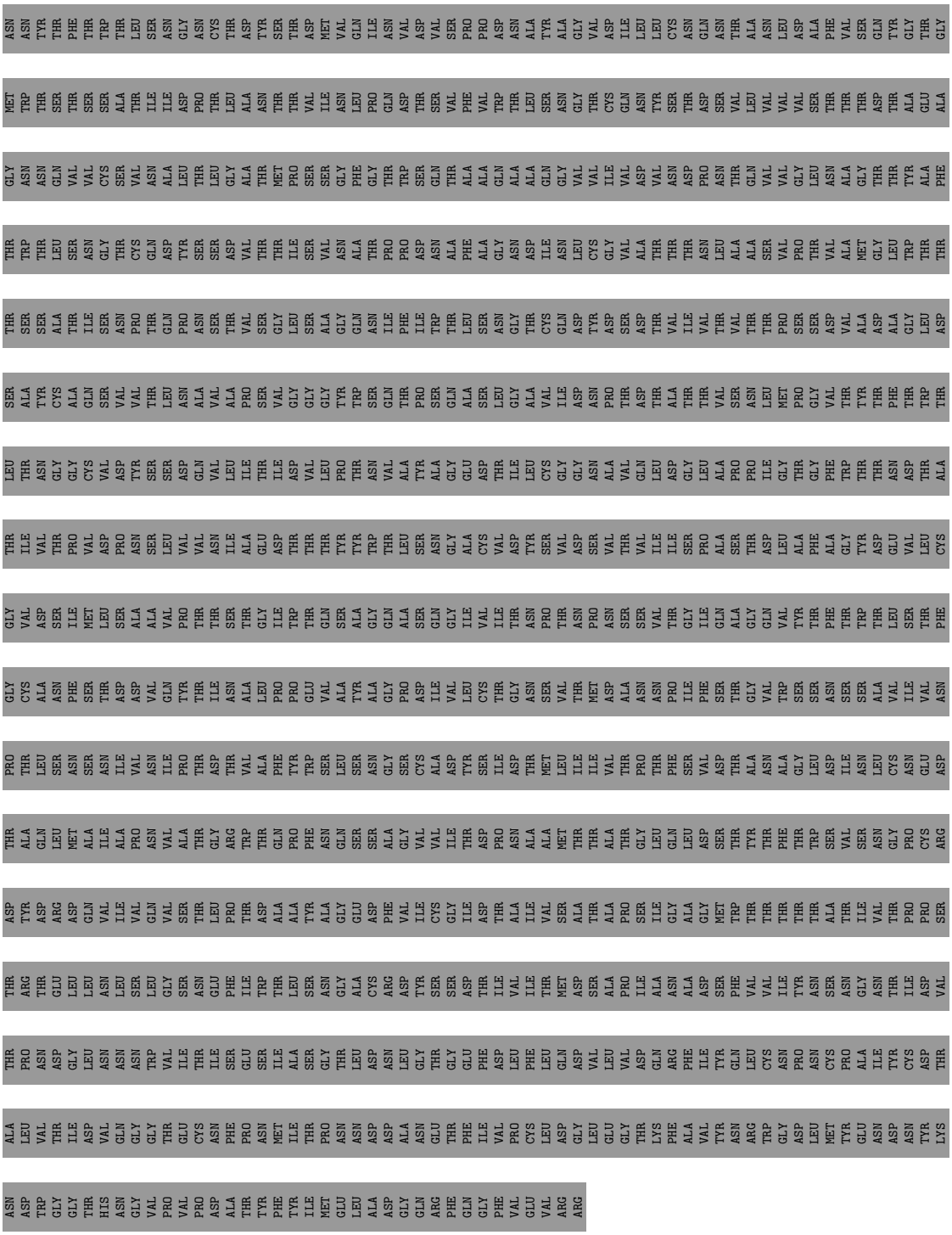
GLY ASP ALA ILE VAL LEU THR THR THR THR ASN ALA SER ALA TYR VAL TRP SER GLY PRO ASN GLY PHE SER SER ASN GLN GLN SER PRO THR VAL ILE ASN ALA ALA THR VAL VAL ASP SER GLY LYS TYR SER LEU TYR VAL ILE ASP ALA ASN GLY CYS ARG SER GLU ASP THR SER

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

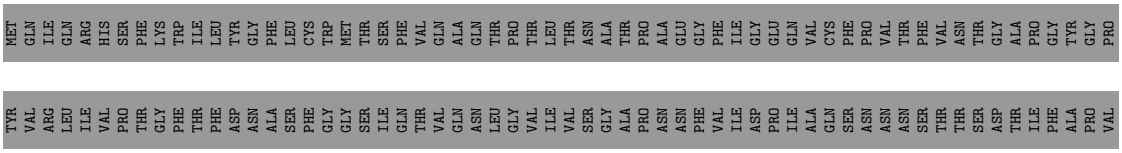
SER ALA THR GLY PHE TRP THR THR ASN SER GLY ALA THR ILE ALA ASN PRO ASN LEU ALA ASN SER ALA VAL TYR ASN LEU PRO THR GLY THR SER THR PHE TYR TRP THR LEU SER ASN GLY ALA CYS ILE ASP PHE SER VAL ASP SER MET VAL VAL GLU VAL THR PRO ALA SER THR

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



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

Chain E: 14% 85%



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 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 A1403 S1409 C1413 E1414 T1419 T1424 S1427 Y1430 A1431 W1432 D1435 A1436 N1440 L1441 V1442 A1443 S1444 T1445 Q1446 N1447 P1448 T1461 F1462 Y1463 V1464 S1468 C1471

L1472 S1473 D1474 T1475 G1517 V1522 L1536 I1556 R1564 P1565 V1566 N1573 V1576 I1582 I1586 T1590 G1591 T1592 T1617 V1627 V1645 N1673 G1681 G1684 M1736 W1761 T1781 L1792 S1820 C1828 T1829 S1841 G1842 L1860 T1873

F1874 Y1875 L1887 Y1895 T1921 V1922 N1932 G1933 F1934 V1942 V1943 N1963 S2085 Y2097 T2098 S2107 T2108 Y2144 A2154 D2155 F2156 I2164 T2170 V2171 G2179 P2180 N2189 S2238 P2239 P2278 Y2283 P2314 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 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 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 SER SER TYR ASN TRP SER GLY PRO ASN GLY PHE THR SER ASN VAL GLN ASN PRO VAL VAL ILE THR ASN ALA THR THR SER ASN ALA GLY VAL TYR THR LEU SER ILE ILE ASP GLY ASN GLY CYS GLU

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

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 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 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

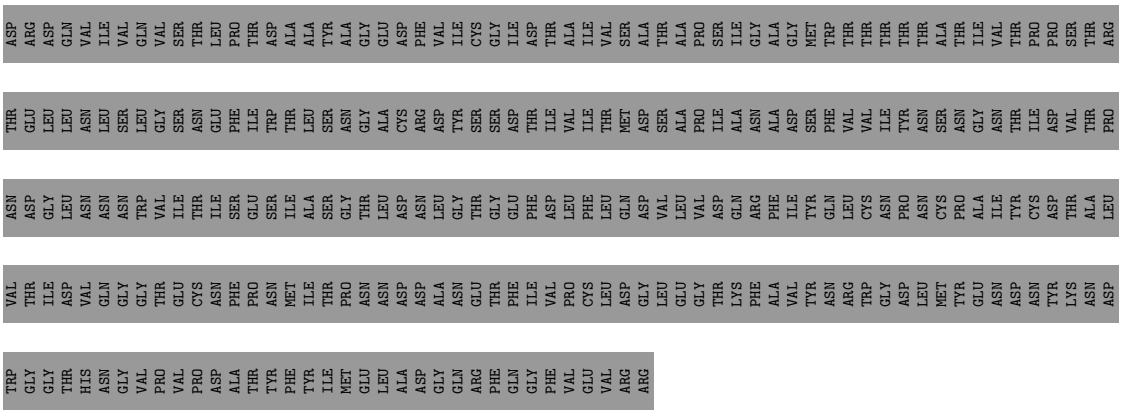
VAL THR PRO VAL ASP PRO ASN SER LEU VAL VAL ASN ILE ALA GLU ASP THR THR THR TYR TYR TRP THR LEU SER ASN GLY ALA CYS VAL ASP TYR SER VAL ASP SER VAL THR VAL ILE ILE SER PRO ALA SER THR ASP LEU ALA PHE ALA GLY TYR ASP GLU VAL LEU CYS GLY VAL

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 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

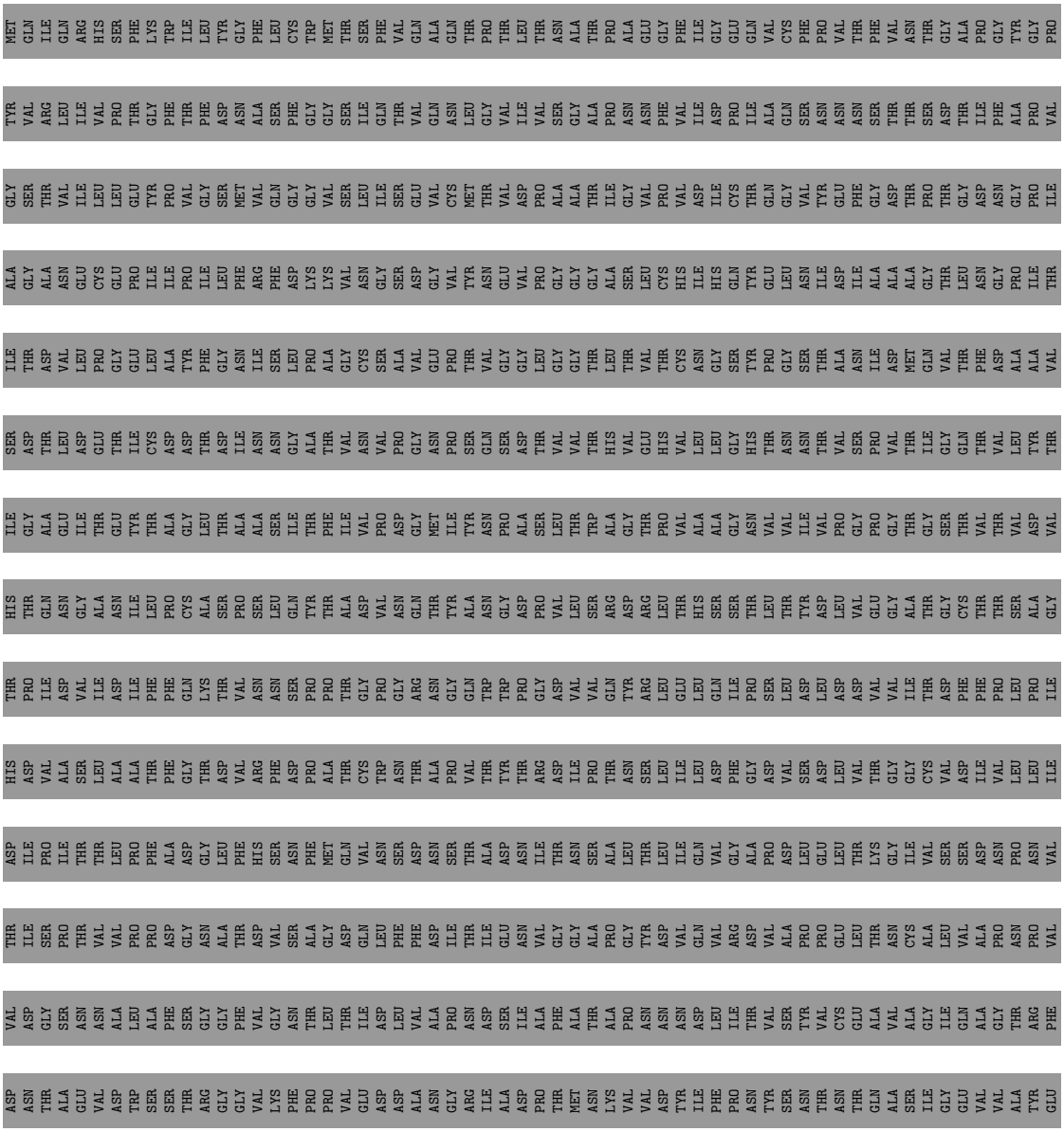
LEU SER ASN SER ASN ILE VAL ASN ILE PRO THR ASP THR VAL ALA PHE TYR TRP SER LEU SER ASN GLY SER CYS ALA ASP TYR SER ILE ASP THR MET LEU ILE ILE VAL THR PRO THR PHE SER VAL ASP THR ALA ASN ALA GLY LEU ASP ILE ASN LEU CYS ASN GLU ASP THR ALA

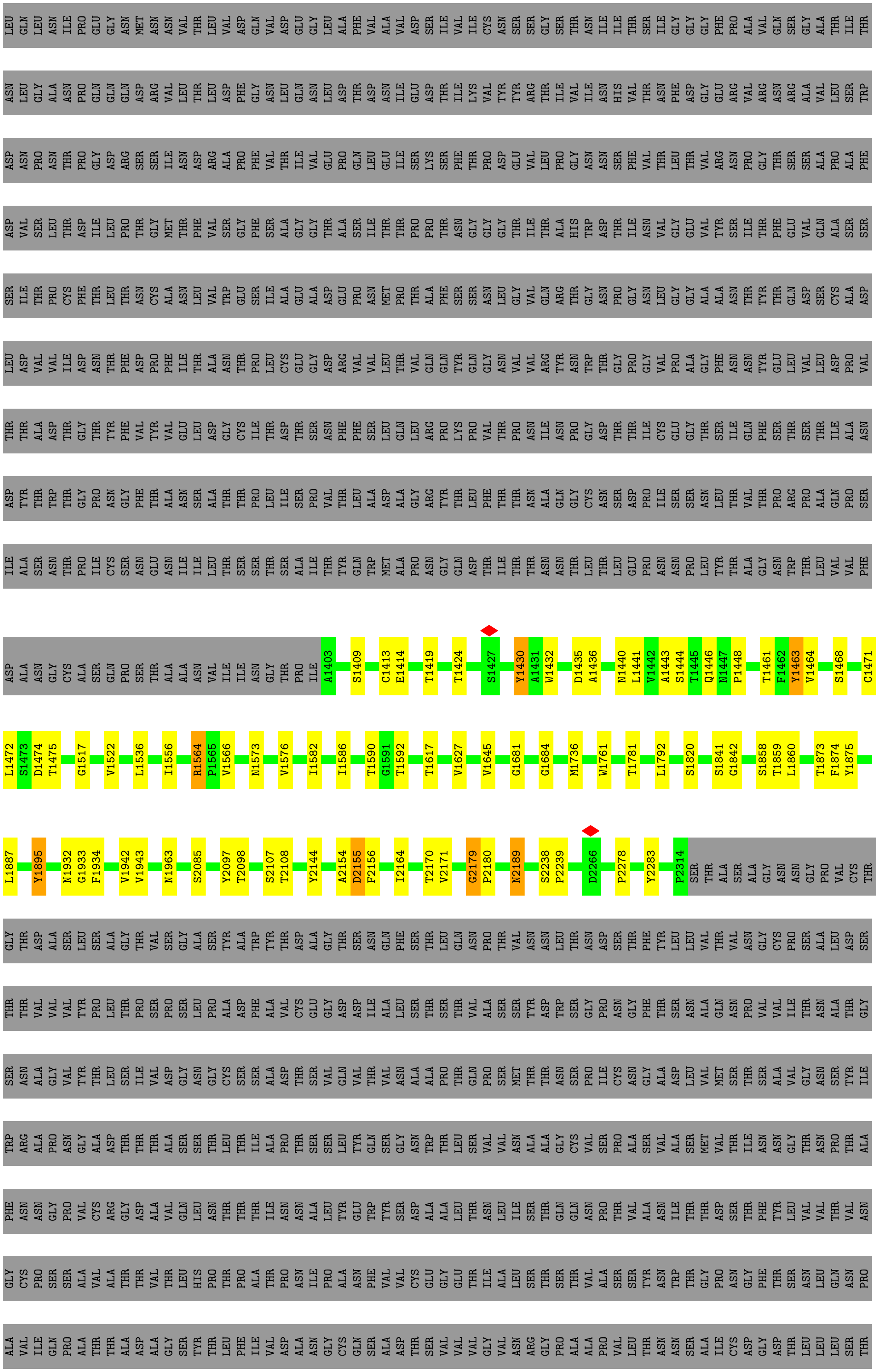
GLN LEU MET ALA ILE ALA PRO ASN VAL ALA THR GLY ARG TRP THR GLN PRO PHE ASN GLN SER SER ALA GLY VAL VAL ILE THR ASP PRO ASN ALA ALA MET THR THR ALA THR GLY LEU GLN LEU ASP SER THR TYR THR PHE THR TRP SER VAL SER ASN GLY PRO CYS ARG ASP TYR



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

Chain F: 14% • 85%

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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
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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
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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 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 A1403 S1409 C1413 E1414 T1419 T1424 S1427 Y1430 A1431 W1432 D1435 A1436 N1440 L1441 V1442 A1443 S1444 T1445 Q1446 N1447 P1448 T1461 F1462 Y1463 V1464 S1468 C1471
L1472 S1473 D1474 T1475 G1517 V1522 L1536 I1556 R1564 P1565 V1566 N1573 V1576 I1582 I1586 T1590 G1591 T1592 T1617 V1627 V1645 G1681 G1684 M1736 W1761 T1781 L1792 S1820 S1841 G1842 S1858 T1859 L1860 T1873 F1874 Y1875
L1887 Y1895 N1932 G1933 F1934 V1942 V1943 N1963 S2085 Y2097 T2098 S2107 T2108 Y2144 A2154 D2155 F2156 I2164 T2170 V2171 G2179 P2180 N2189 S2238 P2239 D2266 P2278 Y2283 P2314 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 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 VAL ALA ASN ILE THR THR ASP SER THR PHE TYR LEU VAL VAL THR VAL ASN
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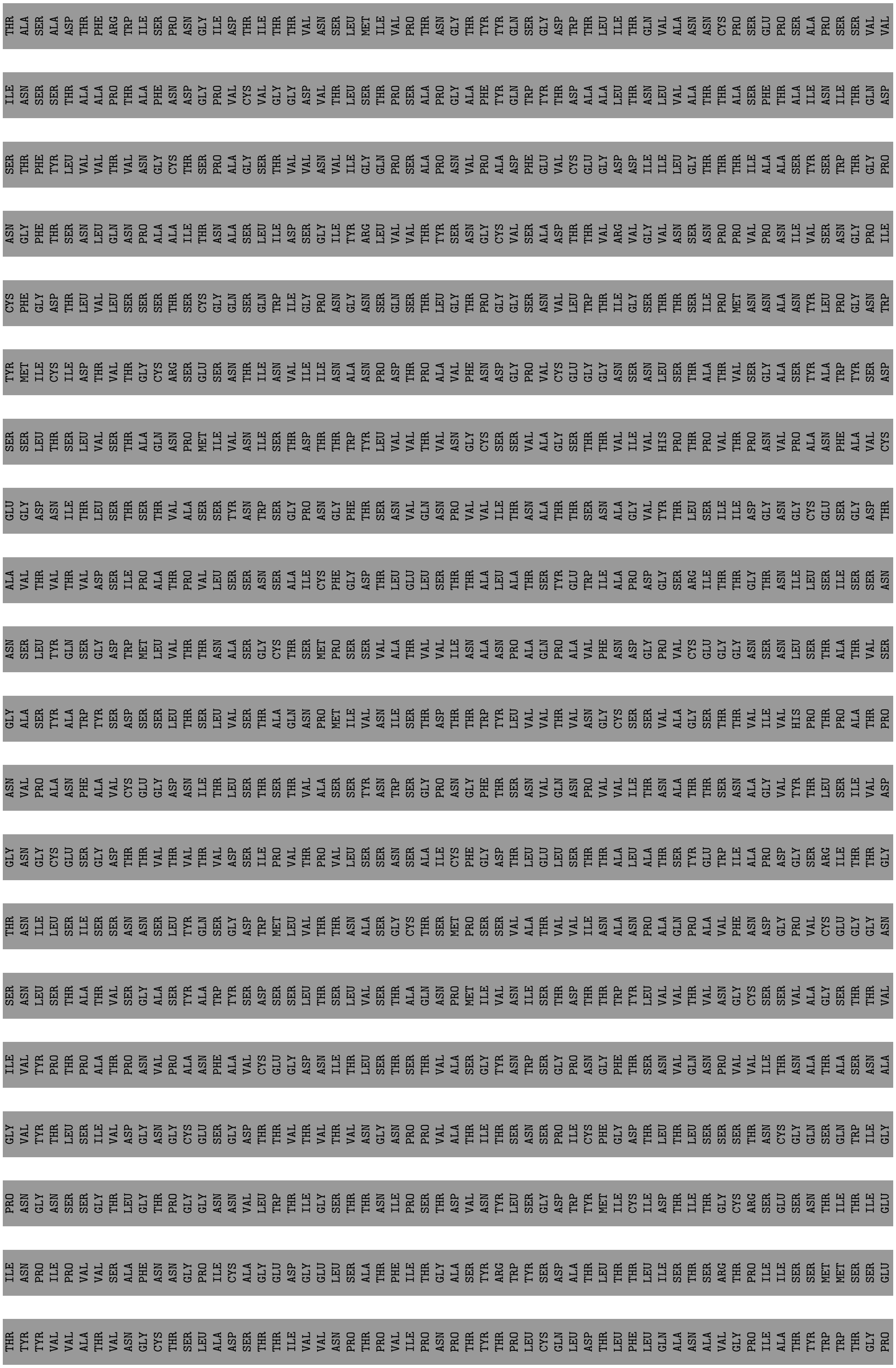
ALA VAL ILE GLN PRO ALA THR THR ALA ASP ALA GLY SER TYR THR LEU PHE ILE VAL ASP ALA ASN GLY CYS GLN SER ALA ASP THR SER VAL VAL VAL GLY VAL ASN ARG GLY PRO ALA ALA PRO VAL LEU THR ASN ASN SER ALA ILE CYS ASP GLY ASP THR LEU LEU LEU SER THR


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

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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

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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

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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 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

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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

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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

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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 in the bacterium Aureispira sp. CCB-QB1

Chain G: 14% • 85%

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 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

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 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 A1403 S1409 C1413 E1414 T1419 T1424 S1427 Y1430 A1431 W1432 D1435 A1436 N1440 L1441 V1442 A1443 S1444 T1445 Q1446 N1447 P1448 T1461 F1462 Y1463 V1464 S1468 C1471

L1472 S1473 D1474 T1475 N1485 P1486 G1517 V1522 L1536 I1556 R1564 P1565 V1566 N1573 V1576 I1582 I1586 T1590 G1591 T1592 T1617 V1627 V1645 G1681 G1684 M1736 W1761 T1781 L1792 S1820 C1828 T1829 S1841 G1842 S1858 T1859

L1860
T1873
F1874
Y1875
L1887
Y1895
T1921
V1922
N1932
G1933
F1934
V1942
V1943
N1963
A2068
S2069
S2085
Y2097
T2098
S2107
T2108
Y2144
A2154
D2155
F2156
I2164
T2170
V2171
G2179
P2180
N2189
S2238
P2239
D2266
P2278
Y2283
P2314
SER

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

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

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

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

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

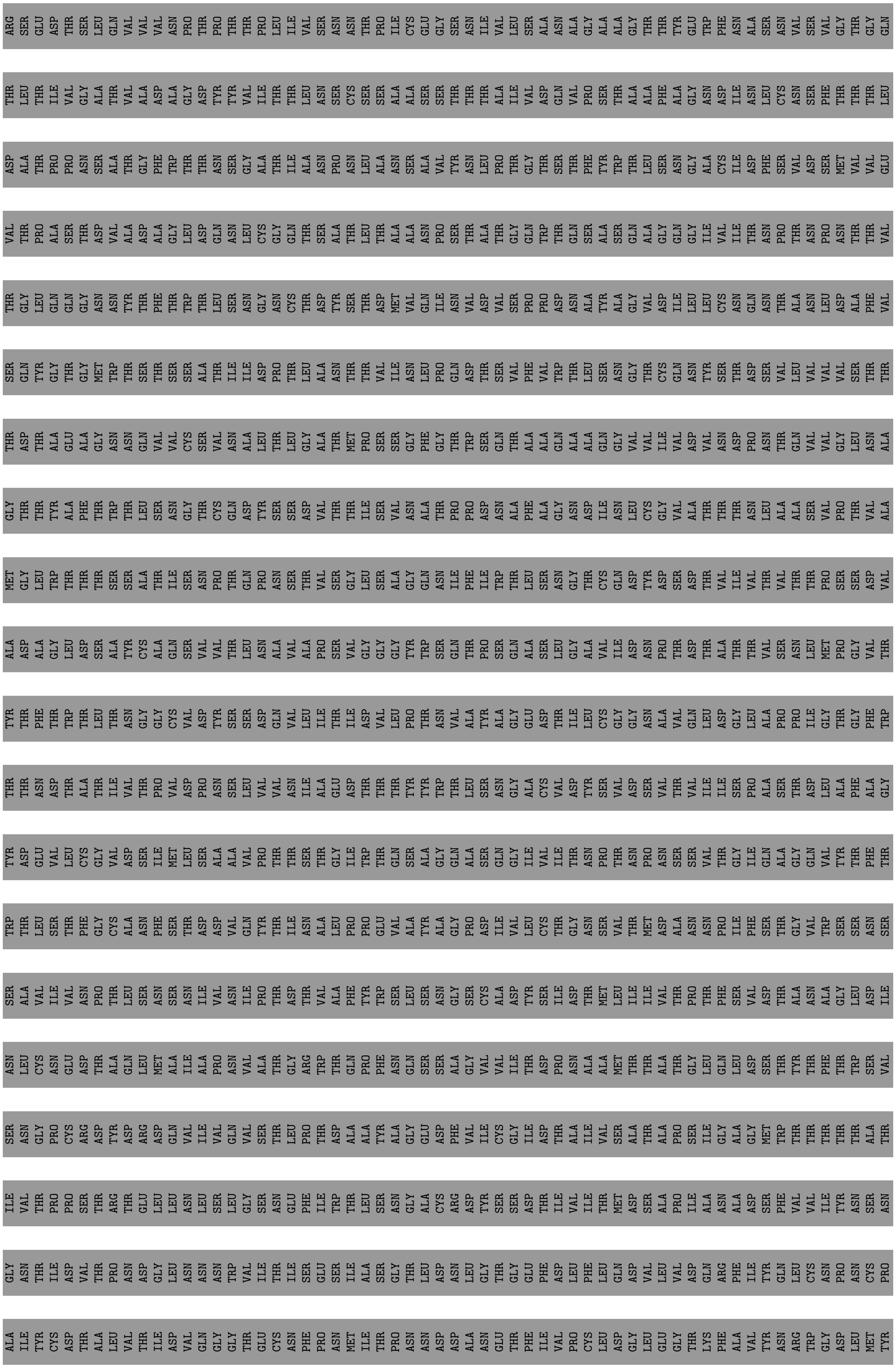
ASN ILE VAL LEU SER THR THR THR VAL ALA ALA GLY TYR ASN TRP THR GLY PRO ASN GLY PHE THR SER ASN LEU GLN ASN PRO SER VAL VAL SER ALA SER LEU VAL ASP SER GLY THR TYR THR LEU PHE ILE ILE ASP ALA ASN GLY CYS PRO SER GLY ASP THR SER VAL GLN VAL

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 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 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 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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	12450	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	4.938	Depositor
Minimum map value	-1.914	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.097	Depositor
Recommended contour level	1	Depositor
Map size (Å)	920.16, 920.16, 920.16	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.704, 1.704, 1.704	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	0.87	0/6579	1.08	20/9107 (0.2%)
1	B	0.87	0/6579	1.08	20/9107 (0.2%)
1	C	0.87	0/6579	1.08	20/9107 (0.2%)
1	D	0.87	0/6579	1.08	20/9107 (0.2%)
1	E	0.87	0/6579	1.08	20/9107 (0.2%)
1	F	0.87	0/6579	1.08	20/9107 (0.2%)
1	G	0.87	0/6579	1.08	20/9107 (0.2%)
All	All	0.87	0/46053	1.08	140/63749 (0.2%)

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 (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	2097	TYR	N-CA-CB	-7.36	97.97	111.37
1	G	2097	TYR	N-CA-CB	-7.36	97.97	111.37
1	D	2097	TYR	N-CA-CB	-7.35	97.99	111.37
1	A	2097	TYR	N-CA-CB	-7.35	98.00	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2097	TYR	N-CA-CB	-7.35	97.99	111.37
1	E	2097	TYR	N-CA-CB	-7.35	98.00	111.37
1	B	2097	TYR	N-CA-CB	-7.34	98.01	111.37
1	G	1781	THR	N-CA-C	-7.20	105.42	114.56
1	E	1781	THR	N-CA-C	-7.19	105.43	114.56
1	B	1781	THR	N-CA-C	-7.18	105.44	114.56
1	C	1781	THR	N-CA-C	-7.18	105.44	114.56
1	D	1781	THR	N-CA-C	-7.18	105.45	114.56
1	A	1781	THR	N-CA-C	-7.17	105.45	114.56
1	F	1781	THR	N-CA-C	-7.16	105.47	114.56
1	G	2144	TYR	N-CA-CB	6.57	119.95	110.03
1	F	2144	TYR	N-CA-CB	6.55	119.93	110.03
1	D	2144	TYR	N-CA-CB	6.55	119.92	110.03
1	A	2144	TYR	N-CA-CB	6.55	119.92	110.03
1	C	2144	TYR	N-CA-CB	6.55	119.91	110.03
1	B	2144	TYR	N-CA-CB	6.54	119.91	110.03
1	E	2144	TYR	N-CA-CB	6.53	119.89	110.03
1	D	2179	GLY	CA-C-N	6.43	126.65	119.32
1	D	2179	GLY	C-N-CA	6.43	126.65	119.32
1	B	2179	GLY	CA-C-N	6.42	126.64	119.32
1	B	2179	GLY	C-N-CA	6.42	126.64	119.32
1	C	2179	GLY	CA-C-N	6.42	126.64	119.32
1	C	2179	GLY	C-N-CA	6.42	126.64	119.32
1	G	2179	GLY	CA-C-N	6.41	126.63	119.32
1	G	2179	GLY	C-N-CA	6.41	126.63	119.32
1	A	2179	GLY	CA-C-N	6.41	126.63	119.32
1	A	2179	GLY	C-N-CA	6.41	126.63	119.32
1	E	2179	GLY	CA-C-N	6.39	126.61	119.32
1	E	2179	GLY	C-N-CA	6.39	126.61	119.32
1	F	2179	GLY	CA-C-N	6.39	126.61	119.32
1	F	2179	GLY	C-N-CA	6.39	126.61	119.32
1	D	1681	GLY	CA-C-N	6.37	126.86	119.47
1	D	1681	GLY	C-N-CA	6.37	126.86	119.47
1	B	1681	GLY	CA-C-N	6.36	126.85	119.47
1	B	1681	GLY	C-N-CA	6.36	126.85	119.47
1	E	1681	GLY	CA-C-N	6.36	126.85	119.47
1	E	1681	GLY	C-N-CA	6.36	126.85	119.47
1	A	1681	GLY	CA-C-N	6.36	126.84	119.47
1	A	1681	GLY	C-N-CA	6.36	126.84	119.47
1	E	1463	TYR	CB-CA-C	6.35	121.00	109.37
1	A	1463	TYR	CB-CA-C	6.35	120.99	109.37
1	B	1463	TYR	CB-CA-C	6.35	120.99	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1681	GLY	CA-C-N	6.35	126.83	119.47
1	C	1681	GLY	C-N-CA	6.35	126.83	119.47
1	F	1681	GLY	CA-C-N	6.35	126.83	119.47
1	F	1681	GLY	C-N-CA	6.35	126.83	119.47
1	G	1463	TYR	CB-CA-C	6.34	120.98	109.37
1	F	1463	TYR	CB-CA-C	6.34	120.98	109.37
1	D	1463	TYR	CB-CA-C	6.34	120.97	109.37
1	C	1463	TYR	CB-CA-C	6.33	120.95	109.37
1	G	1681	GLY	CA-C-N	6.32	126.81	119.47
1	G	1681	GLY	C-N-CA	6.32	126.81	119.47
1	D	2155	ASP	CA-C-N	-6.28	111.65	123.27
1	D	2155	ASP	C-N-CA	-6.28	111.65	123.27
1	E	2155	ASP	CA-C-N	-6.27	111.67	123.27
1	E	2155	ASP	C-N-CA	-6.27	111.67	123.27
1	C	2155	ASP	CA-C-N	-6.27	111.67	123.27
1	C	2155	ASP	C-N-CA	-6.27	111.67	123.27
1	F	2155	ASP	CA-C-N	-6.26	111.68	123.27
1	F	2155	ASP	C-N-CA	-6.26	111.68	123.27
1	G	2155	ASP	CA-C-N	-6.26	111.68	123.27
1	G	2155	ASP	C-N-CA	-6.26	111.68	123.27
1	A	2155	ASP	CA-C-N	-6.26	111.69	123.27
1	A	2155	ASP	C-N-CA	-6.26	111.69	123.27
1	B	2155	ASP	CA-C-N	-6.25	111.70	123.27
1	B	2155	ASP	C-N-CA	-6.25	111.70	123.27
1	F	1517	GLY	CA-C-N	6.12	126.58	119.47
1	F	1517	GLY	C-N-CA	6.12	126.58	119.47
1	G	1517	GLY	CA-C-N	6.12	126.56	119.47
1	G	1517	GLY	C-N-CA	6.12	126.56	119.47
1	C	1517	GLY	CA-C-N	6.11	126.56	119.47
1	C	1517	GLY	C-N-CA	6.11	126.56	119.47
1	B	1517	GLY	CA-C-N	6.10	126.55	119.47
1	B	1517	GLY	C-N-CA	6.10	126.55	119.47
1	E	1517	GLY	CA-C-N	6.10	126.54	119.47
1	E	1517	GLY	C-N-CA	6.10	126.54	119.47
1	A	1517	GLY	CA-C-N	6.09	126.54	119.47
1	A	1517	GLY	C-N-CA	6.09	126.54	119.47
1	D	1517	GLY	CA-C-N	6.07	126.51	119.47
1	D	1517	GLY	C-N-CA	6.07	126.51	119.47
1	E	2144	TYR	CB-CA-C	-5.89	99.79	109.46
1	G	2144	TYR	CB-CA-C	-5.89	99.80	109.46
1	D	2144	TYR	CB-CA-C	-5.89	99.80	109.46
1	A	2144	TYR	CB-CA-C	-5.89	99.81	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2144	TYR	CB-CA-C	-5.89	99.81	109.46
1	B	2144	TYR	CB-CA-C	-5.88	99.81	109.46
1	F	2144	TYR	CB-CA-C	-5.88	99.82	109.46
1	E	2189	ASN	CA-C-N	5.82	126.15	119.92
1	E	2189	ASN	C-N-CA	5.82	126.15	119.92
1	G	1430	TYR	N-CA-CB	-5.81	101.79	111.20
1	C	2189	ASN	CA-C-N	5.80	126.13	119.92
1	C	2189	ASN	C-N-CA	5.80	126.13	119.92
1	B	1430	TYR	N-CA-CB	-5.80	101.81	111.20
1	E	1430	TYR	N-CA-CB	-5.80	101.81	111.20
1	A	1430	TYR	N-CA-CB	-5.79	101.82	111.20
1	C	1430	TYR	N-CA-CB	-5.79	101.82	111.20
1	F	1430	TYR	N-CA-CB	-5.79	101.83	111.20
1	C	1895	TYR	N-CA-CB	5.78	118.55	110.11
1	B	1895	TYR	N-CA-CB	5.78	118.55	110.11
1	D	1430	TYR	N-CA-CB	-5.78	101.83	111.20
1	B	2189	ASN	CA-C-N	5.78	126.10	119.92
1	B	2189	ASN	C-N-CA	5.78	126.10	119.92
1	A	2189	ASN	CA-C-N	5.77	126.09	119.92
1	A	2189	ASN	C-N-CA	5.77	126.09	119.92
1	G	2189	ASN	CA-C-N	5.77	126.09	119.92
1	G	2189	ASN	C-N-CA	5.77	126.09	119.92
1	A	1895	TYR	N-CA-CB	5.76	118.52	110.11
1	F	1895	TYR	N-CA-CB	5.76	118.52	110.11
1	D	2189	ASN	CA-C-N	5.76	126.08	119.92
1	D	2189	ASN	C-N-CA	5.76	126.08	119.92
1	E	1895	TYR	N-CA-CB	5.76	118.52	110.11
1	F	2189	ASN	CA-C-N	5.75	126.07	119.92
1	F	2189	ASN	C-N-CA	5.75	126.07	119.92
1	G	1895	TYR	N-CA-CB	5.75	118.50	110.11
1	D	1895	TYR	N-CA-CB	5.74	118.48	110.11
1	C	2085	SER	N-CA-C	5.15	116.57	107.61
1	D	2085	SER	N-CA-C	5.15	116.57	107.61
1	A	2085	SER	N-CA-C	5.14	116.56	107.61
1	B	2085	SER	N-CA-C	5.14	116.55	107.61
1	E	2085	SER	N-CA-C	5.13	116.55	107.61
1	F	2085	SER	N-CA-C	5.13	116.53	107.61
1	G	2085	SER	N-CA-C	5.11	116.50	107.61
1	E	2098	THR	CB-CA-C	-5.09	99.34	109.99
1	C	2098	THR	CB-CA-C	-5.09	99.35	109.99
1	F	2098	THR	CB-CA-C	-5.08	99.37	109.99
1	G	1684	GLY	N-CA-C	-5.08	108.27	115.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2098	THR	CB-CA-C	-5.08	99.37	109.99
1	B	2098	THR	CB-CA-C	-5.08	99.38	109.99
1	G	2098	THR	CB-CA-C	-5.08	99.38	109.99
1	C	1684	GLY	N-CA-C	-5.07	108.28	115.43
1	D	2098	THR	CB-CA-C	-5.07	99.39	109.99
1	D	1684	GLY	N-CA-C	-5.06	108.29	115.43
1	F	1684	GLY	N-CA-C	-5.06	108.30	115.43
1	A	1684	GLY	N-CA-C	-5.05	108.31	115.43
1	E	1684	GLY	N-CA-C	-5.05	108.31	115.43
1	B	1684	GLY	N-CA-C	-5.04	108.32	115.43

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1564	ARG	Sidechain
1	B	1564	ARG	Sidechain
1	C	1564	ARG	Sidechain
1	D	1564	ARG	Sidechain
1	E	1564	ARG	Sidechain
1	F	1564	ARG	Sidechain
1	G	1564	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	6443	0	6100	100	0
1	B	6443	0	6100	108	0
1	C	6443	0	6100	103	0
1	D	6443	0	6100	103	0
1	E	6443	0	6100	106	0
1	F	6443	0	6100	101	0
1	G	6443	0	6100	102	0
All	All	45101	0	42700	554	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 6.

All (554) 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:B:1576:VAL:CG2	1:B:1645:VAL:HG22	1.73	1.18
1:F:1576:VAL:CG2	1:F:1645:VAL:HG22	1.73	1.17
1:C:1576:VAL:CG2	1:C:1645:VAL:HG22	1.73	1.17
1:E:1576:VAL:CG2	1:E:1645:VAL:HG22	1.73	1.17
1:G:1576:VAL:CG2	1:G:1645:VAL:HG22	1.73	1.17
1:D:1576:VAL:CG2	1:D:1645:VAL:HG22	1.73	1.16
1:A:1576:VAL:CG2	1:A:1645:VAL:HG22	1.73	1.16
1:C:1820:SER:HB2	1:D:1860:LEU:HD21	1.36	1.08
1:F:1566:VAL:HG13	1:G:1590:THR:HG21	1.35	1.08
1:F:1942:VAL:HG22	1:G:1932:ASN:O	1.51	1.08
1:B:1820:SER:HB2	1:C:1860:LEU:HD21	1.37	1.07
1:D:1942:VAL:HG22	1:E:1932:ASN:O	1.55	1.06
1:A:1820:SER:HB2	1:B:1860:LEU:HD21	1.36	1.06
1:A:1590:THR:HG21	1:G:1566:VAL:HG13	1.37	1.06
1:B:1566:VAL:HG13	1:C:1590:THR:HG21	1.38	1.05
1:A:1566:VAL:HG13	1:B:1590:THR:HG21	1.38	1.05
1:A:1932:ASN:O	1:G:1942:VAL:HG22	1.53	1.05
1:D:1566:VAL:HG13	1:E:1590:THR:HG21	1.38	1.05
1:D:1820:SER:HB2	1:E:1860:LEU:HD21	1.37	1.05
1:E:1566:VAL:HG13	1:F:1590:THR:HG21	1.39	1.04
1:E:1820:SER:HB2	1:F:1860:LEU:HD21	1.38	1.03
1:C:1942:VAL:HG22	1:D:1932:ASN:O	1.57	1.03
1:E:1942:VAL:HG22	1:F:1932:ASN:O	1.58	1.03
1:C:1566:VAL:HG13	1:D:1590:THR:HG21	1.41	1.03
1:A:2238:SER:HB2	1:A:2239:PRO:HD2	1.41	1.03
1:F:2238:SER:HB2	1:F:2239:PRO:HD2	1.41	1.02
1:G:2238:SER:HB2	1:G:2239:PRO:HD2	1.41	1.02
1:A:1860:LEU:HD21	1:G:1820:SER:HB2	1.38	1.02
1:B:1942:VAL:HG22	1:C:1932:ASN:O	1.55	1.02
1:C:2238:SER:HB2	1:C:2239:PRO:HD2	1.41	1.02
1:B:2238:SER:HB2	1:B:2239:PRO:HD2	1.41	1.02
1:D:2238:SER:HB2	1:D:2239:PRO:HD2	1.41	1.02
1:E:2238:SER:HB2	1:E:2239:PRO:HD2	1.41	1.02
1:A:1942:VAL:HG22	1:B:1932:ASN:O	1.57	1.01
1:D:1564:ARG:NH2	1:E:1592:THR:HA	1.77	1.00
1:F:1564:ARG:NH2	1:G:1592:THR:HA	1.77	1.00
1:B:1564:ARG:NH2	1:C:1592:THR:HA	1.77	0.99
1:A:1592:THR:HA	1:G:1564:ARG:NH2	1.78	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1820:SER:HB2	1:G:1860:LEU:HD21	1.43	0.97
1:C:1564:ARG:NH2	1:D:1592:THR:HA	1.80	0.97
1:A:1564:ARG:NH2	1:B:1592:THR:HA	1.79	0.96
1:E:1564:ARG:NH2	1:F:1592:THR:HA	1.81	0.96
1:C:1820:SER:HB2	1:D:1860:LEU:CD2	1.99	0.93
1:B:1820:SER:HB2	1:C:1860:LEU:CD2	1.99	0.92
1:D:1820:SER:HB2	1:E:1860:LEU:CD2	1.99	0.92
1:A:1820:SER:HB2	1:B:1860:LEU:CD2	1.99	0.92
1:E:1736:MET:CE	1:E:1792:LEU:HB2	2.01	0.91
1:G:1736:MET:CE	1:G:1792:LEU:HB2	2.01	0.91
1:B:1736:MET:CE	1:B:1792:LEU:HB2	2.01	0.90
1:C:1736:MET:CE	1:C:1792:LEU:HB2	2.01	0.90
1:D:1736:MET:CE	1:D:1792:LEU:HB2	2.01	0.90
1:A:1736:MET:CE	1:A:1792:LEU:HB2	2.01	0.90
1:A:1860:LEU:CD2	1:G:1820:SER:HB2	2.00	0.90
1:E:1820:SER:HB2	1:F:1860:LEU:CD2	2.02	0.89
1:F:1736:MET:CE	1:F:1792:LEU:HB2	2.01	0.89
1:D:1564:ARG:HH21	1:E:1592:THR:HA	1.39	0.85
1:F:1564:ARG:HH21	1:G:1592:THR:HA	1.36	0.85
1:A:1592:THR:HA	1:G:1564:ARG:HH21	1.38	0.85
1:B:1564:ARG:HH21	1:C:1592:THR:HA	1.39	0.84
1:F:1820:SER:HB2	1:G:1860:LEU:CD2	2.06	0.84
1:A:1564:ARG:HH21	1:B:1592:THR:HA	1.40	0.83
1:C:1564:ARG:HH21	1:D:1592:THR:HA	1.42	0.83
1:E:1564:ARG:HH21	1:F:1592:THR:HA	1.41	0.82
1:E:1576:VAL:HG23	1:E:1645:VAL:HG22	1.63	0.81
1:D:1576:VAL:HG23	1:D:1645:VAL:HG22	1.63	0.81
1:G:1576:VAL:HG23	1:G:1645:VAL:HG22	1.63	0.80
1:F:1566:VAL:HG13	1:G:1590:THR:CG2	2.09	0.80
1:G:2238:SER:CB	1:G:2239:PRO:HD2	2.09	0.79
1:F:1576:VAL:HG23	1:F:1645:VAL:HG22	1.63	0.79
1:A:1590:THR:CG2	1:G:1566:VAL:HG13	2.11	0.79
1:A:2238:SER:CB	1:A:2239:PRO:HD2	2.09	0.79
1:B:1566:VAL:HG13	1:C:1590:THR:CG2	2.12	0.79
1:F:2238:SER:CB	1:F:2239:PRO:HD2	2.09	0.79
1:F:1576:VAL:HG22	1:F:1645:VAL:HG22	1.65	0.79
1:E:1576:VAL:HG22	1:E:1645:VAL:HG22	1.65	0.78
1:G:1576:VAL:HG22	1:G:1645:VAL:HG22	1.65	0.78
1:B:1576:VAL:HG23	1:B:1645:VAL:HG22	1.63	0.78
1:D:1566:VAL:HG13	1:E:1590:THR:CG2	2.12	0.78
1:A:1566:VAL:HG13	1:B:1590:THR:CG2	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1576:VAL:HG22	1:A:1645:VAL:HG22	1.65	0.77
1:B:2238:SER:CB	1:B:2239:PRO:HD2	2.09	0.77
1:C:1576:VAL:HG23	1:C:1645:VAL:HG22	1.63	0.77
1:A:1576:VAL:HG23	1:A:1645:VAL:HG22	1.63	0.77
1:D:1576:VAL:HG22	1:D:1645:VAL:HG22	1.65	0.77
1:E:1461:THR:HG22	1:E:1463:TYR:CE1	2.21	0.76
1:E:2238:SER:CB	1:E:2239:PRO:HD2	2.09	0.76
1:B:1461:THR:HG22	1:B:1463:TYR:CE1	2.21	0.76
1:F:1461:THR:HG22	1:F:1463:TYR:CE1	2.21	0.76
1:C:2238:SER:CB	1:C:2239:PRO:HD2	2.09	0.76
1:G:1461:THR:HG22	1:G:1463:TYR:CE1	2.21	0.76
1:D:1461:THR:HG22	1:D:1463:TYR:CE1	2.21	0.76
1:E:1566:VAL:HG13	1:F:1590:THR:CG2	2.14	0.76
1:C:1566:VAL:HG13	1:D:1590:THR:CG2	2.15	0.75
1:A:1461:THR:HG22	1:A:1463:TYR:CE1	2.21	0.75
1:C:1461:THR:HG22	1:C:1463:TYR:CE1	2.21	0.75
1:C:1576:VAL:HG22	1:C:1645:VAL:HG22	1.65	0.75
1:B:1576:VAL:HG22	1:B:1645:VAL:HG22	1.65	0.75
1:D:1820:SER:OG	1:E:1860:LEU:HG	1.87	0.75
1:A:1736:MET:HE3	1:A:1792:LEU:HB2	1.69	0.74
1:F:2189:ASN:HB3	1:G:2180:PRO:HA	1.69	0.74
1:A:2180:PRO:HA	1:G:2189:ASN:HB3	1.70	0.74
1:B:1820:SER:OG	1:C:1860:LEU:HG	1.87	0.74
1:A:1860:LEU:HG	1:G:1820:SER:OG	1.88	0.74
1:C:1736:MET:HE3	1:C:1792:LEU:HB2	1.68	0.74
1:E:1736:MET:HE3	1:E:1792:LEU:HB2	1.69	0.74
1:A:1820:SER:OG	1:B:1860:LEU:HG	1.88	0.74
1:F:1736:MET:HE3	1:F:1792:LEU:HB2	1.69	0.74
1:C:1820:SER:OG	1:D:1860:LEU:HG	1.87	0.73
1:D:1736:MET:HE3	1:D:1792:LEU:HB2	1.69	0.73
1:D:2189:ASN:HB3	1:E:2180:PRO:HA	1.70	0.73
1:D:2238:SER:CB	1:D:2239:PRO:HD2	2.09	0.73
1:G:1736:MET:HE3	1:G:1792:LEU:HB2	1.69	0.73
1:E:1820:SER:OG	1:F:1860:LEU:HG	1.89	0.73
1:B:1736:MET:HE3	1:B:1792:LEU:HB2	1.69	0.72
1:C:2189:ASN:HB3	1:D:2180:PRO:HA	1.72	0.72
1:B:2189:ASN:HB3	1:C:2180:PRO:HA	1.72	0.71
1:D:1820:SER:CB	1:E:1860:LEU:HG	2.20	0.71
1:A:1860:LEU:HG	1:G:1820:SER:CB	2.21	0.71
1:A:1932:ASN:O	1:G:1942:VAL:CG2	2.37	0.70
1:A:1820:SER:CB	1:B:1860:LEU:HG	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2189:ASN:HB3	1:B:2180:PRO:HA	1.74	0.70
1:B:1820:SER:CB	1:C:1860:LEU:HG	2.21	0.70
1:C:1820:SER:CB	1:D:1860:LEU:HG	2.21	0.70
1:F:1820:SER:OG	1:G:1860:LEU:HG	1.91	0.70
1:F:1564:ARG:HH21	1:G:1592:THR:CA	2.06	0.69
1:A:1436:ALA:HA	1:A:1463:TYR:CG	2.27	0.69
1:G:1436:ALA:HA	1:G:1463:TYR:CG	2.27	0.69
1:B:1436:ALA:HA	1:B:1463:TYR:CG	2.27	0.69
1:F:1436:ALA:HA	1:F:1463:TYR:CG	2.27	0.69
1:C:1436:ALA:HA	1:C:1463:TYR:CG	2.27	0.69
1:D:1436:ALA:HA	1:D:1463:TYR:CG	2.27	0.69
1:E:1436:ALA:HA	1:E:1463:TYR:CG	2.27	0.68
1:E:2189:ASN:HB3	1:F:2180:PRO:HA	1.75	0.68
1:D:1564:ARG:HH21	1:E:1592:THR:CA	2.06	0.68
1:C:1820:SER:CB	1:D:1860:LEU:CD2	2.72	0.67
1:F:1820:SER:CB	1:G:1860:LEU:HG	2.25	0.67
1:E:1820:SER:CB	1:F:1860:LEU:HG	2.24	0.67
1:B:1564:ARG:HH21	1:C:1592:THR:CA	2.06	0.67
1:D:1820:SER:CB	1:E:1860:LEU:CD2	2.73	0.67
1:D:1943:VAL:HG23	1:E:1932:ASN:OD1	1.96	0.66
1:A:1564:ARG:HH21	1:B:1592:THR:CA	2.08	0.66
1:A:1592:THR:CA	1:G:1564:ARG:HH21	2.07	0.66
1:A:1820:SER:CB	1:B:1860:LEU:CD2	2.73	0.66
1:F:1942:VAL:CG2	1:G:1932:ASN:O	2.35	0.66
1:A:1860:LEU:CD2	1:G:1820:SER:CB	2.74	0.65
1:B:1942:VAL:CG2	1:C:1932:ASN:O	2.39	0.65
1:C:1564:ARG:HH21	1:D:1592:THR:CA	2.10	0.65
1:C:1943:VAL:HG23	1:D:1932:ASN:OD1	1.97	0.65
1:B:1943:VAL:HG23	1:C:1932:ASN:OD1	1.97	0.65
1:D:1942:VAL:CG2	1:E:1932:ASN:O	2.38	0.65
1:A:1942:VAL:CG2	1:B:1932:ASN:O	2.41	0.65
1:A:1932:ASN:OD1	1:G:1943:VAL:HG23	1.95	0.64
1:C:1736:MET:HE2	1:C:1761:TRP:CZ3	2.32	0.64
1:E:1820:SER:CB	1:F:1860:LEU:CD2	2.74	0.64
1:B:1522:VAL:O	1:C:1556:ILE:HG21	1.96	0.64
1:B:1736:MET:HE2	1:B:1761:TRP:CZ3	2.33	0.64
1:B:1820:SER:CB	1:C:1860:LEU:CD2	2.73	0.64
1:G:1736:MET:HE2	1:G:1761:TRP:CZ3	2.33	0.64
1:A:1556:ILE:HG21	1:G:1522:VAL:O	1.97	0.64
1:D:1522:VAL:O	1:E:1556:ILE:HG21	1.97	0.64
1:A:1943:VAL:HG23	1:B:1932:ASN:OD1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1942:VAL:CG2	1:D:1932:ASN:O	2.40	0.63
1:D:1736:MET:HE2	1:D:1761:TRP:CZ3	2.32	0.63
1:F:1736:MET:HE2	1:F:1761:TRP:CZ3	2.33	0.63
1:E:1736:MET:HE2	1:E:1761:TRP:CZ3	2.33	0.63
1:F:1573:ASN:HD21	1:F:1582:ILE:HA	1.64	0.63
1:A:1736:MET:HE2	1:A:1761:TRP:CZ3	2.33	0.63
1:C:1576:VAL:HG21	1:C:1645:VAL:HG22	1.76	0.63
1:G:1573:ASN:HD21	1:G:1582:ILE:HA	1.64	0.63
1:F:1576:VAL:HG21	1:F:1645:VAL:HG22	1.76	0.62
1:F:1736:MET:HE3	1:F:1792:LEU:CB	2.29	0.62
1:B:1573:ASN:HD21	1:B:1582:ILE:HA	1.64	0.62
1:E:1564:ARG:HH21	1:F:1592:THR:CA	2.10	0.62
1:D:1736:MET:HE3	1:D:1792:LEU:CB	2.29	0.62
1:G:1576:VAL:HG21	1:G:1645:VAL:HG22	1.76	0.62
1:D:1573:ASN:HD21	1:D:1582:ILE:HA	1.64	0.62
1:A:1522:VAL:O	1:B:1556:ILE:HG21	1.99	0.62
1:A:1573:ASN:HD21	1:A:1582:ILE:HA	1.64	0.62
1:E:1943:VAL:HG23	1:F:1932:ASN:OD1	2.00	0.62
1:E:1736:MET:HE3	1:E:1792:LEU:CB	2.29	0.61
1:C:1736:MET:HE3	1:C:1792:LEU:CB	2.29	0.61
1:E:1576:VAL:HG21	1:E:1645:VAL:HG22	1.76	0.61
1:C:1522:VAL:O	1:D:1556:ILE:HG21	1.99	0.61
1:F:1522:VAL:O	1:G:1556:ILE:HG21	1.99	0.61
1:C:1573:ASN:HD21	1:C:1582:ILE:HA	1.64	0.61
1:A:1576:VAL:HG21	1:A:1645:VAL:HG22	1.76	0.61
1:G:1736:MET:HE3	1:G:1792:LEU:CB	2.29	0.61
1:B:1576:VAL:HG21	1:B:1645:VAL:HG22	1.76	0.61
1:E:1573:ASN:HD21	1:E:1582:ILE:HA	1.64	0.61
1:A:1736:MET:HE3	1:A:1792:LEU:CB	2.29	0.61
1:B:1736:MET:HE3	1:B:1792:LEU:CB	2.30	0.61
1:F:1943:VAL:HG23	1:G:1932:ASN:OD1	2.00	0.61
1:E:1942:VAL:CG2	1:F:1932:ASN:O	2.42	0.60
1:A:1590:THR:HG21	1:G:1566:VAL:CG1	2.24	0.59
1:A:1424:THR:HG23	1:A:1446:GLN:HE22	1.68	0.59
1:D:1576:VAL:HG21	1:D:1645:VAL:HG22	1.76	0.59
1:A:1432:TRP:O	1:A:1441:LEU:HD22	2.03	0.59
1:C:1432:TRP:O	1:C:1441:LEU:HD22	2.03	0.59
1:F:1424:THR:HG23	1:F:1446:GLN:HE22	1.68	0.59
1:B:1424:THR:HG23	1:B:1446:GLN:HE22	1.68	0.59
1:B:1432:TRP:O	1:B:1441:LEU:HD22	2.03	0.58
1:C:1424:THR:HG23	1:C:1446:GLN:HE22	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2278:PRO:HA	1:A:2283:TYR:CD1	2.38	0.58
1:C:2278:PRO:HA	1:C:2283:TYR:CD1	2.39	0.58
1:E:1522:VAL:O	1:F:1556:ILE:HG21	2.02	0.58
1:D:1432:TRP:O	1:D:1441:LEU:HD22	2.03	0.58
1:E:2278:PRO:HA	1:E:2283:TYR:CD1	2.38	0.58
1:B:2278:PRO:HA	1:B:2283:TYR:CD1	2.38	0.58
1:D:2278:PRO:HA	1:D:2283:TYR:CD1	2.39	0.58
1:E:1432:TRP:O	1:E:1441:LEU:HD22	2.03	0.58
1:G:1432:TRP:O	1:G:1441:LEU:HD22	2.03	0.58
1:F:1432:TRP:O	1:F:1441:LEU:HD22	2.03	0.58
1:G:2278:PRO:HA	1:G:2283:TYR:CD1	2.38	0.58
1:D:1424:THR:HG23	1:D:1446:GLN:HE22	1.68	0.58
1:E:1424:THR:HG23	1:E:1446:GLN:HE22	1.68	0.58
1:C:1430:TYR:CE2	1:C:1446:GLN:HG3	2.39	0.58
1:F:1820:SER:CB	1:G:1860:LEU:CD2	2.80	0.58
1:G:1430:TYR:CE2	1:G:1446:GLN:HG3	2.39	0.58
1:G:1424:THR:HG23	1:G:1446:GLN:HE22	1.68	0.57
1:F:1430:TYR:CE2	1:F:1446:GLN:HG3	2.39	0.57
1:F:2278:PRO:HA	1:F:2283:TYR:CD1	2.39	0.57
1:D:1820:SER:CB	1:E:1860:LEU:CG	2.83	0.57
1:E:1430:TYR:CE2	1:E:1446:GLN:HG3	2.39	0.57
1:A:1430:TYR:CE2	1:A:1446:GLN:HG3	2.39	0.57
1:B:1430:TYR:CE2	1:B:1446:GLN:HG3	2.39	0.57
1:C:1820:SER:CB	1:D:1860:LEU:CG	2.83	0.57
1:E:1436:ALA:HA	1:E:1463:TYR:CD2	2.41	0.56
1:C:1436:ALA:HA	1:C:1463:TYR:CD2	2.41	0.56
1:D:1436:ALA:HA	1:D:1463:TYR:CD2	2.41	0.56
1:D:1430:TYR:CE2	1:D:1446:GLN:HG3	2.39	0.56
1:F:1436:ALA:HA	1:F:1463:TYR:CD2	2.41	0.56
1:B:1820:SER:CB	1:C:1860:LEU:CG	2.83	0.56
1:B:1436:ALA:HA	1:B:1463:TYR:CD2	2.41	0.56
1:A:1860:LEU:CG	1:G:1820:SER:CB	2.84	0.55
1:G:1436:ALA:HA	1:G:1463:TYR:CD2	2.41	0.55
1:A:1820:SER:CB	1:B:1860:LEU:CG	2.84	0.55
1:C:1820:SER:CB	1:D:1860:LEU:HD21	2.24	0.55
1:D:1564:ARG:HH22	1:E:1592:THR:HA	1.67	0.55
1:C:1566:VAL:CG1	1:D:1590:THR:HG21	2.28	0.55
1:A:1436:ALA:HA	1:A:1463:TYR:CD2	2.41	0.55
1:F:2189:ASN:CB	1:G:2180:PRO:HA	2.37	0.55
1:A:2180:PRO:HA	1:G:2189:ASN:CB	2.37	0.55
1:F:1564:ARG:HH22	1:G:1592:THR:HA	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1736:MET:HE1	1:G:1792:LEU:HB2	1.89	0.55
1:D:1586:ILE:HD11	1:D:1627:VAL:HG21	1.90	0.54
1:F:1586:ILE:HD11	1:F:1627:VAL:HG21	1.90	0.54
1:B:1564:ARG:HH22	1:C:1592:THR:HA	1.68	0.54
1:D:2189:ASN:CB	1:E:2180:PRO:HA	2.37	0.54
1:E:1586:ILE:HD11	1:E:1627:VAL:HG21	1.90	0.54
1:G:1586:ILE:HD11	1:G:1627:VAL:HG21	1.90	0.54
1:C:1586:ILE:HD11	1:C:1627:VAL:HG21	1.90	0.54
1:F:1566:VAL:CG1	1:G:1590:THR:HG21	2.23	0.54
1:A:1586:ILE:HD11	1:A:1627:VAL:HG21	1.90	0.53
1:A:1592:THR:HA	1:G:1564:ARG:HH22	1.69	0.53
1:A:1736:MET:HE1	1:A:1792:LEU:HB2	1.89	0.53
1:A:1566:VAL:CG1	1:B:1590:THR:HG21	2.26	0.53
1:C:2189:ASN:CB	1:D:2180:PRO:HA	2.38	0.53
1:G:1875:TYR:HB3	1:G:1887:LEU:HD11	1.90	0.53
1:B:1875:TYR:HB3	1:B:1887:LEU:HD11	1.90	0.53
1:E:1820:SER:CB	1:F:1860:LEU:CG	2.86	0.53
1:A:1875:TYR:HB3	1:A:1887:LEU:HD11	1.90	0.53
1:B:1586:ILE:HD11	1:B:1627:VAL:HG21	1.90	0.53
1:B:1736:MET:HE1	1:B:1792:LEU:HB2	1.89	0.53
1:C:1875:TYR:HB3	1:C:1887:LEU:HD11	1.90	0.53
1:F:1875:TYR:HB3	1:F:1887:LEU:HD11	1.90	0.53
1:B:1566:VAL:CG1	1:C:1590:THR:HG21	2.25	0.52
1:D:1875:TYR:HB3	1:D:1887:LEU:HD11	1.90	0.52
1:G:1472:LEU:HD23	1:G:1472:LEU:H	1.75	0.52
1:B:1820:SER:CB	1:C:1860:LEU:HD21	2.26	0.52
1:D:1736:MET:HE1	1:D:1792:LEU:HB2	1.89	0.52
1:A:1564:ARG:HH22	1:B:1592:THR:HA	1.70	0.52
1:E:1736:MET:HE1	1:E:1792:LEU:HB2	1.89	0.52
1:B:1472:LEU:HD23	1:B:1472:LEU:H	1.74	0.52
1:B:2189:ASN:CB	1:C:2180:PRO:HA	2.39	0.52
1:D:1566:VAL:CG1	1:E:1590:THR:HG21	2.25	0.52
1:F:1472:LEU:H	1:F:1472:LEU:HD23	1.74	0.52
1:C:1736:MET:HE1	1:C:1792:LEU:HB2	1.89	0.51
1:D:2278:PRO:HA	1:D:2283:TYR:CE1	2.46	0.51
1:E:1566:VAL:CG1	1:F:1590:THR:HG21	2.27	0.51
1:G:2278:PRO:HA	1:G:2283:TYR:CE1	2.46	0.51
1:F:2278:PRO:HA	1:F:2283:TYR:CE1	2.46	0.51
1:C:1472:LEU:H	1:C:1472:LEU:HD23	1.75	0.51
1:D:1472:LEU:HD23	1:D:1472:LEU:H	1.74	0.51
1:E:1875:TYR:HB3	1:E:1887:LEU:HD11	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2278:PRO:HA	1:E:2283:TYR:CE1	2.46	0.51
1:A:2189:ASN:HB3	1:B:2180:PRO:O	2.10	0.51
1:C:2278:PRO:HA	1:C:2283:TYR:CE1	2.46	0.51
1:E:1472:LEU:HD23	1:E:1472:LEU:H	1.74	0.51
1:C:1564:ARG:HH22	1:D:1592:THR:HA	1.70	0.51
1:A:1472:LEU:H	1:A:1472:LEU:HD23	1.74	0.51
1:E:2189:ASN:CB	1:F:2180:PRO:HA	2.41	0.51
1:A:2278:PRO:HA	1:A:2283:TYR:CE1	2.46	0.51
1:B:1461:THR:CG2	1:B:1463:TYR:CE1	2.94	0.51
1:E:1564:ARG:HH22	1:F:1592:THR:HA	1.73	0.51
1:F:1820:SER:CB	1:G:1860:LEU:CG	2.89	0.51
1:A:2180:PRO:O	1:G:2189:ASN:HB3	2.11	0.51
1:D:2189:ASN:HB3	1:E:2180:PRO:O	2.11	0.51
1:G:1440:ASN:OD1	1:G:1440:ASN:N	2.44	0.51
1:B:2278:PRO:HA	1:B:2283:TYR:CE1	2.46	0.51
1:C:1536:LEU:O	1:C:1536:LEU:HG	2.11	0.51
1:E:2189:ASN:HB3	1:F:2180:PRO:O	2.11	0.51
1:F:2238:SER:CB	1:F:2239:PRO:CD	2.88	0.51
1:B:1536:LEU:HG	1:B:1536:LEU:O	2.11	0.50
1:D:1536:LEU:O	1:D:1536:LEU:HG	2.11	0.50
1:D:1440:ASN:OD1	1:D:1440:ASN:N	2.44	0.50
1:A:2189:ASN:CB	1:B:2180:PRO:HA	2.40	0.50
1:E:1536:LEU:HG	1:E:1536:LEU:O	2.11	0.50
1:F:1461:THR:CG2	1:F:1463:TYR:CE1	2.94	0.50
1:F:1536:LEU:O	1:F:1536:LEU:HG	2.11	0.50
1:G:1536:LEU:HG	1:G:1536:LEU:O	2.11	0.50
1:D:2189:ASN:HB3	1:E:2180:PRO:CA	2.41	0.50
1:C:2189:ASN:HB3	1:D:2180:PRO:O	2.11	0.50
1:F:1564:ARG:NH2	1:G:1592:THR:CA	2.64	0.50
1:B:2189:ASN:HB3	1:C:2180:PRO:O	2.11	0.49
1:F:1736:MET:HE1	1:F:1792:LEU:HB2	1.89	0.49
1:A:1536:LEU:O	1:A:1536:LEU:HG	2.11	0.49
1:A:1841:SER:O	1:A:1842:GLY:C	2.54	0.49
1:C:2107:SER:OG	1:C:2108:THR:N	2.46	0.49
1:G:1841:SER:O	1:G:1842:GLY:C	2.54	0.49
1:A:2180:PRO:CA	1:G:2189:ASN:HB3	2.40	0.49
1:E:1461:THR:CG2	1:E:1463:TYR:CE1	2.94	0.49
1:B:1841:SER:O	1:B:1842:GLY:C	2.54	0.49
1:C:1841:SER:O	1:C:1842:GLY:C	2.54	0.49
1:A:1461:THR:CG2	1:A:1463:TYR:CE1	2.94	0.49
1:B:2107:SER:OG	1:B:2108:THR:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1841:SER:O	1:D:1842:GLY:C	2.54	0.49
1:D:2107:SER:OG	1:D:2108:THR:N	2.46	0.49
1:E:2238:SER:CB	1:E:2239:PRO:CD	2.88	0.49
1:E:1841:SER:O	1:E:1842:GLY:C	2.54	0.49
1:E:1440:ASN:OD1	1:E:1440:ASN:N	2.44	0.48
1:F:1841:SER:O	1:F:1842:GLY:C	2.54	0.48
1:D:1586:ILE:CD1	1:D:1627:VAL:HG21	2.44	0.48
1:G:2107:SER:OG	1:G:2108:THR:N	2.46	0.48
1:F:1586:ILE:CD1	1:F:1627:VAL:HG21	2.43	0.48
1:F:2107:SER:OG	1:F:2108:THR:N	2.46	0.48
1:A:2107:SER:OG	1:A:2108:THR:N	2.46	0.48
1:D:1461:THR:CG2	1:D:1463:TYR:CE1	2.94	0.48
1:G:1586:ILE:CD1	1:G:1627:VAL:HG21	2.43	0.48
1:D:1441:LEU:HD11	1:D:1444:SER:HB3	1.96	0.48
1:D:2189:ASN:HB3	1:E:2180:PRO:C	2.38	0.48
1:B:1409:SER:HB3	1:B:1419:THR:OG1	2.14	0.48
1:B:1617:THR:HG22	1:B:1645:VAL:HG11	1.96	0.48
1:C:1441:LEU:HD11	1:C:1444:SER:HB3	1.96	0.48
1:D:1409:SER:HB3	1:D:1419:THR:OG1	2.14	0.48
1:E:1586:ILE:CD1	1:E:1627:VAL:HG21	2.44	0.48
1:E:2107:SER:OG	1:E:2108:THR:N	2.46	0.48
1:F:1617:THR:HG22	1:F:1645:VAL:HG11	1.96	0.48
1:G:1617:THR:HG22	1:G:1645:VAL:HG11	1.96	0.48
1:A:2189:ASN:HB3	1:B:2180:PRO:C	2.39	0.48
1:E:1441:LEU:HD11	1:E:1444:SER:HB3	1.96	0.48
1:E:1617:THR:HG22	1:E:1645:VAL:HG11	1.96	0.48
1:B:1441:LEU:HD11	1:B:1444:SER:HB3	1.96	0.48
1:G:1409:SER:HB3	1:G:1419:THR:OG1	2.14	0.48
1:C:1617:THR:HG22	1:C:1645:VAL:HG11	1.96	0.48
1:D:1617:THR:HG22	1:D:1645:VAL:HG11	1.96	0.48
1:A:1586:ILE:CD1	1:A:1627:VAL:HG21	2.43	0.47
1:A:1617:THR:HG22	1:A:1645:VAL:HG11	1.96	0.47
1:A:2180:PRO:C	1:G:2189:ASN:HB3	2.38	0.47
1:B:1586:ILE:CD1	1:B:1627:VAL:HG21	2.43	0.47
1:B:2189:ASN:HB3	1:C:2180:PRO:C	2.40	0.47
1:C:1461:THR:CG2	1:C:1463:TYR:CE1	2.94	0.47
1:F:1441:LEU:HD11	1:F:1444:SER:HB3	1.96	0.47
1:C:1409:SER:HB3	1:C:1419:THR:OG1	2.14	0.47
1:C:2189:ASN:HB3	1:D:2180:PRO:C	2.39	0.47
1:D:2238:SER:CB	1:D:2239:PRO:CD	2.88	0.47
1:E:1443:ALA:HB1	1:E:1448:PRO:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1586:ILE:CD1	1:C:1627:VAL:HG21	2.43	0.47
1:D:1443:ALA:HB1	1:D:1448:PRO:HG3	1.97	0.47
1:C:1443:ALA:HB1	1:C:1448:PRO:HG3	1.97	0.47
1:F:1409:SER:HB3	1:F:1419:THR:OG1	2.14	0.47
1:F:1443:ALA:HB1	1:F:1448:PRO:HG3	1.97	0.47
1:A:1441:LEU:HD11	1:A:1444:SER:HB3	1.96	0.47
1:E:1409:SER:HB3	1:E:1419:THR:OG1	2.14	0.47
1:F:1440:ASN:OD1	1:F:1440:ASN:N	2.44	0.47
1:A:1409:SER:HB3	1:A:1419:THR:OG1	2.14	0.47
1:G:1441:LEU:HD11	1:G:1444:SER:HB3	1.96	0.47
1:F:2189:ASN:HB3	1:G:2180:PRO:O	2.15	0.46
1:B:1443:ALA:HB1	1:B:1448:PRO:HG3	1.97	0.46
1:B:2189:ASN:HB3	1:C:2180:PRO:CA	2.43	0.46
1:E:2189:ASN:HB3	1:F:2180:PRO:CA	2.45	0.46
1:E:2189:ASN:HB3	1:F:2180:PRO:C	2.41	0.46
1:C:2189:ASN:HB3	1:D:2180:PRO:CA	2.42	0.46
1:D:2189:ASN:HB2	1:E:2179:GLY:O	2.16	0.46
1:G:1443:ALA:HB1	1:G:1448:PRO:HG3	1.97	0.46
1:G:1461:THR:CG2	1:G:1463:TYR:CE1	2.94	0.46
1:A:2179:GLY:O	1:G:2189:ASN:HB2	2.16	0.46
1:G:1895:TYR:CZ	1:G:1963:ASN:HB3	2.51	0.46
1:E:1895:TYR:CZ	1:E:1963:ASN:HB3	2.51	0.45
1:A:1895:TYR:CZ	1:A:1963:ASN:HB3	2.51	0.45
1:F:1895:TYR:CZ	1:F:1963:ASN:HB3	2.51	0.45
1:B:2156:PHE:CZ	1:B:2164:ILE:HG23	2.52	0.45
1:A:1443:ALA:HB1	1:A:1448:PRO:HG3	1.97	0.45
1:C:2156:PHE:CZ	1:C:2164:ILE:HG23	2.52	0.45
1:D:1895:TYR:CZ	1:D:1963:ASN:HB3	2.51	0.45
1:G:2156:PHE:CZ	1:G:2164:ILE:HG23	2.52	0.45
1:A:2156:PHE:CZ	1:A:2164:ILE:HG23	2.52	0.45
1:F:2156:PHE:CZ	1:F:2164:ILE:HG23	2.52	0.45
1:C:2238:SER:CB	1:C:2239:PRO:CD	2.88	0.45
1:A:1673:ASN:OD1	1:A:1673:ASN:N	2.49	0.45
1:B:1895:TYR:CZ	1:B:1963:ASN:HB3	2.51	0.45
1:C:1895:TYR:CZ	1:C:1963:ASN:HB3	2.51	0.45
1:D:1443:ALA:HB1	1:D:1448:PRO:CB	2.47	0.45
1:D:2154:ALA:O	1:D:2155:ASP:C	2.60	0.45
1:E:1443:ALA:HB1	1:E:1448:PRO:CB	2.47	0.45
1:E:2154:ALA:O	1:E:2155:ASP:C	2.60	0.44
1:E:2156:PHE:CZ	1:E:2164:ILE:HG23	2.52	0.44
1:B:1443:ALA:HB1	1:B:1448:PRO:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1673:ASN:OD1	1:B:1673:ASN:N	2.49	0.44
1:D:2156:PHE:CZ	1:D:2164:ILE:HG23	2.52	0.44
1:C:2189:ASN:HB2	1:D:2179:GLY:O	2.18	0.44
1:E:1820:SER:CB	1:F:1860:LEU:HD21	2.26	0.44
1:F:1443:ALA:HB1	1:F:1448:PRO:CB	2.47	0.44
1:A:1443:ALA:HB1	1:A:1448:PRO:CB	2.47	0.44
1:A:1474:ASP:CG	1:A:1475:THR:H	2.26	0.44
1:A:2189:ASN:HB2	1:B:2179:GLY:O	2.17	0.44
1:C:2154:ALA:O	1:C:2155:ASP:C	2.60	0.44
1:F:2189:ASN:HB3	1:G:2180:PRO:CA	2.42	0.44
1:A:1435:ASP:OD1	1:A:1436:ALA:N	2.51	0.44
1:C:1921:THR:OG1	1:C:1922:VAL:N	2.51	0.44
1:G:1443:ALA:HB1	1:G:1448:PRO:CB	2.48	0.44
1:B:1474:ASP:CG	1:B:1475:THR:H	2.26	0.44
1:E:1413:CYS:O	1:E:1414:GLU:C	2.61	0.44
1:F:1432:TRP:CZ3	1:F:1464:VAL:HG22	2.53	0.44
1:F:2154:ALA:O	1:F:2155:ASP:C	2.60	0.44
1:G:1435:ASP:OD1	1:G:1436:ALA:N	2.51	0.44
1:B:1921:THR:OG1	1:B:1922:VAL:N	2.51	0.43
1:G:1474:ASP:CG	1:G:1475:THR:H	2.26	0.43
1:C:1440:ASN:O	1:C:1441:LEU:C	2.61	0.43
1:C:1443:ALA:HB1	1:C:1448:PRO:CB	2.48	0.43
1:D:2170:THR:OG1	1:D:2171:VAL:N	2.51	0.43
1:E:1432:TRP:CZ3	1:E:1464:VAL:HG22	2.53	0.43
1:G:1440:ASN:O	1:G:1441:LEU:C	2.61	0.43
1:B:1435:ASP:OD1	1:B:1436:ALA:N	2.51	0.43
1:C:1474:ASP:CG	1:C:1475:THR:H	2.26	0.43
1:D:1440:ASN:O	1:D:1441:LEU:C	2.61	0.43
1:G:1921:THR:OG1	1:G:1922:VAL:N	2.51	0.43
1:B:1432:TRP:CZ3	1:B:1464:VAL:HG22	2.53	0.43
1:C:1435:ASP:OD1	1:C:1436:ALA:N	2.51	0.43
1:D:1432:TRP:CZ3	1:D:1464:VAL:HG22	2.53	0.43
1:D:1921:THR:OG1	1:D:1922:VAL:N	2.51	0.43
1:E:1921:THR:OG1	1:E:1922:VAL:N	2.51	0.43
1:G:1432:TRP:CZ3	1:G:1464:VAL:HG22	2.53	0.43
1:C:1432:TRP:CZ3	1:C:1464:VAL:HG22	2.53	0.43
1:D:1435:ASP:OD1	1:D:1436:ALA:N	2.51	0.43
1:A:1432:TRP:CZ3	1:A:1464:VAL:HG22	2.53	0.43
1:C:2170:THR:OG1	1:C:2171:VAL:N	2.51	0.43
1:F:1474:ASP:CG	1:F:1475:THR:H	2.26	0.43
1:A:1921:THR:OG1	1:A:1922:VAL:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1435:ASP:OD1	1:F:1436:ALA:N	2.51	0.43
1:F:2156:PHE:HZ	1:F:2164:ILE:HG23	1.84	0.43
1:B:1440:ASN:O	1:B:1441:LEU:C	2.61	0.43
1:B:2189:ASN:HB2	1:C:2179:GLY:O	2.18	0.43
1:F:2189:ASN:HB3	1:G:2180:PRO:C	2.43	0.43
1:G:2154:ALA:O	1:G:2155:ASP:C	2.61	0.43
1:G:2156:PHE:HZ	1:G:2164:ILE:HG23	1.84	0.43
1:A:2156:PHE:HZ	1:A:2164:ILE:HG23	1.84	0.42
1:D:2238:SER:O	1:D:2239:PRO:C	2.62	0.42
1:E:2156:PHE:HZ	1:E:2164:ILE:HG23	1.84	0.42
1:F:2170:THR:OG1	1:F:2171:VAL:N	2.51	0.42
1:D:1413:CYS:O	1:D:1414:GLU:C	2.61	0.42
1:C:2238:SER:O	1:C:2239:PRO:C	2.62	0.42
1:D:2156:PHE:HZ	1:D:2164:ILE:HG23	1.84	0.42
1:F:1440:ASN:O	1:F:1441:LEU:C	2.61	0.42
1:A:2238:SER:O	1:A:2239:PRO:C	2.62	0.42
1:C:1673:ASN:OD1	1:C:1673:ASN:N	2.49	0.42
1:D:1474:ASP:CG	1:D:1475:THR:H	2.26	0.42
1:E:2170:THR:OG1	1:E:2171:VAL:N	2.51	0.42
1:A:1424:THR:HG23	1:A:1446:GLN:NE2	2.33	0.42
1:A:1468:SER:HB3	1:A:1471:CYS:HB2	2.02	0.42
1:B:2154:ALA:O	1:B:2155:ASP:C	2.61	0.42
1:B:2156:PHE:HZ	1:B:2164:ILE:HG23	1.84	0.42
1:C:2156:PHE:HZ	1:C:2164:ILE:HG23	1.84	0.42
1:E:1440:ASN:O	1:E:1441:LEU:C	2.61	0.42
1:F:1468:SER:HB3	1:F:1471:CYS:HB2	2.02	0.42
1:F:2238:SER:O	1:F:2239:PRO:C	2.62	0.42
1:A:2154:ALA:O	1:A:2155:ASP:C	2.60	0.42
1:D:1933:GLY:O	1:D:1934:PHE:C	2.63	0.42
1:E:1435:ASP:OD1	1:E:1436:ALA:N	2.51	0.42
1:G:1933:GLY:O	1:G:1934:PHE:C	2.63	0.42
1:G:2170:THR:OG1	1:G:2171:VAL:N	2.51	0.42
1:E:1474:ASP:CG	1:E:1475:THR:H	2.26	0.42
1:E:1933:GLY:O	1:E:1934:PHE:C	2.63	0.42
1:G:1424:THR:HG23	1:G:1446:GLN:NE2	2.33	0.42
1:G:2238:SER:O	1:G:2239:PRO:C	2.62	0.42
1:F:1933:GLY:O	1:F:1934:PHE:C	2.63	0.42
1:B:1468:SER:HB3	1:B:1471:CYS:HB2	2.02	0.42
1:E:1468:SER:HB3	1:E:1471:CYS:HB2	2.02	0.42
1:G:1468:SER:HB3	1:G:1471:CYS:HB2	2.02	0.42
1:F:1424:THR:HG23	1:F:1446:GLN:NE2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1933:GLY:O	1:A:1934:PHE:C	2.63	0.41
1:B:1413:CYS:O	1:B:1414:GLU:C	2.61	0.41
1:B:1424:THR:HG23	1:B:1446:GLN:NE2	2.33	0.41
1:D:1820:SER:CB	1:E:1860:LEU:HD21	2.26	0.41
1:G:1435:ASP:O	1:G:1463:TYR:HB2	2.20	0.41
1:B:1831:THR:OG1	1:B:1832:ASP:N	2.54	0.41
1:B:1873:THR:C	1:B:1874:PHE:CD1	2.99	0.41
1:C:1831:THR:OG1	1:C:1832:ASP:N	2.54	0.41
1:E:2189:ASN:HB2	1:F:2179:GLY:O	2.20	0.41
1:A:2189:ASN:HB3	1:B:2180:PRO:CA	2.43	0.41
1:E:1873:THR:C	1:E:1874:PHE:CD1	2.99	0.41
1:G:1443:ALA:HB1	1:G:1448:PRO:CG	2.51	0.41
1:G:1828:CYS:O	1:G:1829:THR:C	2.64	0.41
1:A:1873:THR:C	1:A:1874:PHE:CD1	2.99	0.41
1:C:1873:THR:C	1:C:1874:PHE:CD1	2.99	0.41
1:D:1435:ASP:O	1:D:1463:TYR:HB2	2.20	0.41
1:D:1468:SER:HB3	1:D:1471:CYS:HB2	2.02	0.41
1:E:1424:THR:HG23	1:E:1446:GLN:NE2	2.33	0.41
1:E:1435:ASP:O	1:E:1463:TYR:HB2	2.20	0.41
1:E:1673:ASN:OD1	1:E:1673:ASN:N	2.49	0.41
1:G:1413:CYS:O	1:G:1414:GLU:C	2.61	0.41
1:A:1820:SER:CB	1:B:1860:LEU:HD21	2.25	0.41
1:A:2068:ALA:O	1:A:2069:SER:C	2.64	0.41
1:C:1468:SER:HB3	1:C:1471:CYS:HB2	2.02	0.41
1:D:1831:THR:OG1	1:D:1832:ASP:N	2.54	0.41
1:F:1443:ALA:HB1	1:F:1448:PRO:CG	2.50	0.41
1:A:1440:ASN:O	1:A:1441:LEU:C	2.61	0.41
1:C:1435:ASP:O	1:C:1463:TYR:HB2	2.20	0.41
1:F:1873:THR:C	1:F:1874:PHE:CD1	2.99	0.41
1:A:1443:ALA:HB1	1:A:1448:PRO:CG	2.51	0.41
1:A:2170:THR:OG1	1:A:2171:VAL:N	2.51	0.41
1:B:1933:GLY:O	1:B:1934:PHE:C	2.63	0.41
1:B:2068:ALA:O	1:B:2069:SER:C	2.64	0.41
1:E:1443:ALA:HB1	1:E:1448:PRO:CG	2.50	0.41
1:B:1564:ARG:HH21	1:C:1592:THR:N	2.19	0.41
1:B:2238:SER:CB	1:B:2239:PRO:CD	2.88	0.41
1:B:2238:SER:O	1:B:2239:PRO:C	2.62	0.41
1:C:1413:CYS:O	1:C:1414:GLU:C	2.61	0.41
1:E:1828:CYS:O	1:E:1829:THR:C	2.64	0.41
1:F:1413:CYS:O	1:F:1414:GLU:C	2.61	0.41
1:G:2068:ALA:O	1:G:2069:SER:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2170:THR:OG1	1:B:2171:VAL:N	2.51	0.41
1:F:1858:SER:OG	1:F:1859:THR:N	2.54	0.41
1:G:1873:THR:C	1:G:1874:PHE:CD1	2.99	0.40
1:B:1435:ASP:O	1:B:1463:TYR:HB2	2.20	0.40
1:B:1828:CYS:O	1:B:1829:THR:C	2.64	0.40
1:C:2068:ALA:O	1:C:2069:SER:C	2.64	0.40
1:D:1443:ALA:HB1	1:D:1448:PRO:CG	2.50	0.40
1:D:1873:THR:C	1:D:1874:PHE:CD1	2.99	0.40
1:F:1435:ASP:O	1:F:1463:TYR:HB2	2.20	0.40
1:A:1435:ASP:O	1:A:1463:TYR:CD1	2.75	0.40
1:B:1435:ASP:O	1:B:1463:TYR:CD1	2.75	0.40
1:B:1443:ALA:HB1	1:B:1448:PRO:CG	2.50	0.40
1:D:1940:ASN:O	1:E:1933:GLY:N	2.54	0.40
1:G:1485:ASN:HA	1:G:1486:PRO:HD3	1.97	0.40
1:A:1940:ASN:O	1:B:1933:GLY:N	2.55	0.40
1:C:1858:SER:OG	1:C:1859:THR:N	2.54	0.40
1:C:1933:GLY:O	1:C:1934:PHE:C	2.63	0.40
1:D:1424:THR:HG23	1:D:1446:GLN:NE2	2.34	0.40
1:E:2238:SER:O	1:E:2239:PRO:C	2.62	0.40
1:B:1485:ASN:HA	1:B:1486:PRO:HD3	1.97	0.40
1:E:1435:ASP:O	1:E:1463:TYR:CD1	2.75	0.40
1:E:1582:ILE:HD11	1:E:1645:VAL:HG21	2.04	0.40
1:F:1435:ASP:O	1:F:1463:TYR:CD1	2.75	0.40
1:G:1858:SER:OG	1:G:1859:THR:N	2.54	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	910/5898 (15%)	896 (98%)	14 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	910/5898 (15%)	896 (98%)	14 (2%)	0	100	100
1	C	910/5898 (15%)	896 (98%)	14 (2%)	0	100	100
1	D	910/5898 (15%)	896 (98%)	14 (2%)	0	100	100
1	E	910/5898 (15%)	896 (98%)	14 (2%)	0	100	100
1	F	910/5898 (15%)	896 (98%)	14 (2%)	0	100	100
1	G	910/5898 (15%)	896 (98%)	14 (2%)	0	100	100
All	All	6370/41286 (15%)	6272 (98%)	98 (2%)	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	743/4919 (15%)	743 (100%)	0	100	100
1	B	743/4919 (15%)	743 (100%)	0	100	100
1	C	743/4919 (15%)	743 (100%)	0	100	100
1	D	743/4919 (15%)	743 (100%)	0	100	100
1	E	743/4919 (15%)	743 (100%)	0	100	100
1	F	743/4919 (15%)	743 (100%)	0	100	100
1	G	743/4919 (15%)	743 (100%)	0	100	100
All	All	5201/34433 (15%)	5201 (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 (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1446	GLN
1	A	1465	GLN
1	A	1583	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1585	ASN
1	A	1613	ASN
1	A	1963	ASN
1	B	1446	GLN
1	B	1465	GLN
1	B	1583	GLN
1	B	1585	ASN
1	B	1613	ASN
1	B	1963	ASN
1	C	1446	GLN
1	C	1465	GLN
1	C	1583	GLN
1	C	1585	ASN
1	C	1613	ASN
1	D	1465	GLN
1	D	1583	GLN
1	D	1585	ASN
1	D	1613	ASN
1	E	1446	GLN
1	E	1465	GLN
1	E	1583	GLN
1	E	1585	ASN
1	E	1613	ASN
1	F	1446	GLN
1	F	1465	GLN
1	F	1485	ASN
1	G	1446	GLN
1	G	1465	GLN
1	G	1485	ASN
1	G	1583	GLN
1	G	1585	ASN
1	G	1613	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.

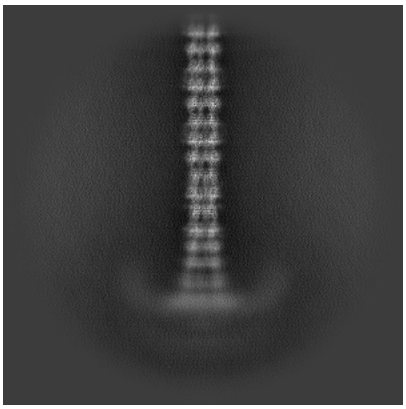
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-50537. These allow visual inspection of the internal detail of the map and identification of artifacts.

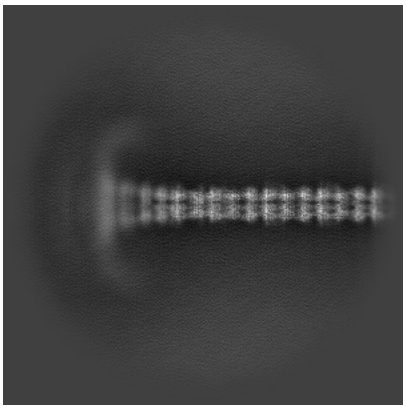
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

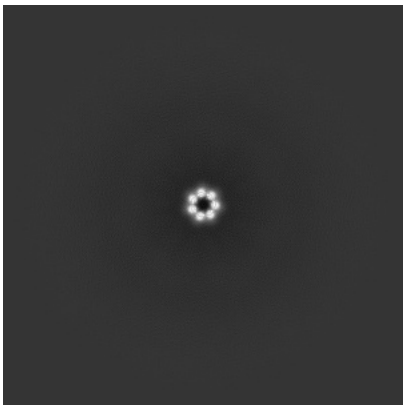
6.1.1 Primary map



X

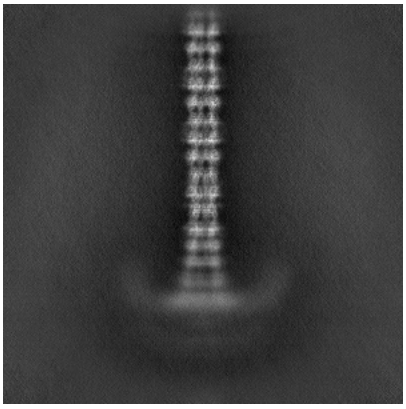


Y

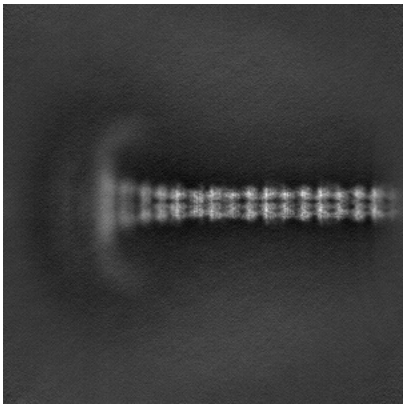


Z

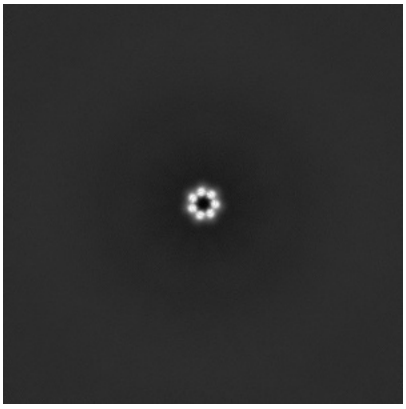
6.1.2 Raw map



X



Y

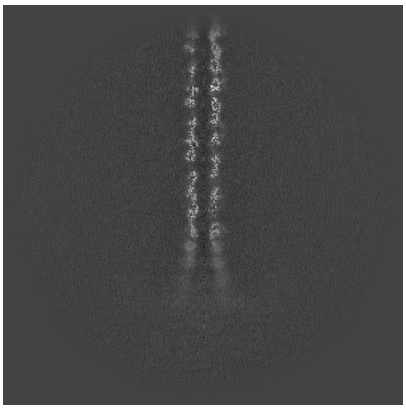


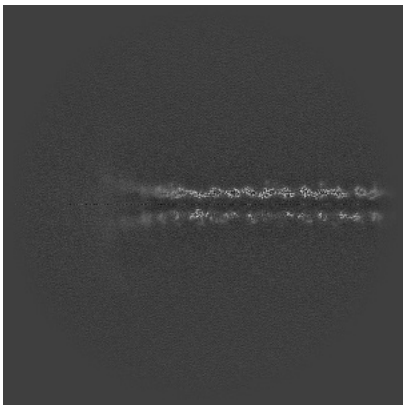
Z

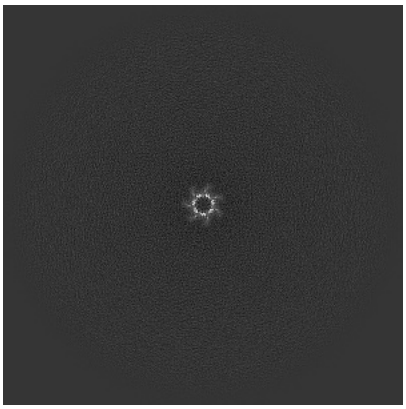
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

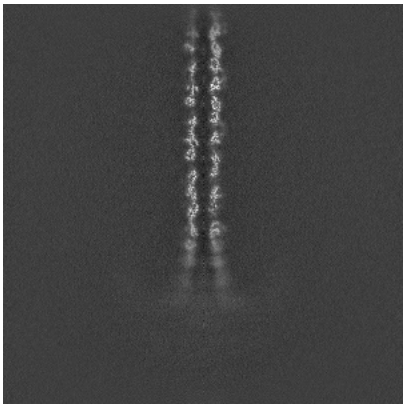
6.2.1 Primary map

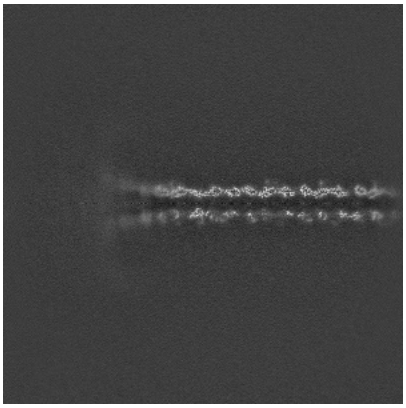

X Index: 270

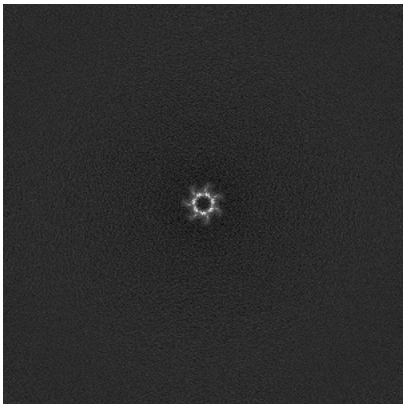

Y Index: 270


Z Index: 270

6.2.2 Raw map


X Index: 270

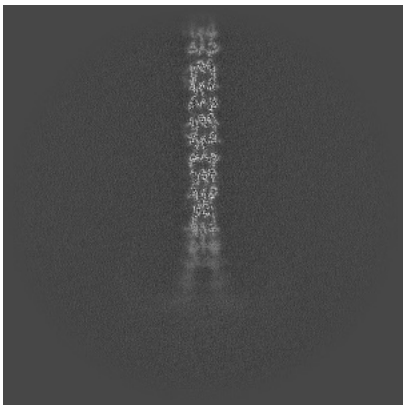

Y Index: 270

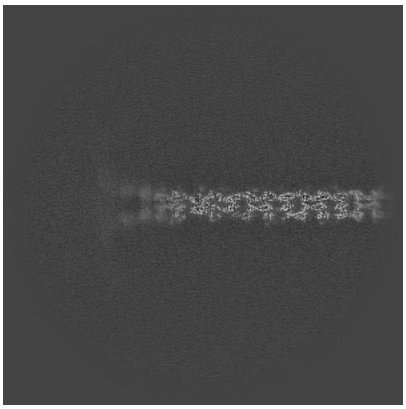

Z Index: 270

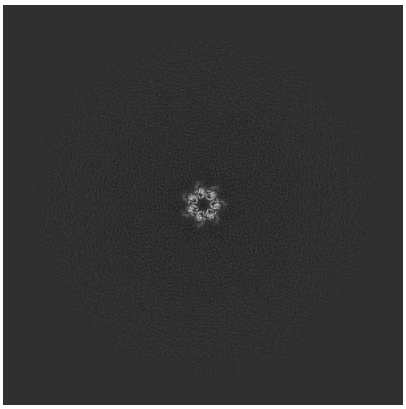
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

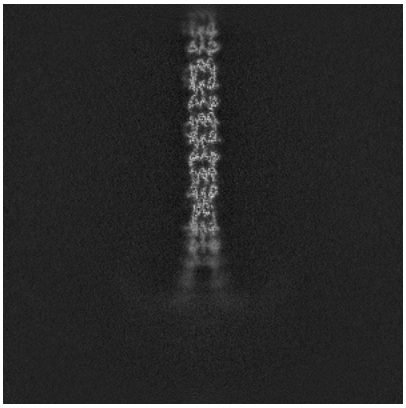
6.3.1 Primary map

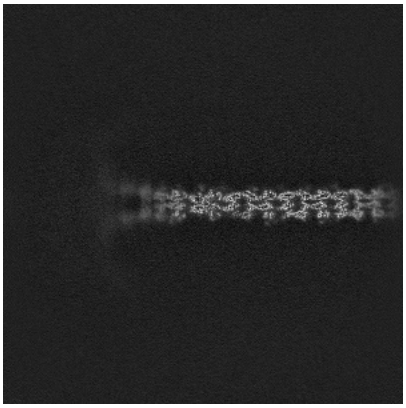

X Index: 282

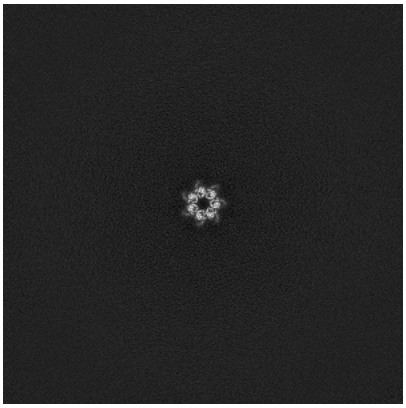

Y Index: 282


Z Index: 355

6.3.2 Raw map


X Index: 282

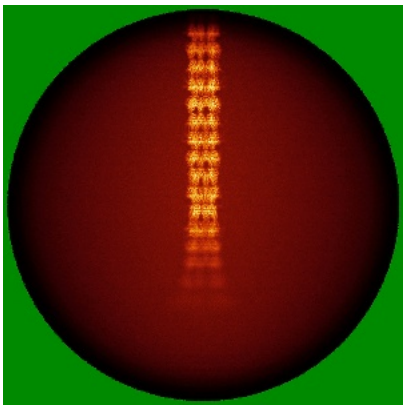

Y Index: 282

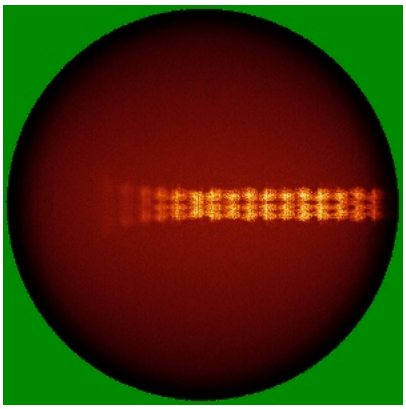

Z Index: 355

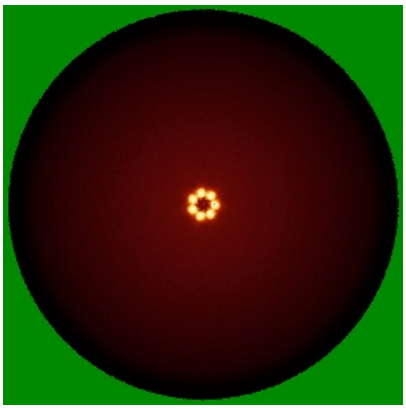
The images above show the largest variance slices of the map in three orthogonal directions.

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

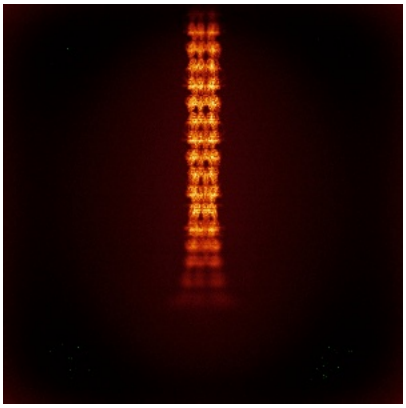
6.4.1 Primary map

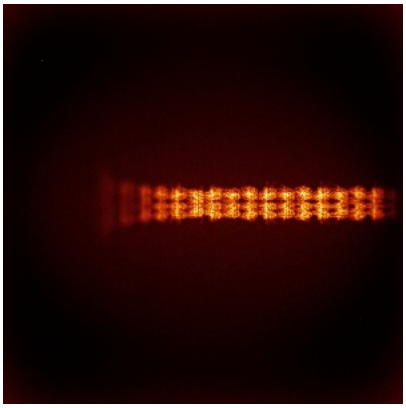

X

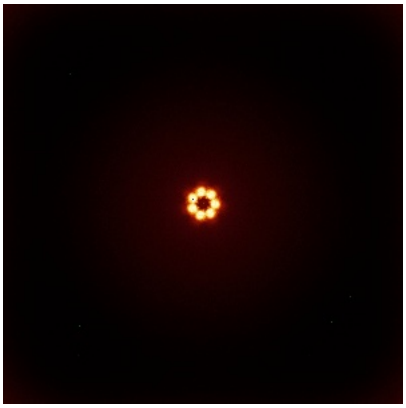

Y


Z

6.4.2 Raw map


X

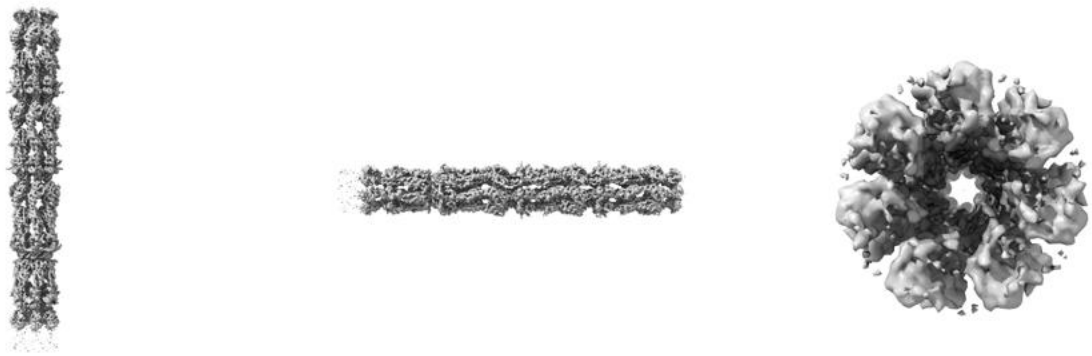

Y


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)

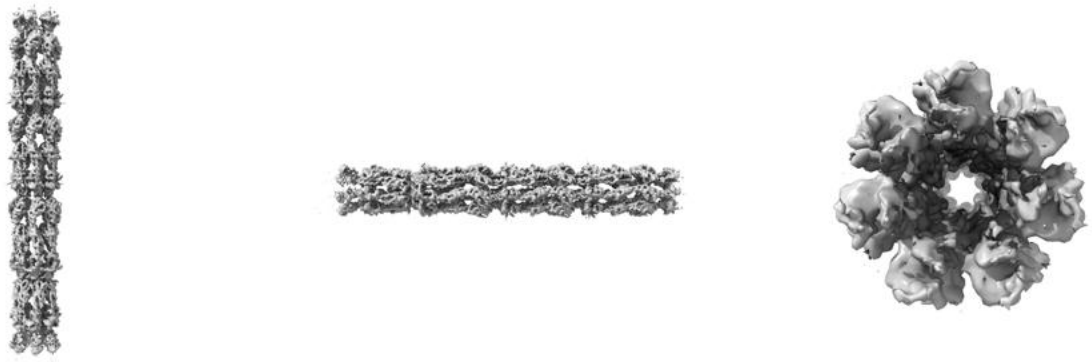
6.5.1 Primary map



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.

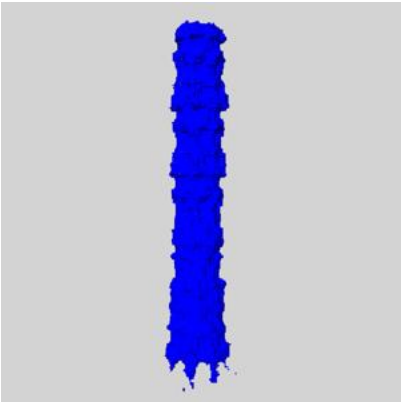
6.6 Mask visualisation (i)

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

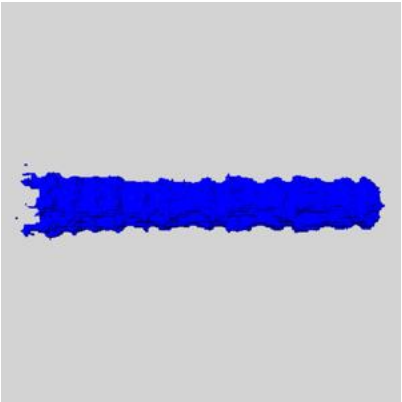
A mask typically either:

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

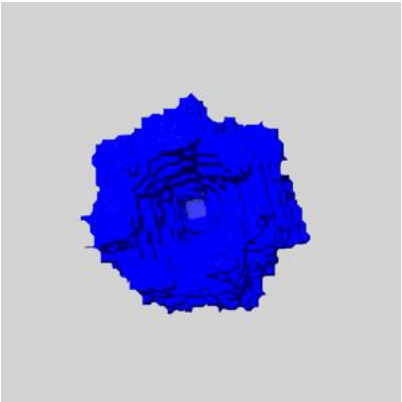
6.6.1 emd_50537_msk_1.map (i)



X



Y

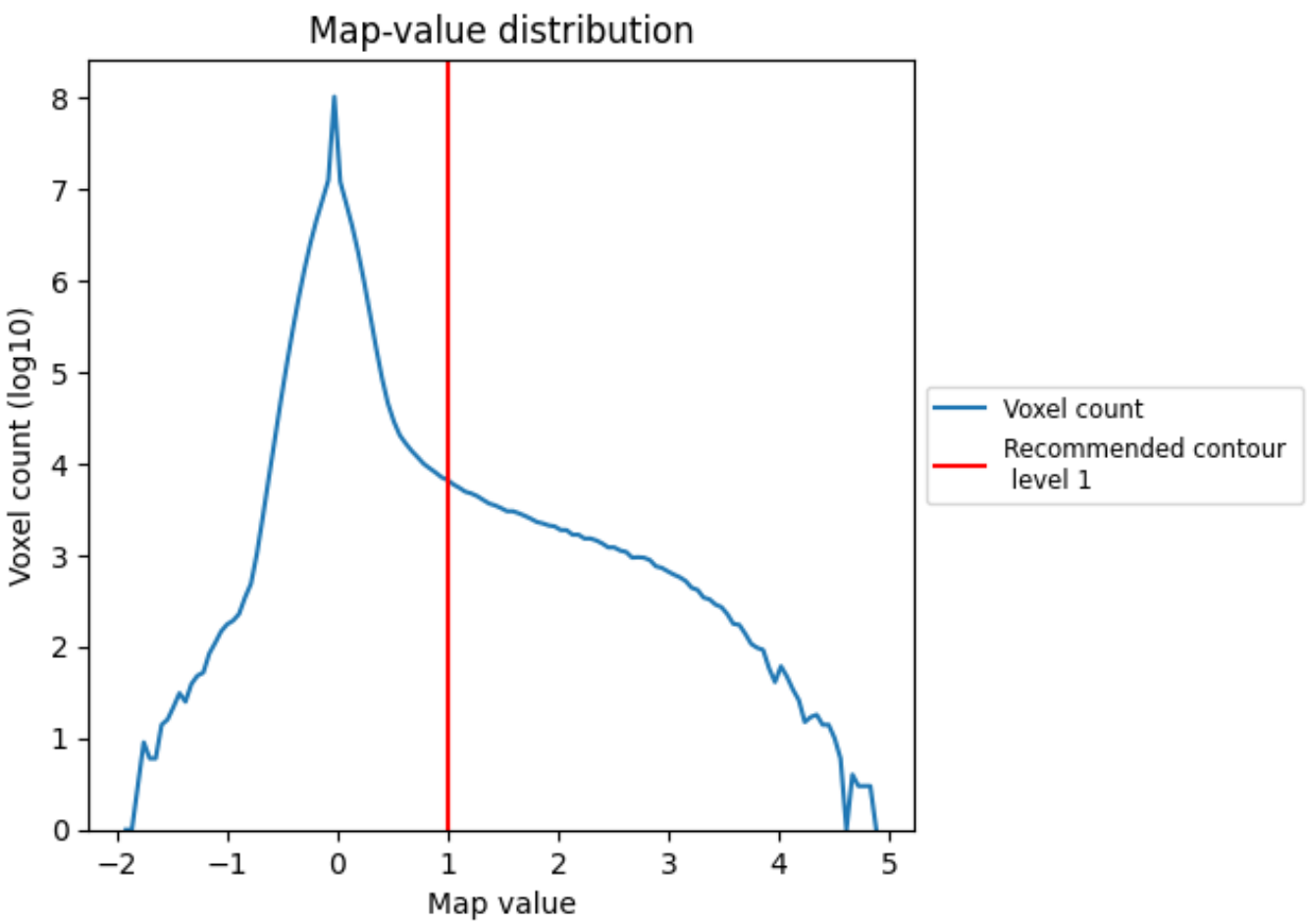


Z

7 Map analysis (i)

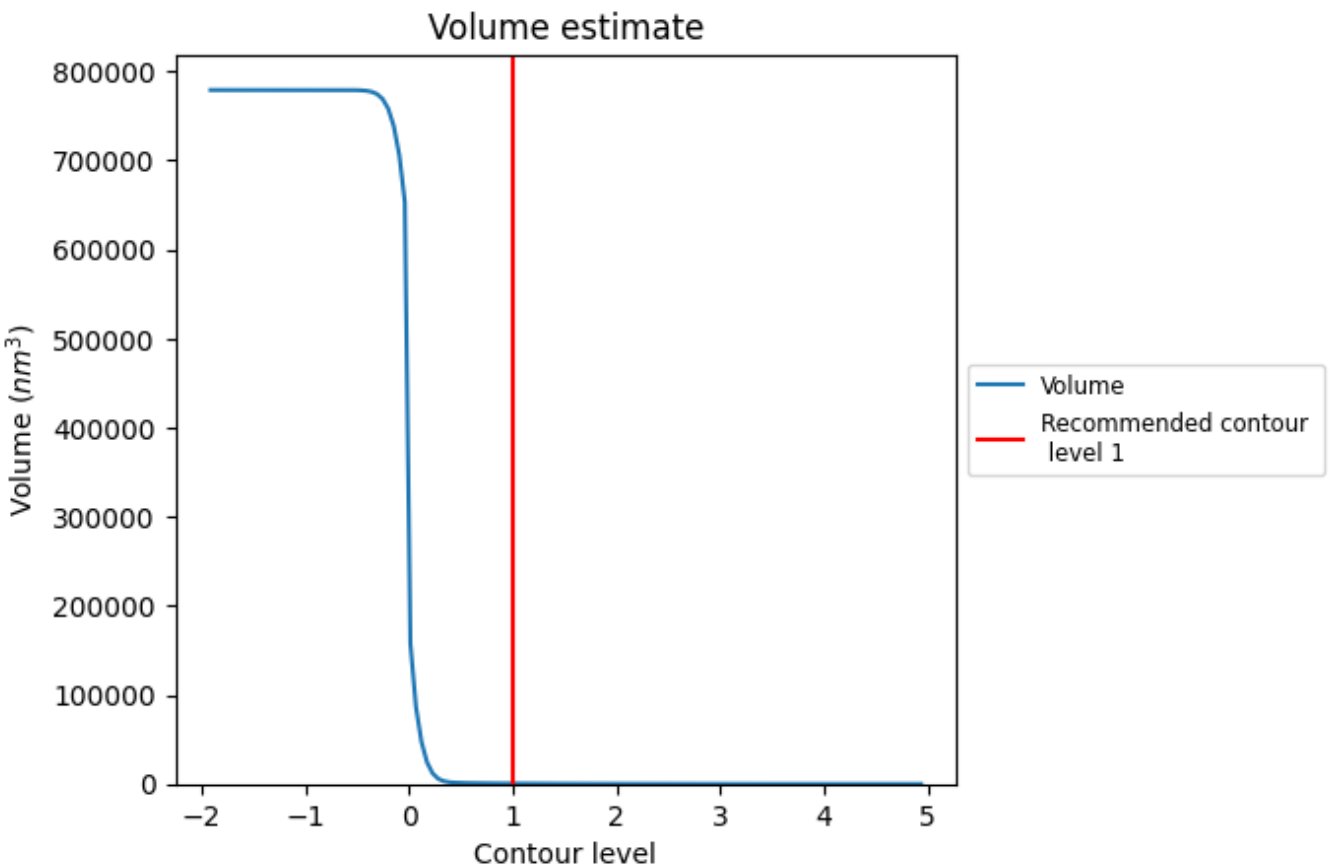
This section contains the results of statistical analysis of the map.

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.

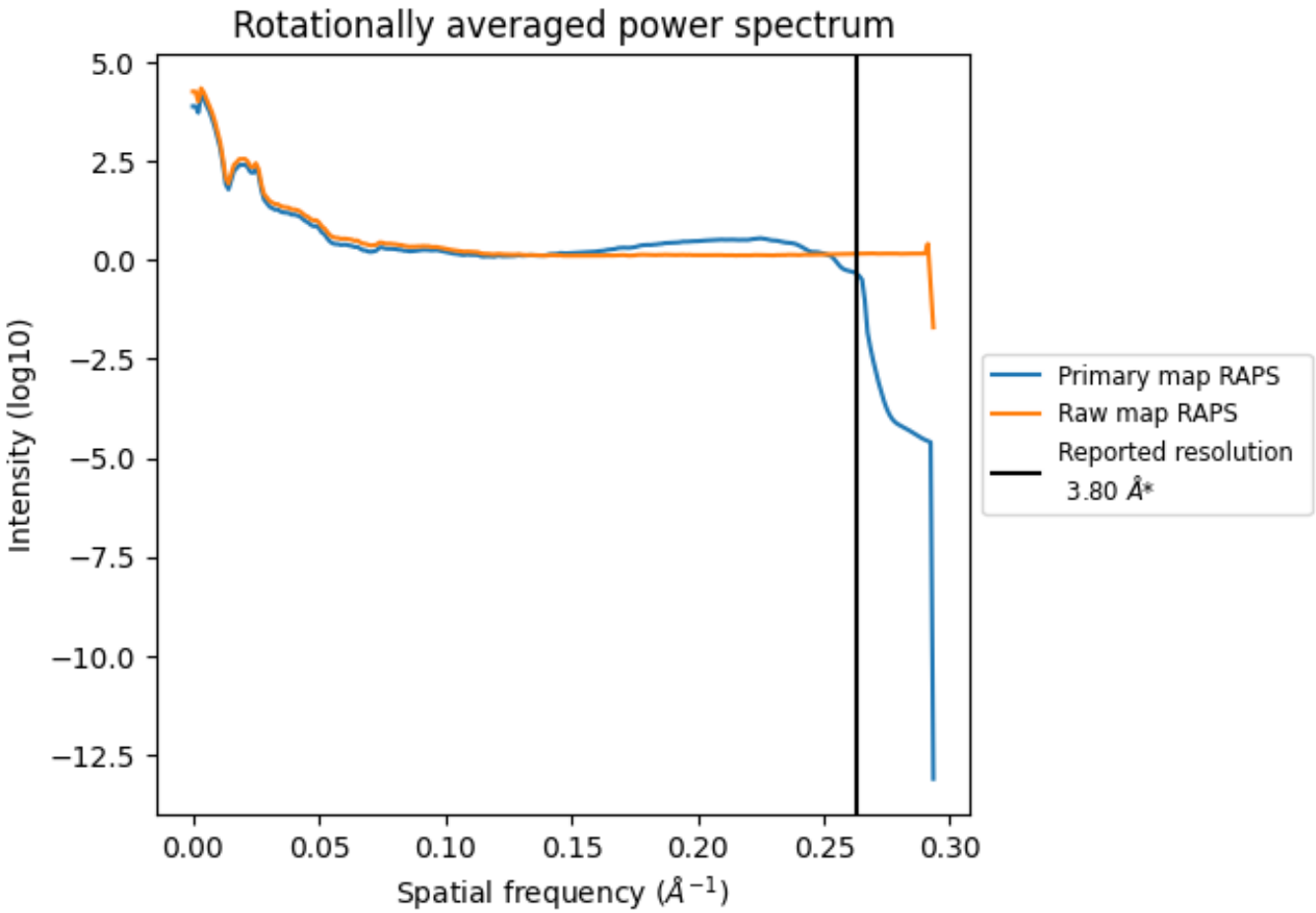
7.2 Volume estimate (i)



The volume at the recommended contour level is 482 nm^3; this corresponds to an approximate mass of 436 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)

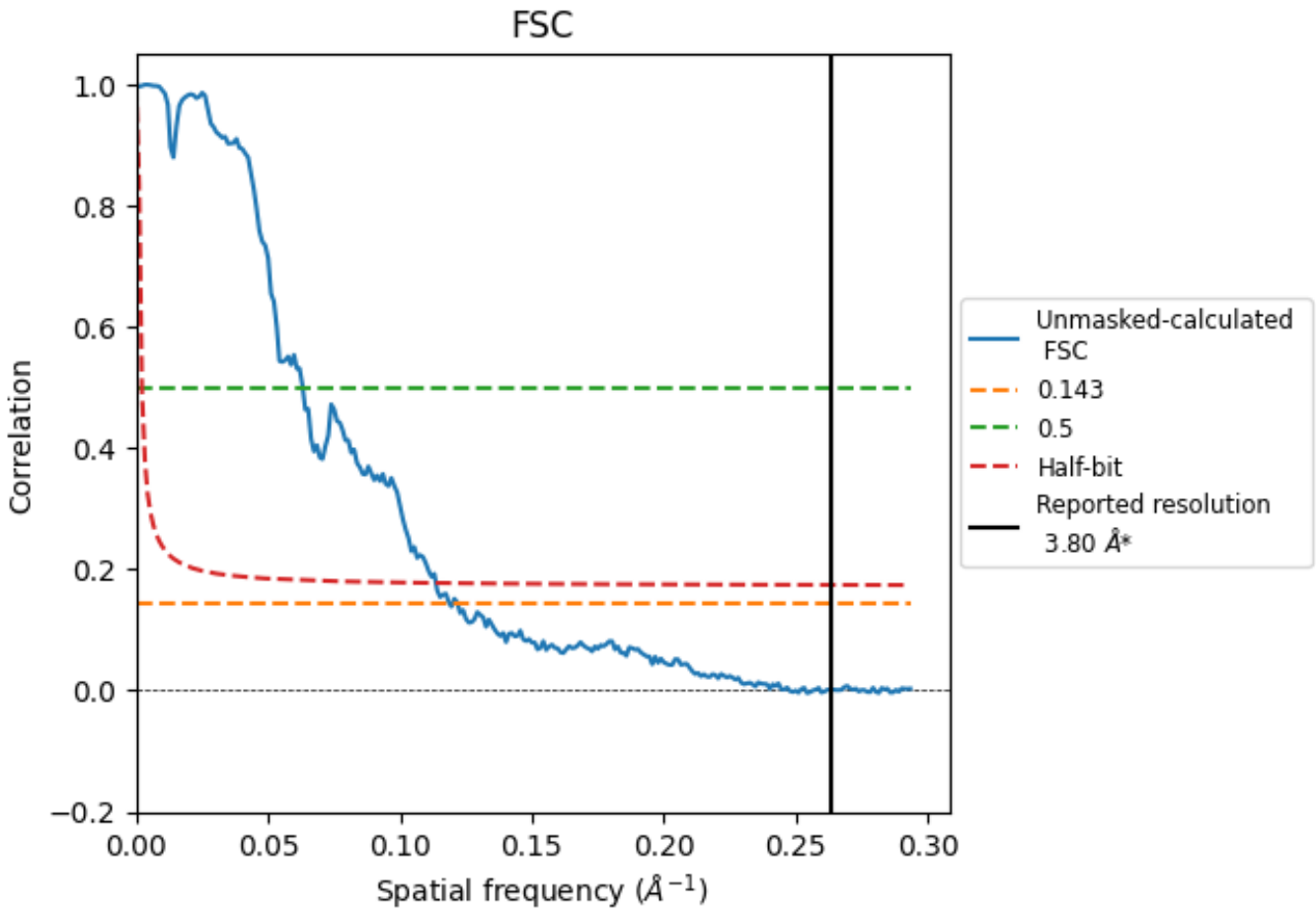


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.42	15.85	8.80

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.42 differs from the reported value 3.8 by more than 10 %

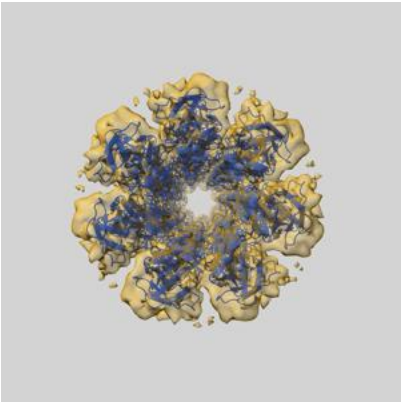
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-50537 and PDB model 9FLP. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay (i)

X

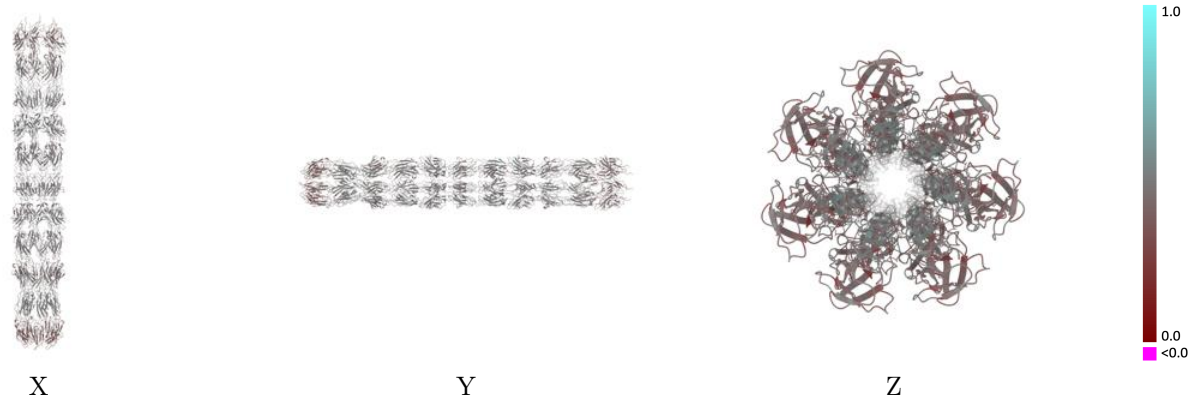
Y



Z

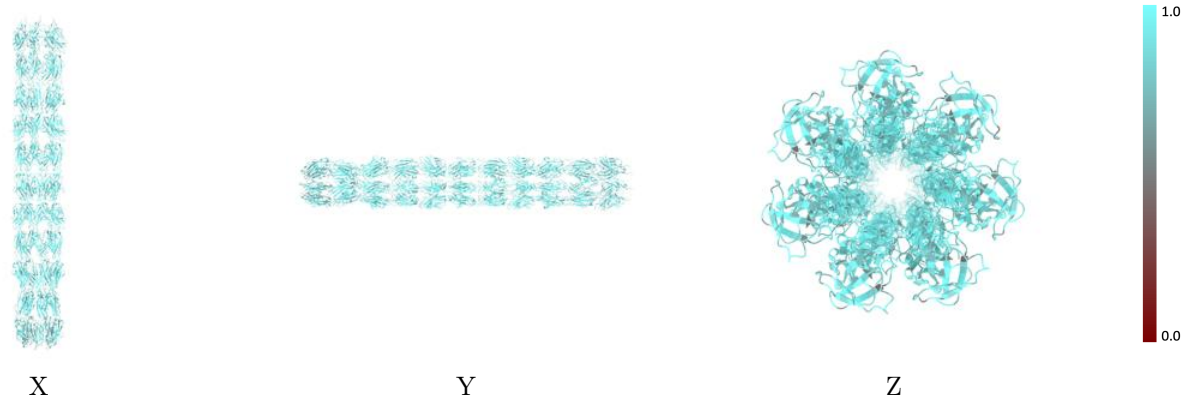
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



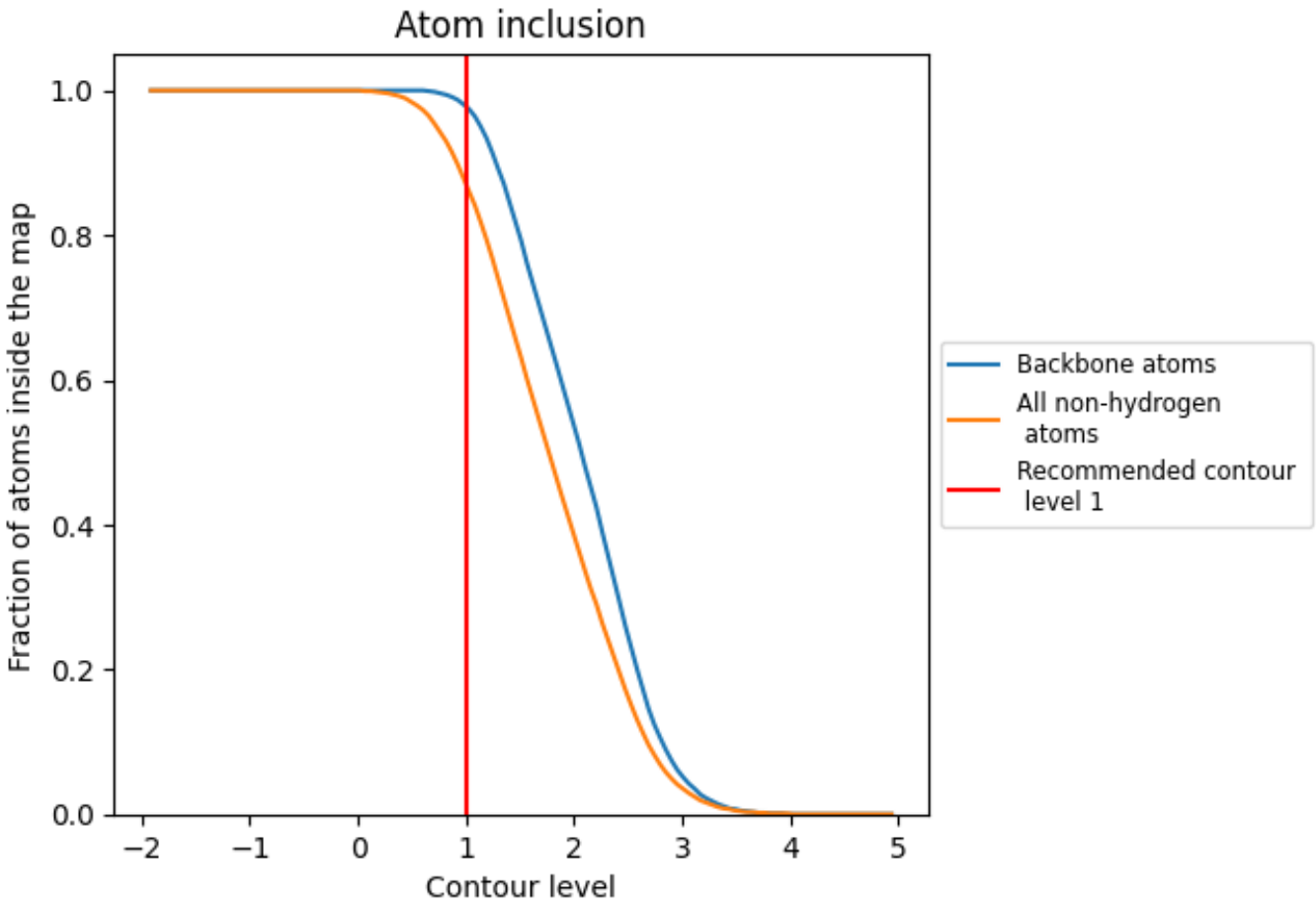
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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, 98% of all backbone atoms, 87% 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	0.8710	0.4360
A	0.8720	0.4390
B	0.8700	0.4340
C	0.8740	0.4360
D	0.8710	0.4360
E	0.8710	0.4370
F	0.8700	0.4350
G	0.8690	0.4350