Full wwPDB EM Validation Report (i)

Mar 9, 2026 – 04:23 AM UTC

PDB ID	:	6X6L / pdb_00006x6l
EMDB ID	:	EMD-22077
Title	:	Cryo-EM Structure of CagX and CagY within the dCag3 Helicobacter pylori PR
Authors	:	Sheedlo, M.J.; Chung, J.M.; Sawhney, N.; Durie, C.L.; Cover, T.L.; Ohi, M.D.; Lacy, D.B.
Deposited on	:	2020-05-28
Resolution	:	3.00 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:

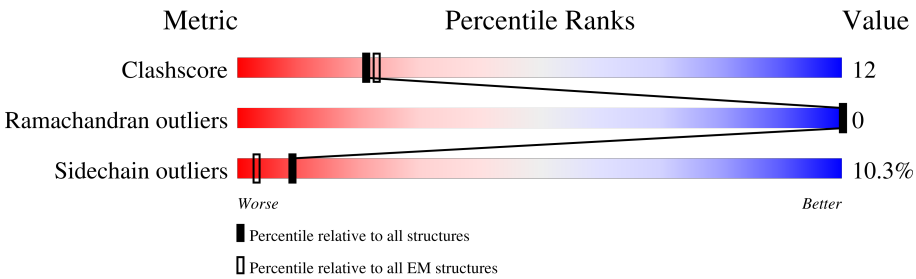
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

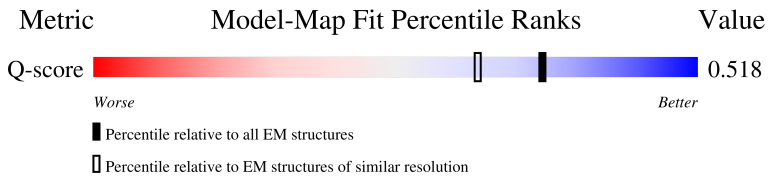
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	AX	521	20% 10% • 69%
1	BX	521	20% 10% • 69%
1	CX	521	20% 10% • 69%
1	DX	521	21% 9% • 69%

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Mol	Chain	Length	Quality of chain
1	EX	521	20% 10% 69%
1	FX	521	20% 10% 69%
1	GX	521	19% 10% 69%
1	HX	521	19% 10% 69%
1	IX	521	21% 9% 69%
1	JX	521	20% 10% 69%
1	KX	521	19% 10% 69%
1	LX	521	19% 11% 69%
1	MX	521	21% 9% 69%
1	NX	521	20% 9% 69%
1	OX	521	20% 10% 69%
1	PX	521	20% 10% 69%
1	QX	521	20% 11% 69%
2	AY	1927	5% 93%
2	BY	1927	5% 93%
2	CY	1927	5% 93%
2	DY	1927	5% 93%
2	EY	1927	5% 93%
2	FY	1927	5% 93%
2	GY	1927	5% 93%
2	HY	1927	5% 93%
2	IY	1927	5% 93%
2	JY	1927	5% 93%
2	KY	1927	93%
2	LY	1927	5% 93%

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Mol	Chain	Length	Quality of chain
2	MY	1927	5% 93%
2	NY	1927	5% 93%
2	OY	1927	5% 93%
2	PY	1927	5% 93%
2	QY	1927	5% 93%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 40613 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 Cag pathogenicity island protein (Cag8).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AX	164	1339	858	227	252	2	0	0
1	BX	164	1339	858	227	252	2	0	0
1	CX	164	1339	858	227	252	2	0	0
1	DX	164	1339	858	227	252	2	0	0
1	EX	164	1339	858	227	252	2	0	0
1	FX	164	1339	858	227	252	2	0	0
1	GX	164	1339	858	227	252	2	0	0
1	HX	164	1339	858	227	252	2	0	0
1	IX	164	1339	858	227	252	2	0	0
1	JX	164	1339	858	227	252	2	0	0
1	KX	164	1339	858	227	252	2	0	0
1	LX	164	1339	858	227	252	2	0	0
1	MX	164	1339	858	227	252	2	0	0
1	NX	164	1339	858	227	252	2	0	0
1	OX	164	1339	858	227	252	2	0	0
1	PX	164	1339	858	227	252	2	0	0
1	QX	164	1339	858	227	252	2	0	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AX	?	-	GLU	deletion	UNP O25263
AX	516	GLU	LEU	conflict	UNP O25263
BX	?	-	GLU	deletion	UNP O25263
BX	516	GLU	LEU	conflict	UNP O25263
CX	?	-	GLU	deletion	UNP O25263
CX	516	GLU	LEU	conflict	UNP O25263
DX	?	-	GLU	deletion	UNP O25263
DX	516	GLU	LEU	conflict	UNP O25263
EX	?	-	GLU	deletion	UNP O25263
EX	516	GLU	LEU	conflict	UNP O25263
FX	?	-	GLU	deletion	UNP O25263
FX	516	GLU	LEU	conflict	UNP O25263
GX	?	-	GLU	deletion	UNP O25263
GX	516	GLU	LEU	conflict	UNP O25263
HX	?	-	GLU	deletion	UNP O25263
HX	516	GLU	LEU	conflict	UNP O25263
IX	?	-	GLU	deletion	UNP O25263
IX	516	GLU	LEU	conflict	UNP O25263
JX	?	-	GLU	deletion	UNP O25263
JX	516	GLU	LEU	conflict	UNP O25263
KX	?	-	GLU	deletion	UNP O25263
KX	516	GLU	LEU	conflict	UNP O25263
LX	?	-	GLU	deletion	UNP O25263
LX	516	GLU	LEU	conflict	UNP O25263
MX	?	-	GLU	deletion	UNP O25263
MX	516	GLU	LEU	conflict	UNP O25263
NX	?	-	GLU	deletion	UNP O25263
NX	516	GLU	LEU	conflict	UNP O25263
OX	?	-	GLU	deletion	UNP O25263
OX	516	GLU	LEU	conflict	UNP O25263
PX	?	-	GLU	deletion	UNP O25263
PX	516	GLU	LEU	conflict	UNP O25263
QX	?	-	GLU	deletion	UNP O25263
QX	516	GLU	LEU	conflict	UNP O25263

- Molecule 2 is a protein called Cag pathogenicity island protein (Cag7).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	AY	135	1050	649	177	220	4	0	0
			Total	C	N	O	S		
2	BY	135	1050	649	177	220	4	0	0

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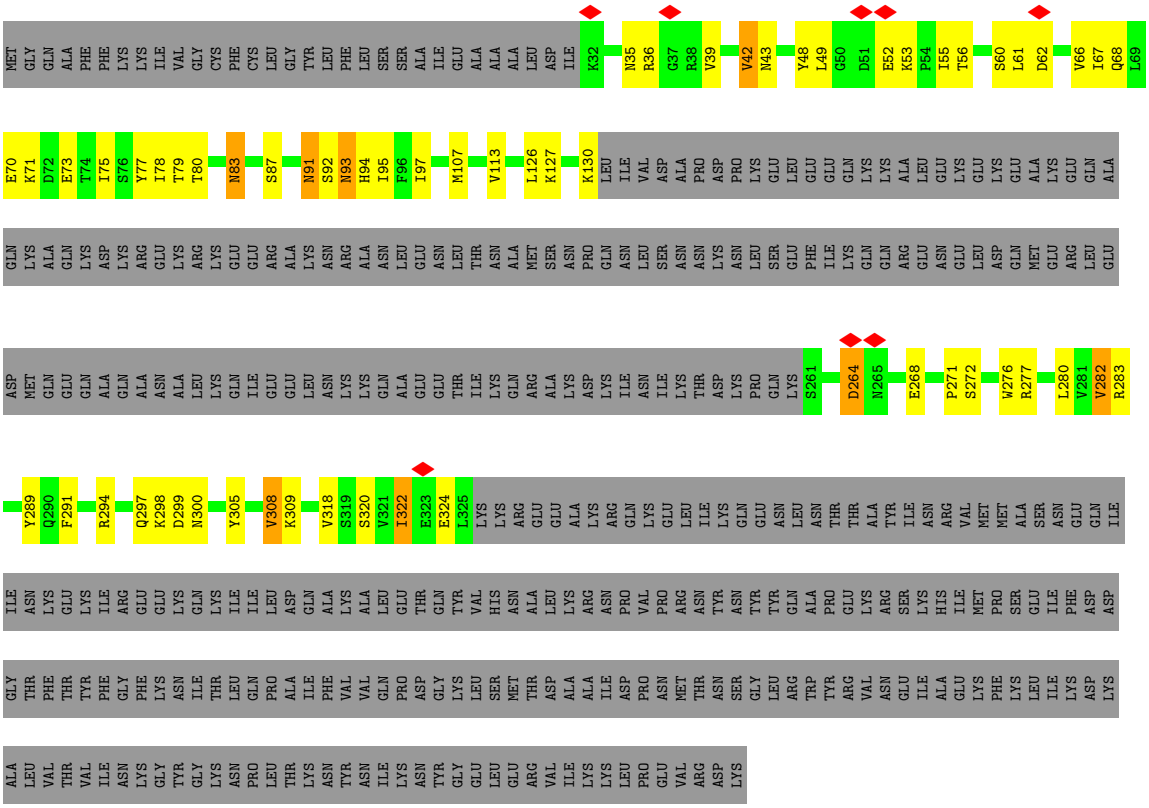
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	CY	135	1050	649	177	220	4	0	0
			Total	C	N	O	S		
2	DY	135	1050	649	177	220	4	0	0
			Total	C	N	O	S		
2	EY	135	1050	649	177	220	4	0	0
			Total	C	N	O	S		
2	FY	135	1050	649	177	220	4	0	0
			Total	C	N	O	S		
2	GY	135	1050	649	177	220	4	0	0
			Total	C	N	O	S		
2	HY	135	1050	649	177	220	4	0	0
			Total	C	N	O	S		
2	IY	135	1050	649	177	220	4	0	0
			Total	C	N	O	S		
2	JY	135	1050	649	177	220	4	0	0
			Total	C	N	O	S		
2	KY	135	1050	649	177	220	4	0	0
			Total	C	N	O	S		
2	LY	135	1050	649	177	220	4	0	0
			Total	C	N	O	S		
2	MY	135	1050	649	177	220	4	0	0
			Total	C	N	O	S		
2	NY	135	1050	649	177	220	4	0	0
			Total	C	N	O	S		
2	OY	135	1050	649	177	220	4	0	0
			Total	C	N	O	S		
2	PY	135	1050	649	177	220	4	0	0
			Total	C	N	O	S		
2	QY	135	1050	649	177	220	4	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.

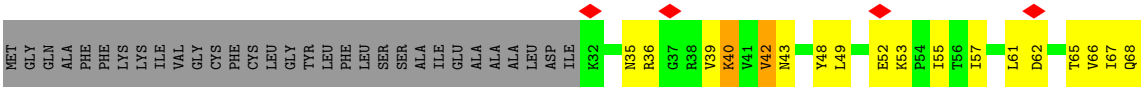
- Molecule 1: Cag pathogenicity island protein (Cag8)

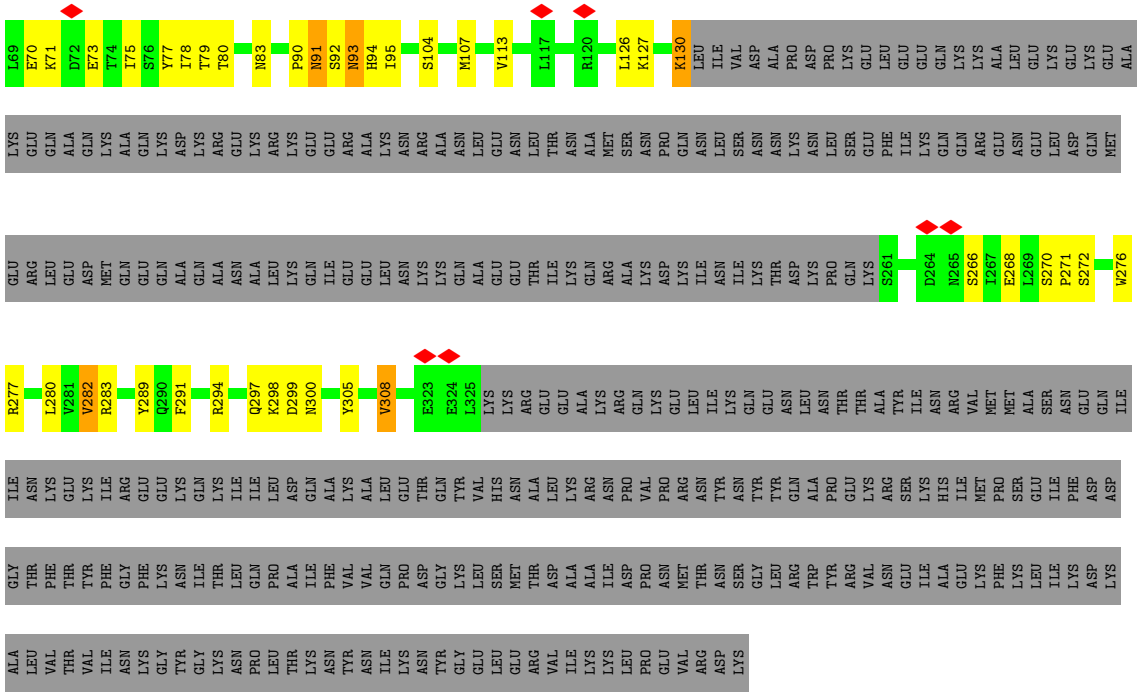
Chain AX:



- Molecule 1: Cag pathogenicity island protein (Cag8)

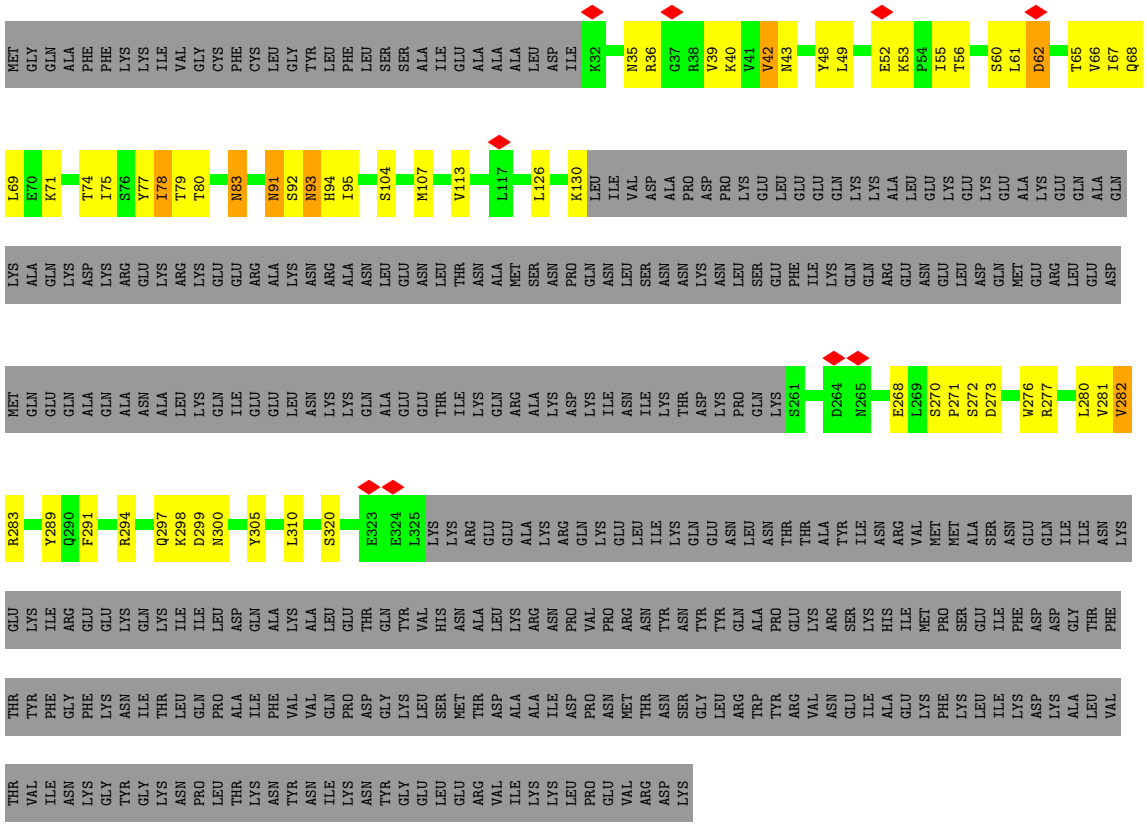
Chain BX:





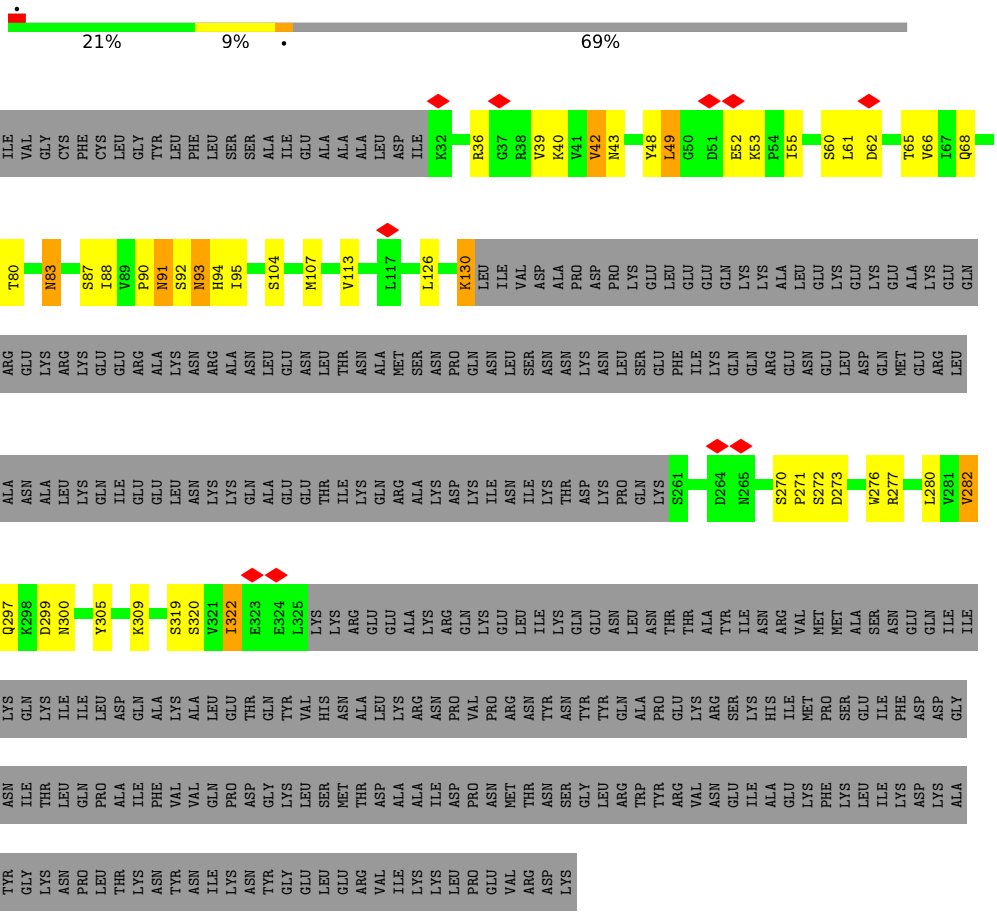
• Molecule 1: Cag pathogenicity island protein (Cag8)

Chain CX:



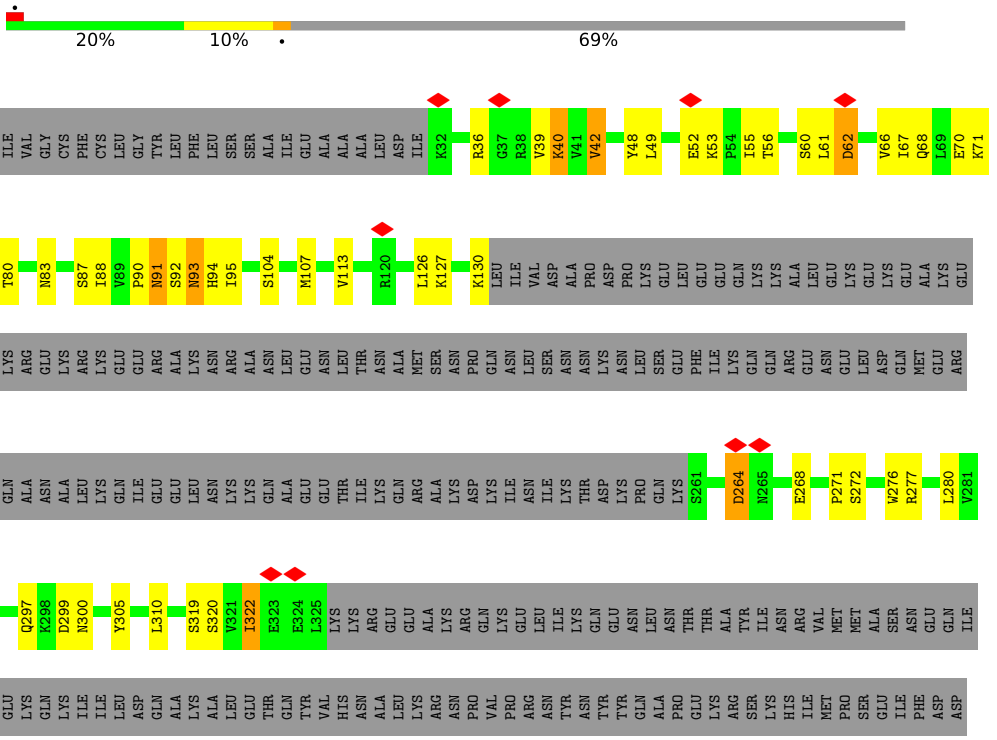
• Molecule 1: Cag pathogenicity island protein (Cag8)

Chain DX:



- Molecule 1: Cag pathogenicity island protein (Cag8)

Chain EX:



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

ALA LEU VAL THR VAL ILE ASN LYS GLY TYR GLY LYS ASN PRO LEU THR LYS ASN TYR ASN ILE LYS ASN TYR GLY GLU LEU GLU ARG VAL ILE LYS LYS LEU PRO GLU VAL ARG ASP LYS

- Molecule 1: Cag pathogenicity island protein (Cag8)

Chain FX:

MET GLY GLN ALA PHE PHE LYS LYS ILE VAL GLY CYS PHE CYS LEU GLY TYR LEU PHE LEU SER SER ALA ILE GLU ALA ALA ALA LEU ASP ILE K32 N35 R36 G37 R38 V39 V42 N43 Y48 L49 E52 K53 P54 I55 T56 S60 L61 D62 V66 I67 Q68 K71

D72 I75 S76 Y77 I78 T79 T80 N83 S87 I88 V89 P90 N91 S92 N93 H94 I95 F96 M107 V113 L126 K127 K130 LEU ILE VAL ASP ALA PRO ASP PRO LYS GLU LEU GLU GLU GLN LYS LYS ALA LEU GLU LYS GLU LYS GLU ALA LYS GLU GLU GLN ALA GLN LYS

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

GLN GLU GLN ALA GLN ALA ASN ALA LEU LYS LYS GLN ILE GLU GLU LEU ASN LYS LYS GLN ALA GLU GLU THR ILE LYS GLN ARG ALA LYS ASP LYS ILE ASN ILE LYS THR ASP LYS PRO GLN LYS S261 D264 N265 E268 P271 S272 D273 S274 A275 W276 R277 L280 V281 V282 R283

Y289 Q290 F291 R294 Q297 K298 D299 N300 Y305 L310 V318 S319 S320 V321 I322 E323 E324 L325 LYS LYS ARG GLU GLU ALA LYS ARG GLN LYS GLU LEU ILE LYS GLN GLU ASN LEU ASN THR THR ALA TYR ILE ASN ARG VAL MET MET ALA SER ASN GLU GLN ILE ILE

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

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

LEU VAL THR VAL ILE ASN LYS GLY TYR GLY LYS ASN PRO LEU THR LYS ASN TYR ASN ILE LYS ASN TYR GLY GLU LEU GLU ARG VAL ILE LYS LYS LEU PRO GLU VAL ARG ASP LYS

- Molecule 1: Cag pathogenicity island protein (Cag8)

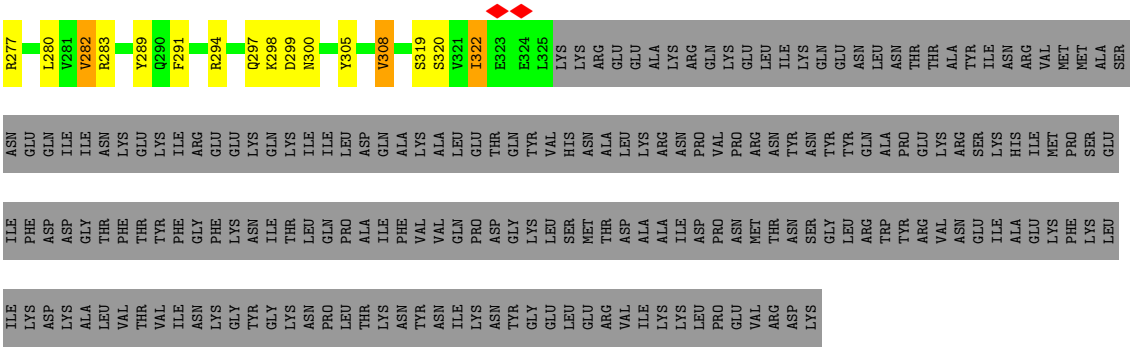
Chain GX:

MET GLY GLN ALA PHE PHE LYS LYS ILE VAL GLY CYS PHE CYS LEU GLY TYR LEU PHE LEU SER SER ALA ILE GLU ALA ALA ALA LEU ASP ILE K32 N35 R36 G37 R38 V39 V42 N43 Y48 L49 G50 D51 E52 K53 P54 I55 T56 S60 L61 D62 N63 V64 T65 V66 I67

Q68 L69 E70 K71 D72 E73 T74 I75 S76 Y77 I78 T79 T80 N83 S87 P90 N91 S92 N93 H94 I95 Q98 S104 M107 V113 L126 K130 LEU ILE VAL ASP ALA PRO ASP PRO LYS GLU LEU GLU GLU GLN LYS LYS ALA LEU GLU LYS GLU LYS GLU ALA

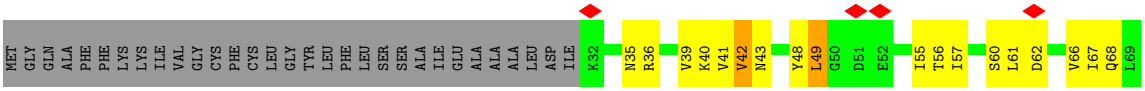
LYS GLU GLN ALA GLN LYS ALA GLN LYS ASP LYS ARG GLU LYS ARG LYS GLU GLU ARG ALA LYS ASN ARG ALA ASN LEU GLU ASN LEU THR ASN ALA MET SER ASN PRO GLN ASN LEU SER ASN ASN LYS ASN LEU SER GLU PHE ILE LYS GLN GLN ARG GLU ASN GLU LEU ASP GLN MET

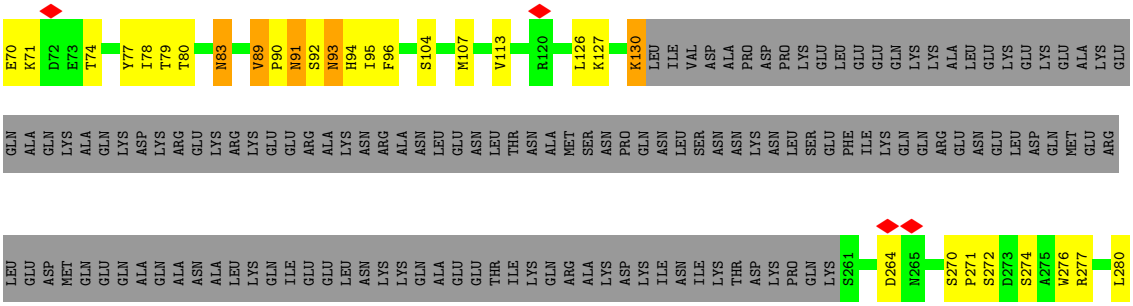
GLU ARG LEU GLU ASP MET GLN GLU GLN ALA GLN ALA ASN ALA LEU LYS GLN ILE GLU GLU LEU ASN LYS LYS GLN ALA GLU GLU THR ILE LYS GLN ARG ALA LYS ASP LYS ILE ASN ILE LYS THR ASP LYS PRO GLN LYS S261 D264 N265 S266 I267 E268 L269 S270 P271 S272 W276

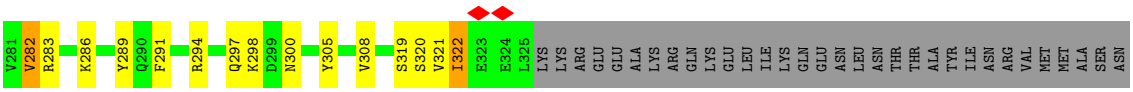


• Molecule 1: Cag pathogenicity island protein (Cag8)

Chain HX:

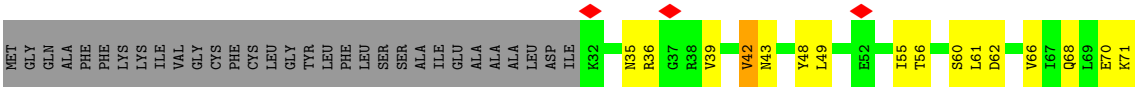


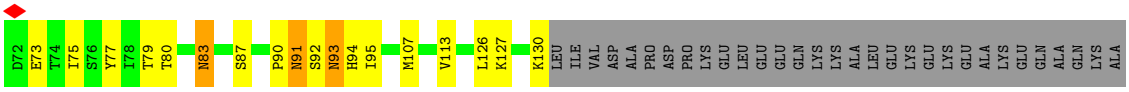


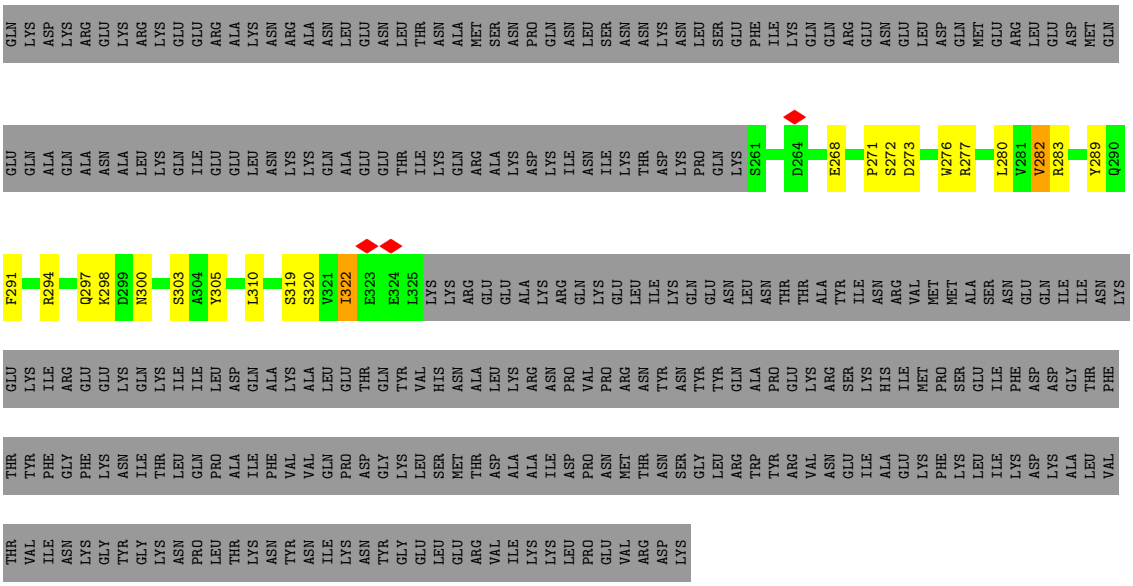


• Molecule 1: Cag pathogenicity island protein (Cag8)

Chain IX:

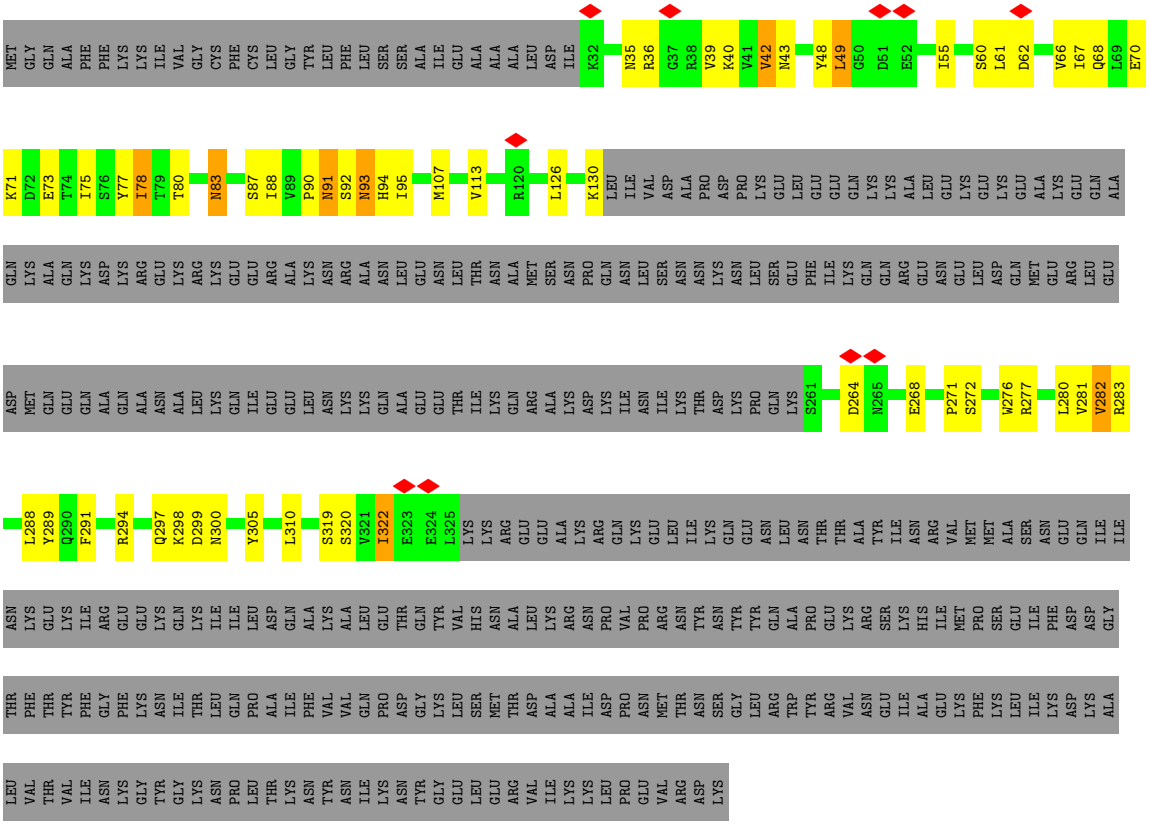






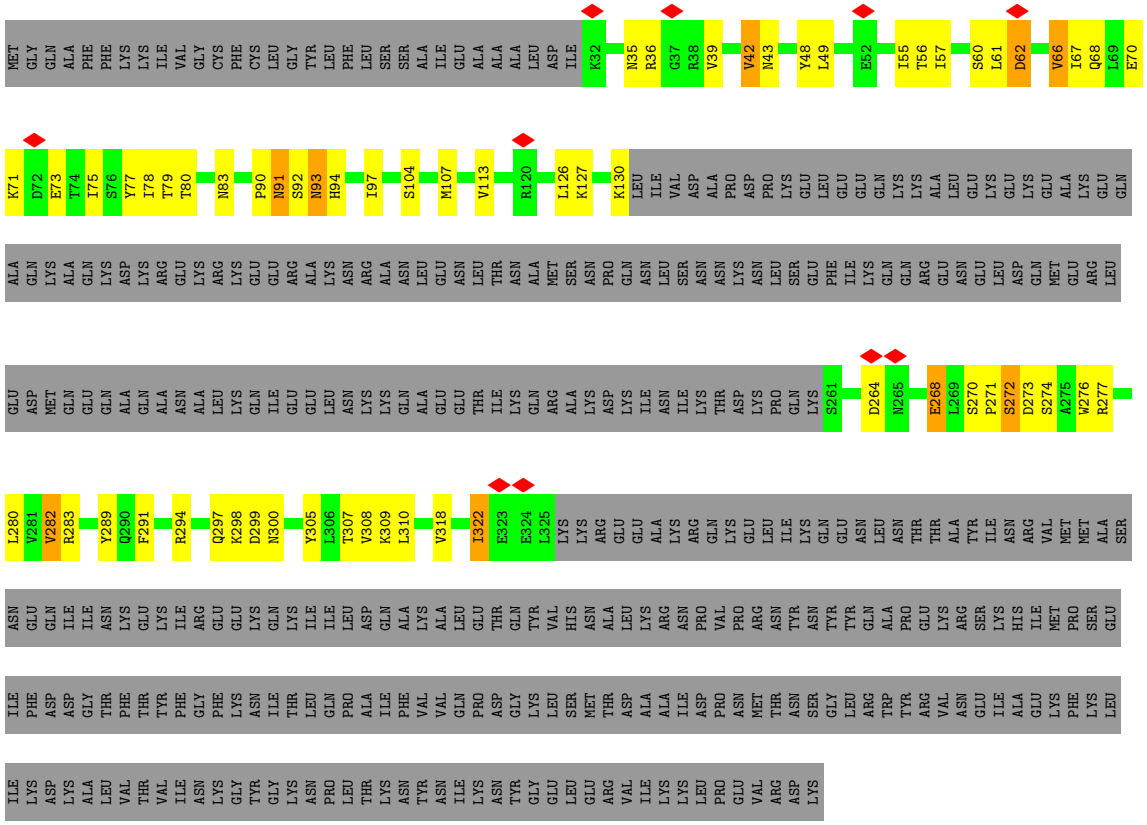
• Molecule 1: Cag pathogenicity island protein (Cag8)

Chain JX:



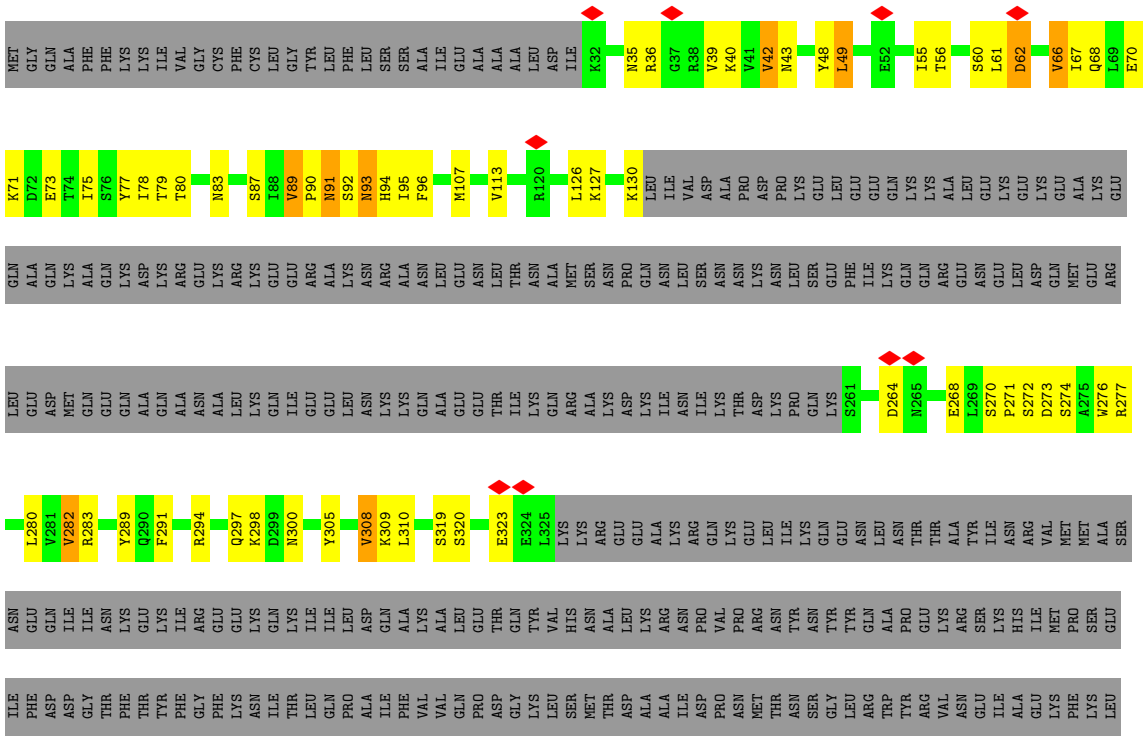
• Molecule 1: Cag pathogenicity island protein (Cag8)

Chain KX:



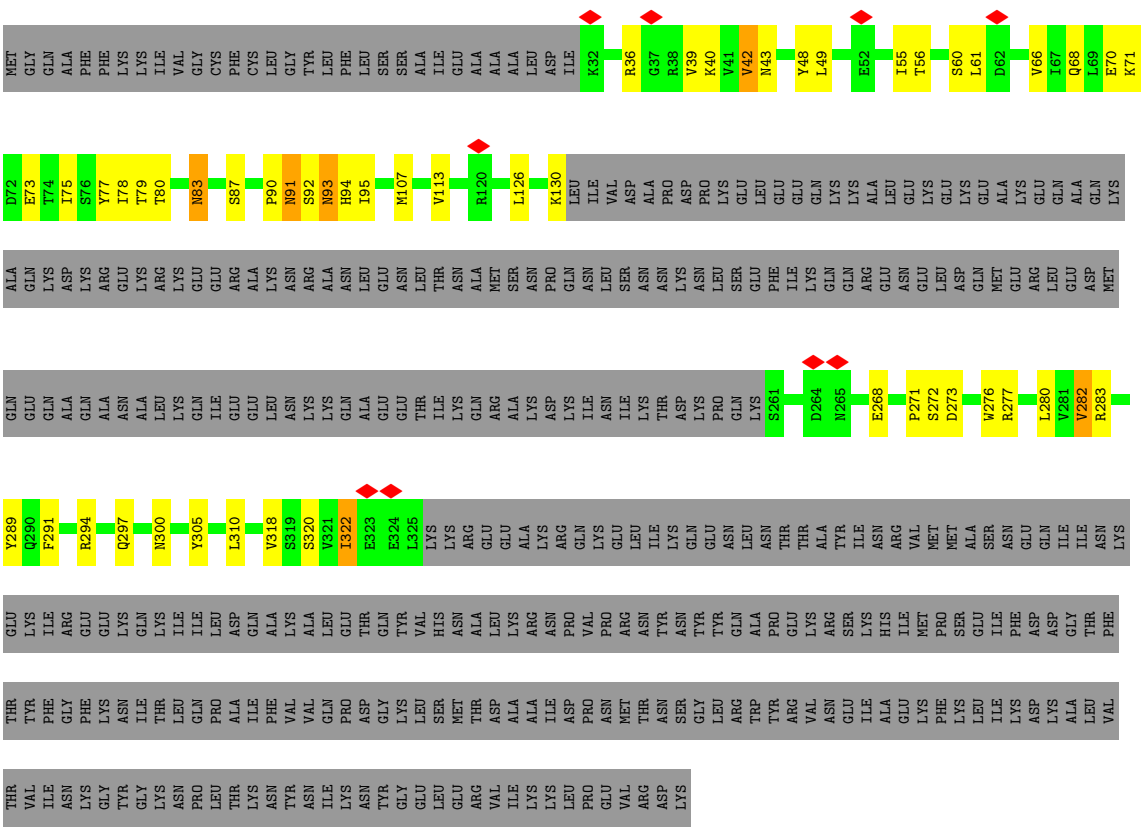
• Molecule 1: Cag pathogenicity island protein (Cag8)

Chain LX:



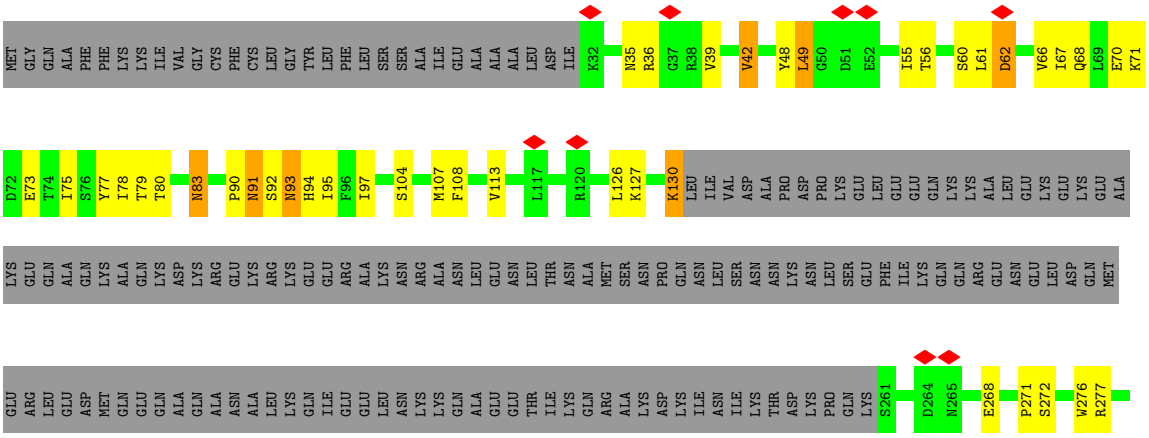
• Molecule 1: Cag pathogenicity island protein (Cag8)

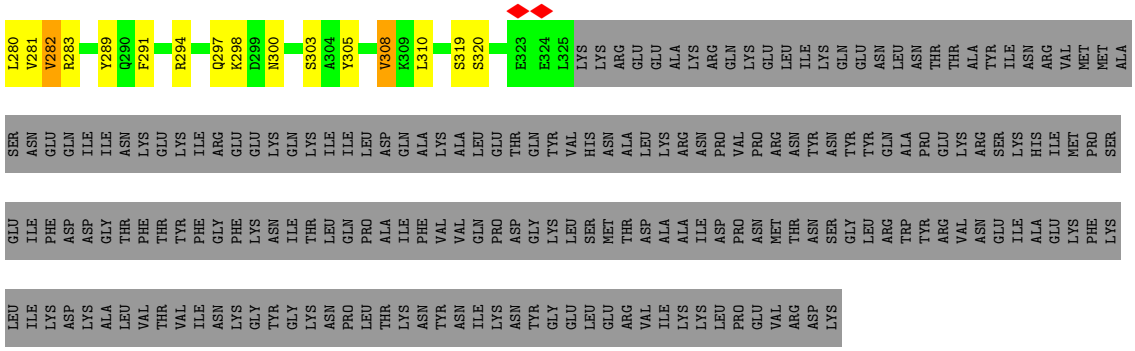
Chain MX:



• Molecule 1: Cag pathogenicity island protein (Cag8)

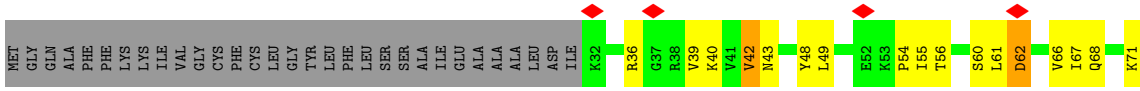
Chain NX:

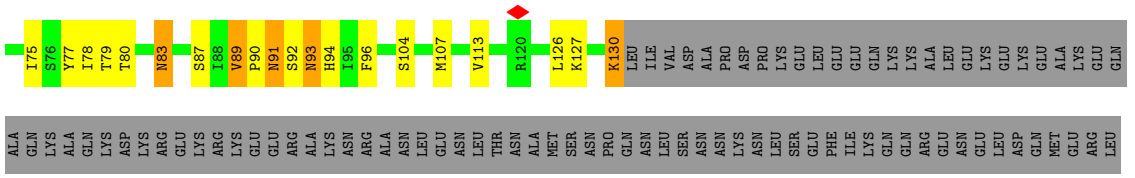


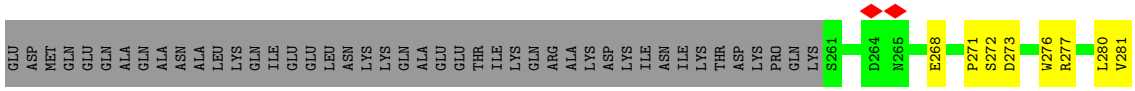


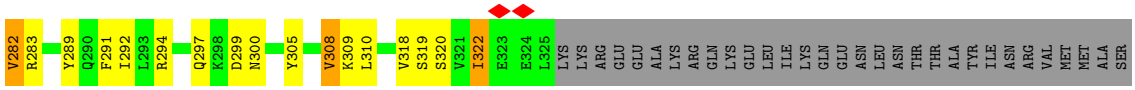
• Molecule 1: Cag pathogenicity island protein (Cag8)

Chain OX:



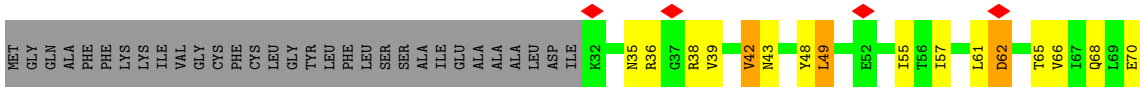


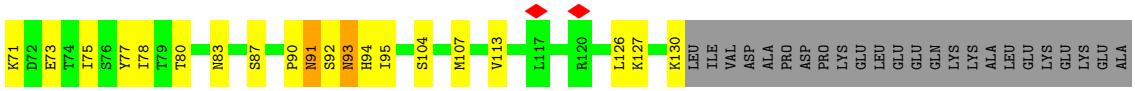


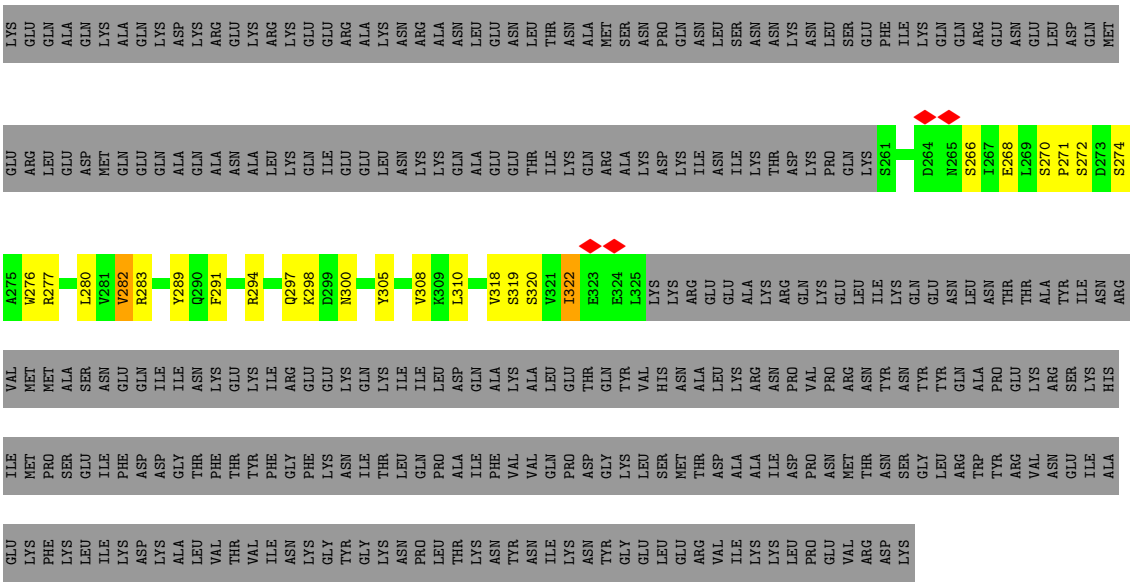


• Molecule 1: Cag pathogenicity island protein (Cag8)

Chain PX:

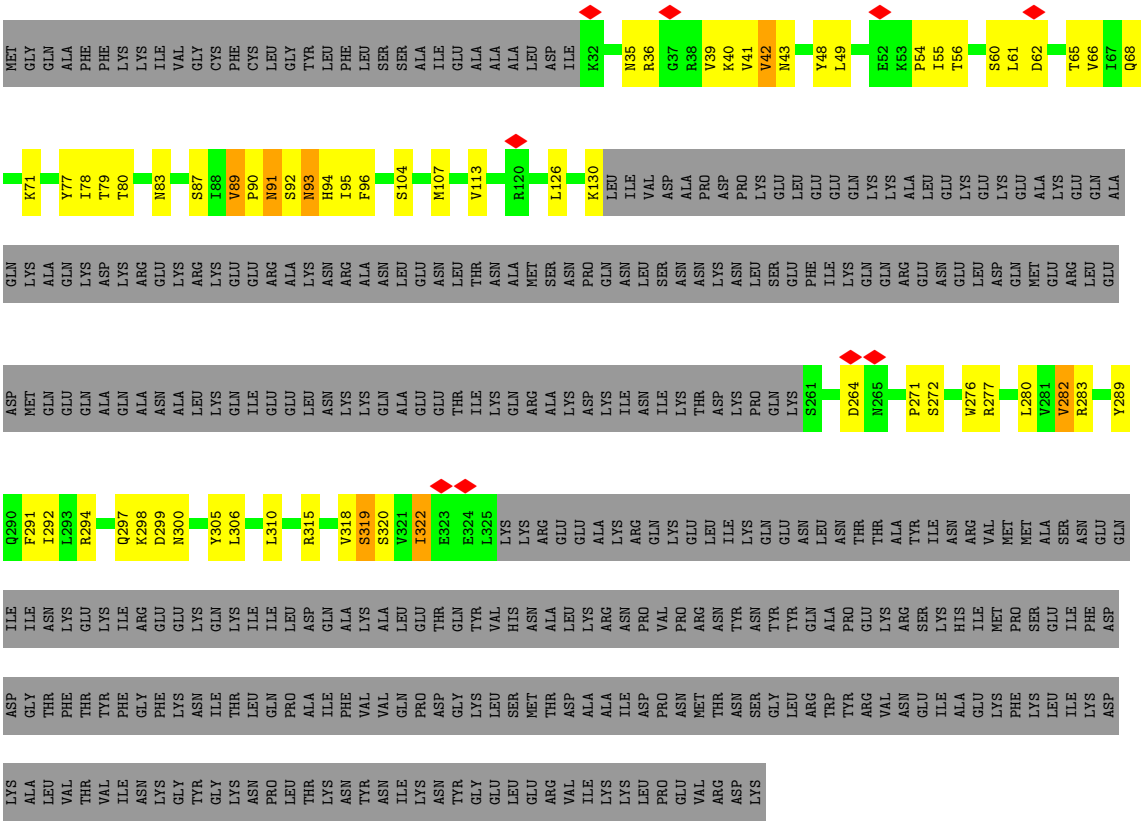




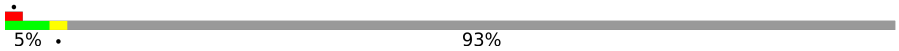


• Molecule 1: Cag pathogenicity island protein (Cag8)

Chain QX:



• Molecule 2: Cag pathogenicity island protein (Cag7)

Chain AY: 

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

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

ASP GLN GLU ASN ASN GLU TYR GLN GLU GLU THR GLN THR ASP LEU ILE ASP ASP GLU THR SER LYS LYS THR GLN GLN HIS SER PRO GLN ASP LEU SER ASN GLU GLU ALA THR GLU ALA ASN HIS PHE GLU ASN LEU LEU LYS GLU SER LYS GLU SER SER ASP HIS HIS LEU ASP ASN

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

GLU GLU THR GLN GLU LEU ASN GLU GLU ASP ASP GLN GLU ASN ASN GLU TYR GLN GLU GLU THR GLN THR ASP LEU ILE ASP ASP GLU THR SER LYS LYS THR GLN GLN HIS SER PRO GLN ASP LEU SER ASN GLU GLU ALA THR GLU ALA ASN HIS PHE GLU ASN LEU LEU LYS GLU SER

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

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

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

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

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

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

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

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

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

CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA ARG LYS LEU LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA

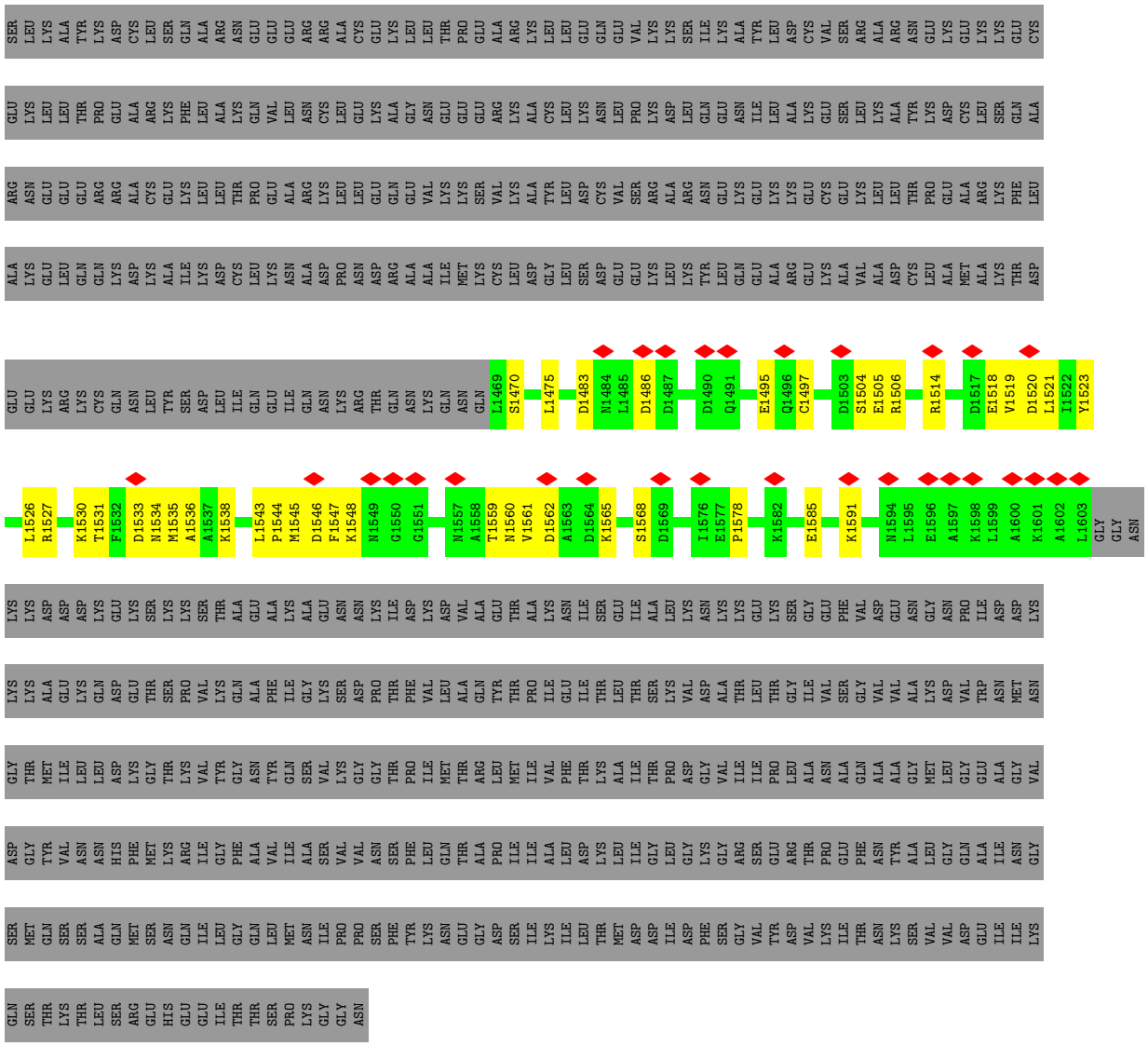
ARG LYS LEU LEU GLU GLU UNK ALA LYS GLU SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS ASN GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR LEU GLU SER LYS LYS LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA

LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LEU LEU GLU GLN GLN ALA LEU ASP CYS LEU LYS ASN ALA LYS THR GLU ALA ASP LYS LYS ARG CYS VAL LYS ASP LEU PRO LYS ASP LEU GLN LYS LYS VAL LEU ALA LYS GLU SER LEU LYS

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

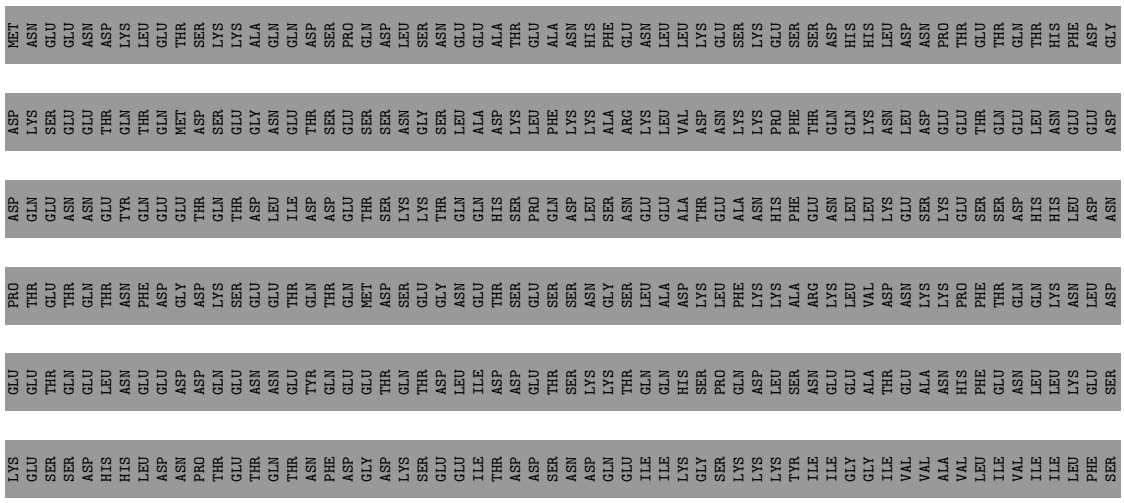
THR PRO GLU ALA ARG LYS LEU LEU GLU GLU ALA LYS GLU SER VAL LYS ALA TYR LYS ASP CYS VAL SER LYS ALA ARG ASN GLU LYS GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LEU LEU GLU GLN GLN VAL LEU ASP CYS LEU LYS ASN ALA LYS THR GLU

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



• Molecule 2: Cag pathogenicity island protein (Cag7)

Chain BY: 5% • 93%



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K1471
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S1479
D1483
D1486
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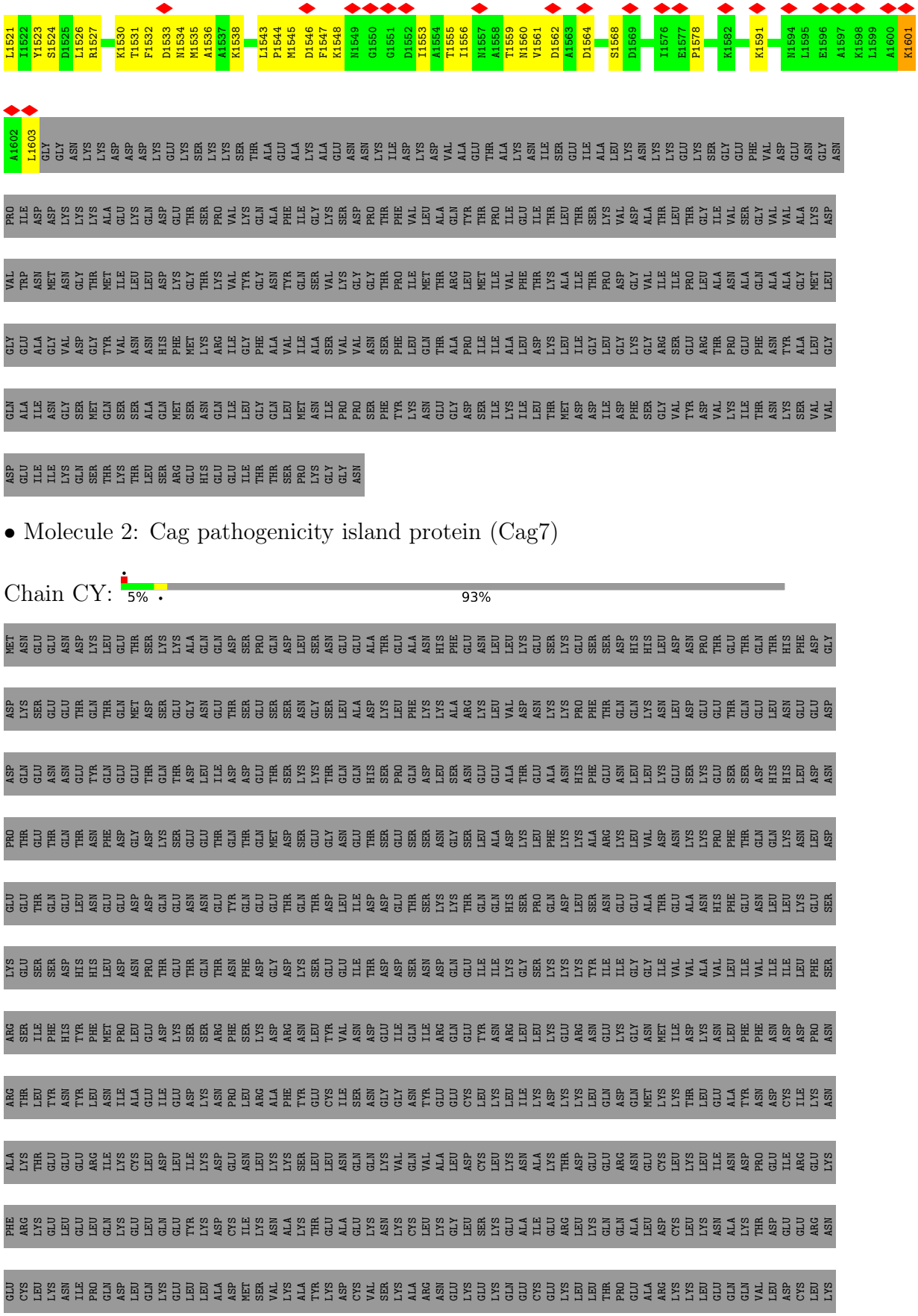
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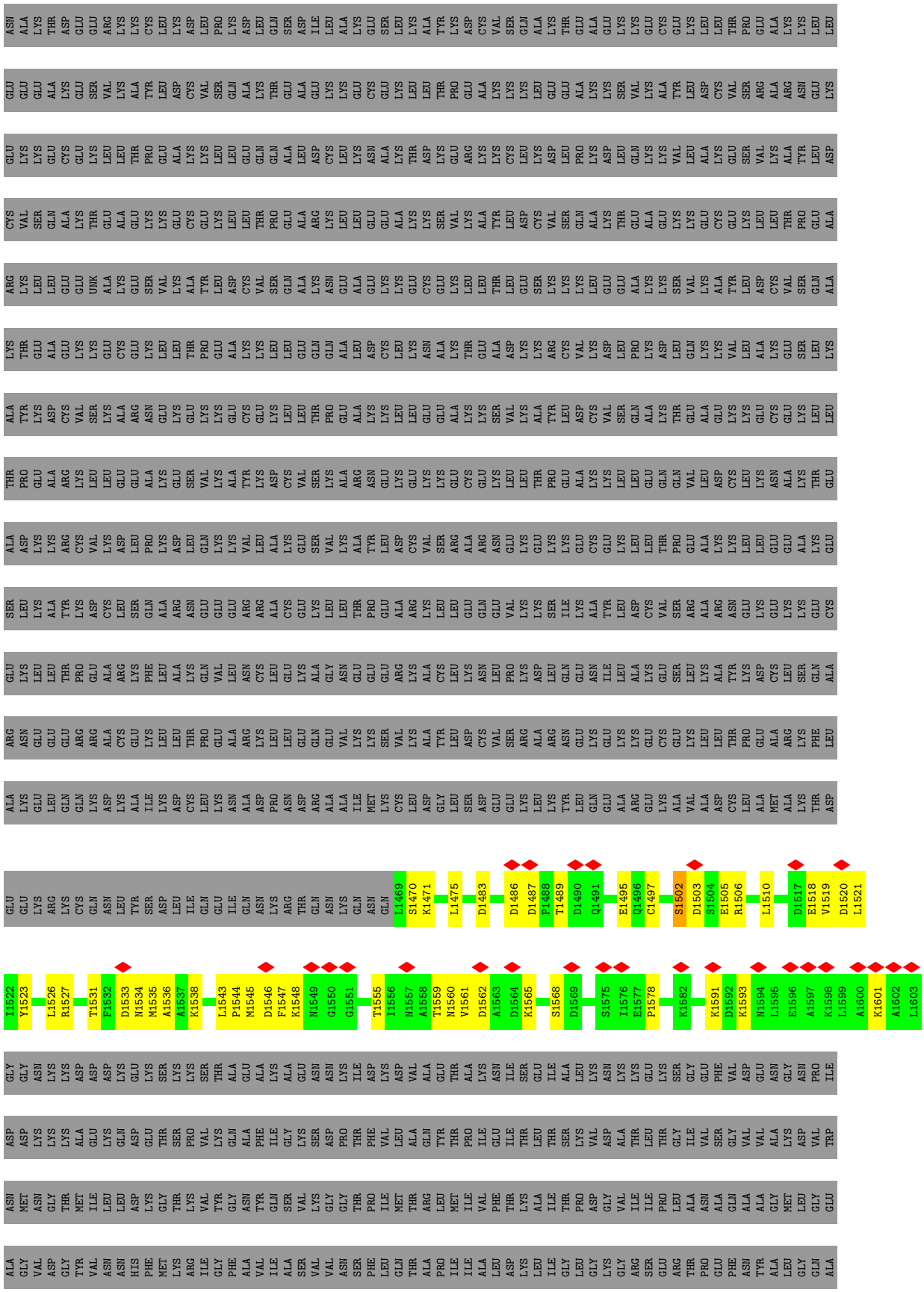
A1602 L1603 GLY GLY ASN LYS LYS ASP ASP ASP LYS GLU LYS THR SER LYS LYS SER THR ALA GLU ALA LYS ALA GLU ASN ASN LYS ILE ASP LYS ASP VAL ALA GLU ILE ILE ALA LEU LYS ASN GLY ASP GLY ASN
PRO ILE ASP ASP LYS LYS LYS ALA GLU LYS GLN ASP GLU THR SER PRO VAL LYS GLN ALA PHE ILE GLY LYS SER ASP PRO THR PHE VAL LEU ALA GLN TYR THR PRO ILE GLU ILE THR LEU THR SER LYS VAL ASP ALA THR LEU THR GLY ILE VAL SER GLY VAL VAL ALA LYS ASP
VAL TRP ASN MET ASN GLY THR MET ILE LEU LEU LEU ASP LYS GLY THR LYS VAL TYR GLY ASN TYR GLN SER VAL LYS GLY GLY THR PRO ILE MET THR ARG LEU MET ILE VAL PHE THR LYS ALA ILE THR PRO ASP GLY VAL ILE ILE PRO LEU ALA ASN ALA GLN ALA ALA GLY MET MET LEU
GLY GLU ALA GLY VAL ASP GLY GLY TYR VAL ASN ASN HIS PHE MET LYS ARG ILE GLY PHE ALA VAL ILE ALA SER VAL VAL ASN SER PHE LEU GLN THR ALA PRO ILE ILE ALA LEU ASP LYS LEU ILE GLY LEU GLY LYS GLY ARG SER GLU ARG THR PRO GLU PHE ASN TYR ALA LEU GLY
GLN ALA ILE ASN GLY SER MET GLN SER SER ALA GLN MET SER ASN GLN ILE LEU GLY GLN LEU MET ASN ILE PRO PRO SER PHE TYR LYS ASN GLU GLY ASP SER ILE LYS ILE LEU THR MET ASP ASP ILE ASP PHE SER GLY VAL TYR ASP VAL LYS ILE THR ASN LYS SER VAL VAL
ASP GLU ILE ILE LYS GLN SER THR LYS THR LEU SER ARG GLU HIS GLU GLU ILE THR THR SER PRO LYS GLY GLY ASN
• Molecule 2: Cag pathogenicity island protein (Cag7)
Chain CY: 5% 93%
MET ASN GLU GLU ASN ASP LYS LEU THR SER LYS LYS ALA GLN GLN ASP SER PRO GLN ASP LEU SER ASN GLU GLU ALA THR GLU ALA ASN HIS PHE GLU ASN LEU LEU LYS GLU SER LYS GLU SER SER ASP HIS HIS LEU ASP ASN PRO THR GLU THR GLN THR HIS PHE ASP GLY
ASP LYS SER GLU GLU THR GLN THR GLN MET ASP SER GLU GLY ASN GLU THR SER GLU SER SER ASN GLY SER LEU ALA ASP LYS LEU PHE LYS LYS ALA ARG LYS LEU VAL ASP ASN LYS LYS PRO PHE THR GLN GLN LYS ASN LEU ASP GLU GLU THR GLN GLU LEU ASN GLU GLU ASP
ASP GLN GLU ASN ASN GLU TYR GLN GLU GLU THR GLN THR ASP LEU ILE ASP GLU THR GLN GLN HIS SER PRO GLN ASP LEU SER ASN GLU GLU GLU THR GLU ALA ASN HIS PHE GLU ASN LEU LEU LYS GLU SER LYS GLU SER SER ASP HIS HIS LEU ASP ASN
PRO THR GLU THR GLN THR ASN PHE ASP GLY ASP LYS SER GLU GLU THR GLN THR GLN MET ASP SER GLU GLY ASN GLU THR SER GLU SER SER ASN GLY SER LEU ALA ASP LYS LYS LYS ALA ARG LYS LEU LEU VAL ASP ASN ASN LYS LYS GLU GLU THR GLN GLN LYS ASN LEU ASP GLU GLU THR GLN GLU LEU LYS LYS
GLU GLU THR GLN GLU LEU ASN GLU GLU ASP ASP GLN GLU ASN ASN GLU TYR GLN GLU GLU THR GLN THR SER GLU GLU ILE ASP ASP GLU THR SER SER LYS LYS THR GLN GLN HIS SER PRO GLN ASP LEU SER ASN GLU GLU ALA THR GLU GLU ASN HIS PHE GLU GLU ASN LYS LYS GLU SER
LYS GLU SER SER ASP HIS HIS LEU ASP ASN PRO THR GLU THR GLN THR ASN PHE ASP GLY ASP LYS SER GLU GLU ILE THR ASP ASP SER ASN GLY SER LEU ALA ASP LYS LEU PHE LYS LYS ALA ARG LYS LEU LEU VAL ASP ASN LYS LYS PRO PHE THR GLN GLN LYS ASN LEU ASP
ARG SER ILE PHE HIS TYR PHE MET PRO LEU GLU ASP LYS SER SER ARG PHE SER LYS ASP ARG ASN LEU LEU TYR VAL ASN ASP GLU ILE GLN ILE ARG GLN GLU TYR ASN ARG LEU LEU LYS GLU LYS LYS GLU GLU ILE ILE GLY GLY ASN MET ILE VAL VAL ALA VAL LEU ILE VAL ILE ILE LEU PHE ASN ASP PRO ASN
ARG THR LEU TYR ASN TYR LEU ASN ILE ALA GLU ILE GLU ASP LYS ASN PRO LEU ARG LYS ASN ALA PHE TYR GLU CYS ILE SER ASN GLY GLY ASN TYR GLU ILE ILE SER ASN GLU GLN GLN ASP GLN GLU CYS LEU LYS LEU LEU ILE LYS ASP LYS LYS LEU GLN GLN MET LYS LYS THR LEU GLU ALA TYR ASN ASP CYS ILE LYS ASN
ALA LYS THR GLU GLU GLU ARG ILE LYS CYS LEU ASP LEU ILE LYS ASP GLU CYS ASN LEU LYS SER LEU LEU ASN GLN GLN LYS VAL GLN VAL ALA LEU ASP CYS LEU LYS ASN ALA LYS THR ASP GLU GLU ARG ASN GLU CYS LEU LYS LEU ILE ASN ALA PRO GLU ILE LYS GLU
PHE ARG LYS GLU LEU LYS GLU GLU GLN LYS GLU GLU TYR LYS ASP CYS ILE LYS ASN ALA ALA LYS THR GLU ALA ASP LYS SER GLY LEU LYS GLU ILE ALA LEU LYS ASN ALA LEU ASP ASP LEU LYS ASN ALA ALA ALA ASP CYS LEU LYS LEU ILE ALA ARG GLU LYS
GLU CYS LEU LYS ASN ILE PRO GLN ASP LEU LEU LYS GLU LEU ALA ASP MET SER VAL ALA LYS ALA TYR LYS ASP CYS VAL SER LYS ALA ARG ASN GLU LYS GLN LYS GLU LYS GLN CYS GLU LYS LEU LEU THR PRO GLU ALA ARG LYS LYS LEU GLU GLN VAL LEU ASP CYS LYS LEU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GLU GLU GLU ALA LYS GLU SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LYS LEU GLU SER VAL LYS ALA ARG ASN GLU LYS
GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LYS LEU LEU GLU GLN ALA LEU ASP CYS LEU LYS ASN ALA LYS THR ASP LYS GLU ARG LYS CYS LEU LYS ASP LEU GLN LYS LYS LYS LEU ALA LYS GLU SER GLN LYS LYS ASP
CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LYS LEU LEU THR THR PRO GLU ALA ARG LYS LEU LYS GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LYS LEU LEU THR PRO GLU ALA
ARG LYS LEU LEU GLU GLU UNK ALA ALA LYS GLU SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA ALA LYS ASN GLU ALA LEU GLU LYS LYS LEU LEU LYS LYS GLU ALA LYS LYS LEU LEU THR LEU GLU SER GLN ALA
LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LYS LEU THR PRO GLU ALA LYS LYS LEU LEU GLU GLN GLN ALA LEU ASP CYS LEU LYS ASN ALA LYS THR GLU LYS LYS ASP LYS LYS LYS ARG CYS VAL LYS ASP LEU PRO LYS ASP LEU GLN LYS LYS VAL LEU LEU LYS
ALA TYR LYS ASP CYS VAL SER LYS LYS ALA ARG ASN GLU LYS GLU LYS LYS LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LEU LEU LEU LEU LYS LYS SER VAL LYS LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS LYS LEU LEU LYS LYS GLU CYS GLU LYS LYS LEU LEU
THR PRO GLU ALA ARG LYS LEU LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LYS ASP CYS VAL SER LYS ALA ARG ASN GLU LYS GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LEU LEU LEU LEU GLN GLN VAL LEU ASP CYS LEU LYS ASN ALA LYS THR GLU
ALA ASP LYS LYS ARG CYS VAL LYS ASP LEU PRO LYS ASP LEU GLN LYS LYS VAL LEU ALA LYS GLU SER VAL LYS ALA TYR LEU ASP CYS VAL SER ARG ALA ARG ASN GLU LYS GLU CYS GLU LYS LYS LEU LEU THR PRO GLU ALA LYS LYS LEU LEU GLU GLU ALA LYS LYS GLU
SER LEU LYS ALA TYR LYS ASP CYS LEU SER GLN ALA ARG ASN GLU GLU GLU ARG ARG ALA CYS GLU LYS LYS LEU LEU THR PRO GLU ALA ARG LYS LEU LEU GLU GLN GLU LYS LYS SER ILE LYS ALA TYR LEU ASP CYS VAL SER ARG ALA ARG ASN GLU LYS GLU LYS LYS GLU CYS
GLU LYS LEU LEU THR PRO GLU ALA ARG LYS PHE LEU ALA LYS GLN VAL LEU ASN CYS LEU GLU LYS LYS LYS ASP LEU GLN GLU ASN ILE LEU ALA LYS GLU SER GLN GLN VAL LEU LYS ALA TYR LYS ASP CYS GLU LYS LYS LEU LEU LYS ASN CYS GLU LYS LYS LEU SER GLN ALA
ARG ASN GLU GLU GLU ARG ARG ALA CYS GLU LYS LEU LEU THR PRO GLU ALA ARG LYS LYS LEU LEU GLU GLN GLU VAL LYS LYS SER ARG ALA ARG ASN GLU LYS GLU LYS LYS GLU CYS GLU LYS LYS LEU LEU LEU THR PRO GLU ALA ARG LYS PHE LEU
ALA LYS GLU LEU GLN GLN LYS ASP LYS ALA LYS ILE LYS ASP CYS LEU LYS ASN ALA ALA ASP PRO ASN ASP ARG ALA ALA LYS GLY ASN GLU GLU GLU LYS LYS LEU LEU LYS ASP GLY LEU SER ASP GLU GLU LYS LEU LYS TYR LEU GLN GLU ASN ILE LEU ALA ARG GLU LYS THR ASP
GLU GLU LYS ARG LYS CYS TYR SER ASP LEU ILE GLN GLU ILE GLN ASN LEU TYR SER LYS ARG THR GLN ASN LYS GLN ASN GLN L1469 S1470 K1471 L1475 D1483 D1486 D1487 P1488 T1489 D1490 Q1491 E1495 Q1496 C1497 S1502 D1503 S1504 E1505 R1506 L1510 D1517 E1518 V1519 D1520 L1521
I1522 Y1523 L1526 R1527 T1531 F1532 D1533 N1534 M1535 A1536 A1537 K1538 L1543 P1544 M1545 D1546 F1547 K1548 N1549 G1550 G1551 T1555 I1556 N1557 A1558 T1559 N1560 V1561 D1562 A1563 D1564 K1565 S1568 D1569 S1575 I1576 E1577 P1578 K1582 K1591 D1592 K1593 N1594 L1595 E1596 A1597 K1598 L1599 A1600 K1601 A1602 L1603
GLY GLY ASN LYS LYS ASP ASP ASP LYS GLU LYS SER LYS LYS ALA GLU ASN ASN ASN LYS ASP LYS ILE ASP LYS ASP VAL ALA GLU TYR THR PHE ILE ALA GLU LYS ASN ILE SER GLU ILE ALA LEU LYS ASN LYS LYS LYS GLU SER GLY GLU PHE VAL ASP GLU ASN GLY ASN PRO ILE
ASP ASP LYS LYS LYS ALA GLU LYS GLN ALA PHE ILE GLY LYS SER ASP PRO THR PHE VAL LEU ALA GLN TYR THR PHE VAL SER GLY LYS GLU THR GLY ILE VAL SER GLY VAL VAL ALA LYS ASP VAL TRP
ASN MET ASN GLY THR MET ILE LEU LEU ASP LYS GLY THR LYS VAL TYR GLN ILE SER VAL GLY GLY THR PRO ILE MET THR ARG LEU MET ILE VAL PHE THR LYS ALA ILE THR PRO ASP GLY VAL ILE ILE ILE LEU LEU ASN ALA GLN ALA ALA GLY MET LEU GLY GLU
ALA GLY VAL ASP GLY TYR VAL ASN ASN HIS PHE MET LYS ARG ILE ALA VAL ALA SER VAL VAL ASN SER PHE LEU GLN THR ALA PRO ILE ILE LEU GLY LYS LYS GLY ARG SER GLU ARG THR PRO GLU PHE ASN TYR ALA LEU GLY GLN ALA

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

ILE ILE LYS GLN SER THR LYS THR LEU SER ARG GLU HIS GLU GLU ILE THR THR SER PRO LYS GLY GLY ASN

• Molecule 2: Cag pathogenicity island protein (Cag7)

Chain DY: 5% 93%

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

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

ASP GLN GLU ASN ASN GLU TYR GLN GLU GLU THR GLN THR ASP GLU THR SER LYS LYS THR GLN GLN HIS SER PRO GLN ASP LEU SER ASN GLU GLU ALA ASN HIS PHE GLU ASN LEU LEU LYS GLU SER LYS GLU SER SER ASP HIS HIS LEU ASP ASN

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

GLU GLU THR GLN GLU LEU ASN GLU GLU ASP ASP GLN GLU ASN ASN GLU TYR GLN GLU GLU THR GLN THR ASP LEU ILE ASP ASP GLU THR SER LYS LYS THR GLN GLN HIS SER PRO GLN ASP LEU SER ASN GLU GLU ALA THR GLU ALA ASN HIS PHE GLU ASN LEU LEU LYS GLU SER

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

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

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

ALA LYS THR GLU GLU ARG ILE LYS CYS LEU ASP LEU ILE LYS ASP GLU ASN LEU LYS LYS LYS SER LEU LEU ASN GLN GLN LYS VAL GLN VAL ALA LEU ASP CYS LEU LYS ASN ALA LYS THR ASP GLU GLU ARG ASN GLU CYS LEU LYS LEU ILE ARG GLU LYS

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

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

ASN ALA LYS THR ASP GLU GLU ARG LYS LYS LEU LYS ASP LEU LEU ALA LYS GLU SER LYS LYS ALA ALA LYS ASP ILE LEU ALA LYS GLN LEU LYS ALA ASP CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS LYS LEU LEU

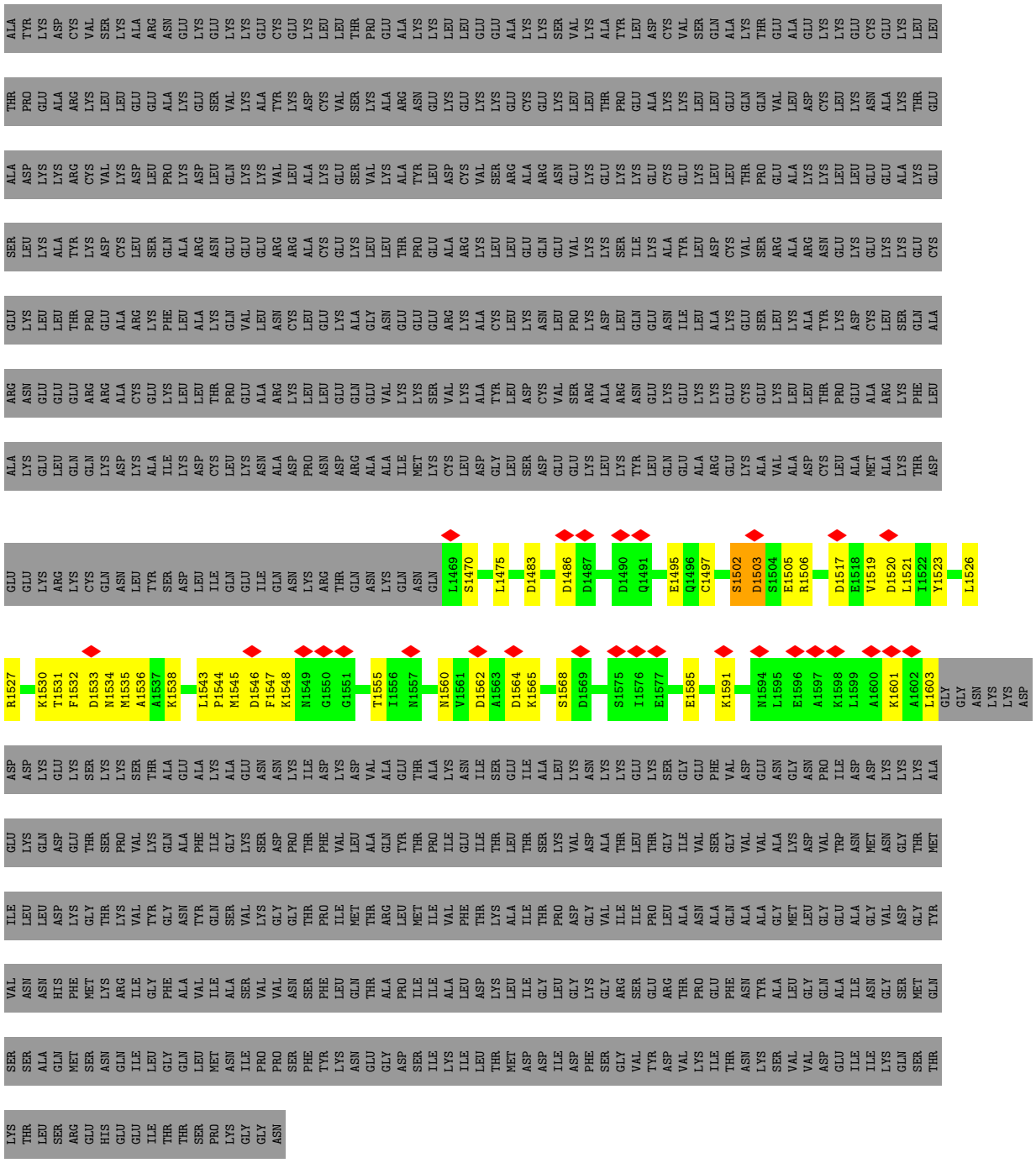
GLU GLU GLU ALA LYS GLU SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS THR GLU ALA ALA LYS GLU GLU CYS GLU LEU LEU THR PRO GLU ALA LYS LYS LEU GLU GLU ALA TYR LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER ARG ALA ARG ASN GLU LYS

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

CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS THR PRO GLU ALA ARG LYS LEU LEU THR GLU LYS LEU LEU GLU CYS GLU LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS THR GLU GLU ALA GLU LYS LYS LYS LEU GLU CYS GLU LYS LEU LEU ALA

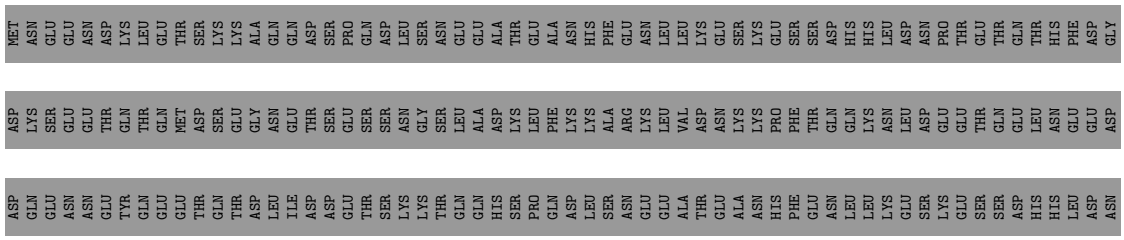
ARG LYS LEU LEU GLU UNK ALA LYS GLU SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS LYS ASN GLU ALA LEU GLU CYS LYS LYS GLU CYS GLU LEU THR LEU GLU GLU SER LYS LYS LYS LEU GLU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS LYS LYS LEU GLU

LYS THR GLU ALA GLU LYS LYS GLU GLN GLN ALA LEU ASP CYS LEU LYS ASN ALA LYS THR GLU ALA ASP LYS LYS ARG CYS VAL LYS ASP LEU PRO LYS ASP LEU GLN LYS LYS VAL LEU ALA LYS GLU SER LEU LYS



- Molecule 2: Cag pathogenicity island protein (Cag7)

Chain EY: 5% 93%



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

GLU GLU THR GLN GLU LEU ASN GLU GLU ASP ASP GLN GLU ASN ASN GLU TYR GLN GLU GLU THR GLN THR ASP LEU ILE ASP ASP GLU THR SER LYS LYS THR GLN GLN HIS SER PRO GLN ASP LEU SER ASN GLU GLU ALA THR GLU ALA ASN HIS PHE GLU ASN LEU LEU LYS GLU SER

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

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

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

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

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

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

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

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

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

CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA ARG LYS LEU LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA

ARG LYS LEU LEU GLU GLU UNK ALA LYS GLU SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS ASN GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR LEU GLU SER LYS LYS LYS LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA

LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LEU LEU GLU GLN GLN ALA LEU ASP CYS LEU LYS ASN ALA LYS THR GLU ALA ASP LYS LYS ARG CYS VAL LYS ASP LEU PRO LYS ASP LEU GLN LYS LYS VAL LEU ALA LYS GLU SER LEU LYS

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

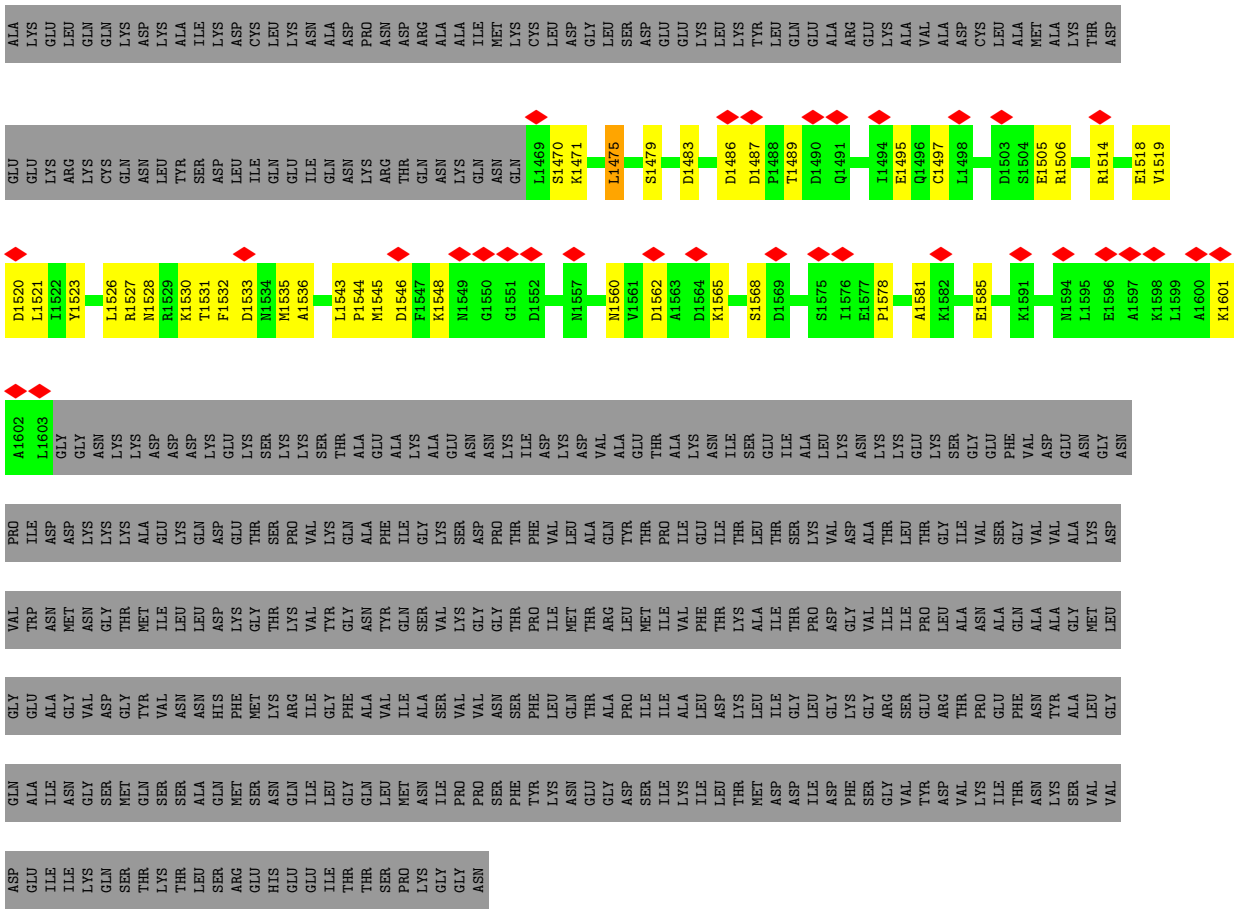
THR PRO GLU ALA ARG LYS LEU LEU GLU GLU ALA LYS GLU SER VAL LYS ALA TYR LYS ASP CYS VAL SER LYS ALA ARG ASN GLU LYS GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LEU LEU GLU GLN GLN VAL LEU ASP CYS LEU LYS ASN ALA LYS THR GLU

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

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

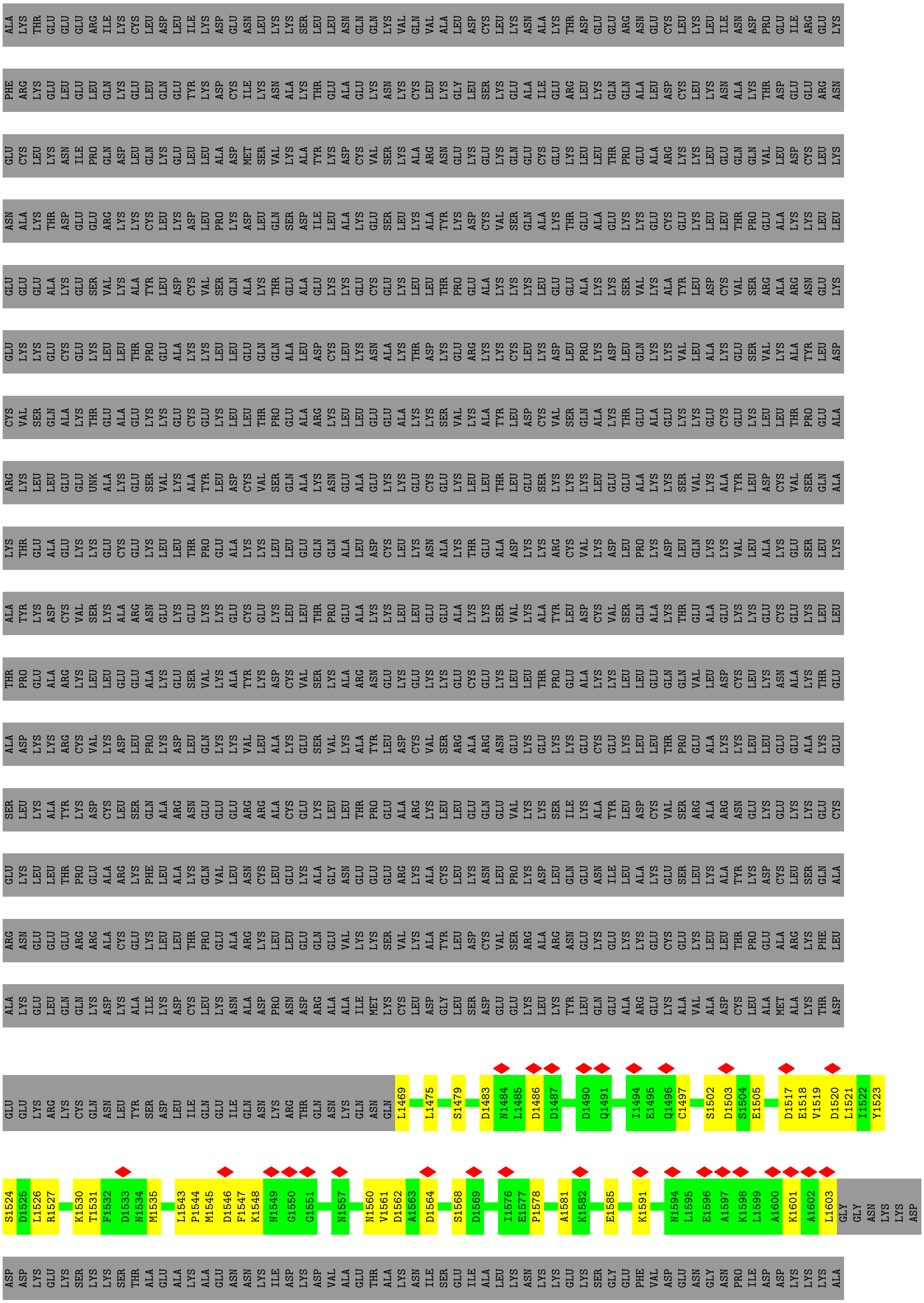
GLU LYS LEU LEU THR PRO GLU ALA ARG LYS PHE LEU ALA LYS GLN VAL LEU ASN CYS LEU GLU LYS ALA GLY ASN GLU GLU GLU ARG LYS ALA CYS LEU LYS ASN LEU PRO LYS ASP LEU GLN GLU ASN ILE LEU ALA LYS GLU SER LEU LYS ALA TYR LYS ASP CYS LEU SER GLN ALA

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



• Molecule 2: Cag pathogenicity island protein (Cag7)

Chain FY: 5% • 93%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L1475
S1479
D1483
N1484
L1485
D1486
D1487
D1490
Q1491
I1494
E1495
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C1497
S1502
D1503
S1504
E1505
D1517
E1518
V1519
D1520
L1521
I1522
Y1523
S1524
D1525
L1526
R1527
K1530
T1531
F1532
D1533
N1534
M1535
L1543
P1544
M1545
D1546
F1547
K1548
N1549
G1550
G1551
N1557
N1560
V1561
D1562
A1563
D1564
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I1576
E1577
P1578
A1581
K1582
E1585
K1591
N1594
L1595
E1596
A1597
K1598
L1599
A1600
K1601
A1602
L1603
GLY
GLY
ASN
LYS
LYS
ASP

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

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

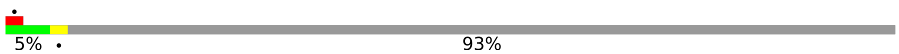
VAL ASN ASN HIS PHE MET LYS ARG ILE GLY PHE ALA VAL ILE ALA SER VAL VAL ASN SER PHE LEU GLN THR ALA PRO ILE ILE ALA LEU ASP LYS LEU ILE GLY LEU GLY LYS GLY ARG SER GLU ARG THR PRO GLU PHE ASN TYR ALA LEU GLY GLN ALA ILE ASN GLY SER MET GLN

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

LYS THR LEU SER ARG GLU HIS GLU GLU ILE THR THR SER PRO LYS GLY ASN

- Molecule 2: Cag pathogenicity island protein (Cag7)

Chain GY:



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

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

ASP GLN GLU ASN ASN GLU TYR GLN GLU GLU THR GLN THR ASP LEU ILE ASP ASP GLU THR SER LYS LYS THR GLN GLN HIS SER PRO GLN ASP LEU SER ASN GLU GLU ALA THR GLU ALA ASN HIS PHE GLU ASN LEU LEU LYS GLU SER LYS GLU SER SER ASP HIS HIS LEU ASP ASN

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

GLU GLU THR GLN GLU LEU ASN GLU GLU ASP ASP GLN GLU ASN ASN GLU TYR GLN GLU GLU THR GLN THR ASP LEU ILE ASP ASP GLU THR SER LYS LYS THR GLN GLN HIS SER PRO GLN ASP LEU SER ASN GLU GLU ALA THR GLU ALA ASN HIS PHE GLU ASN LEU LEU LYS GLU SER

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

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

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

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

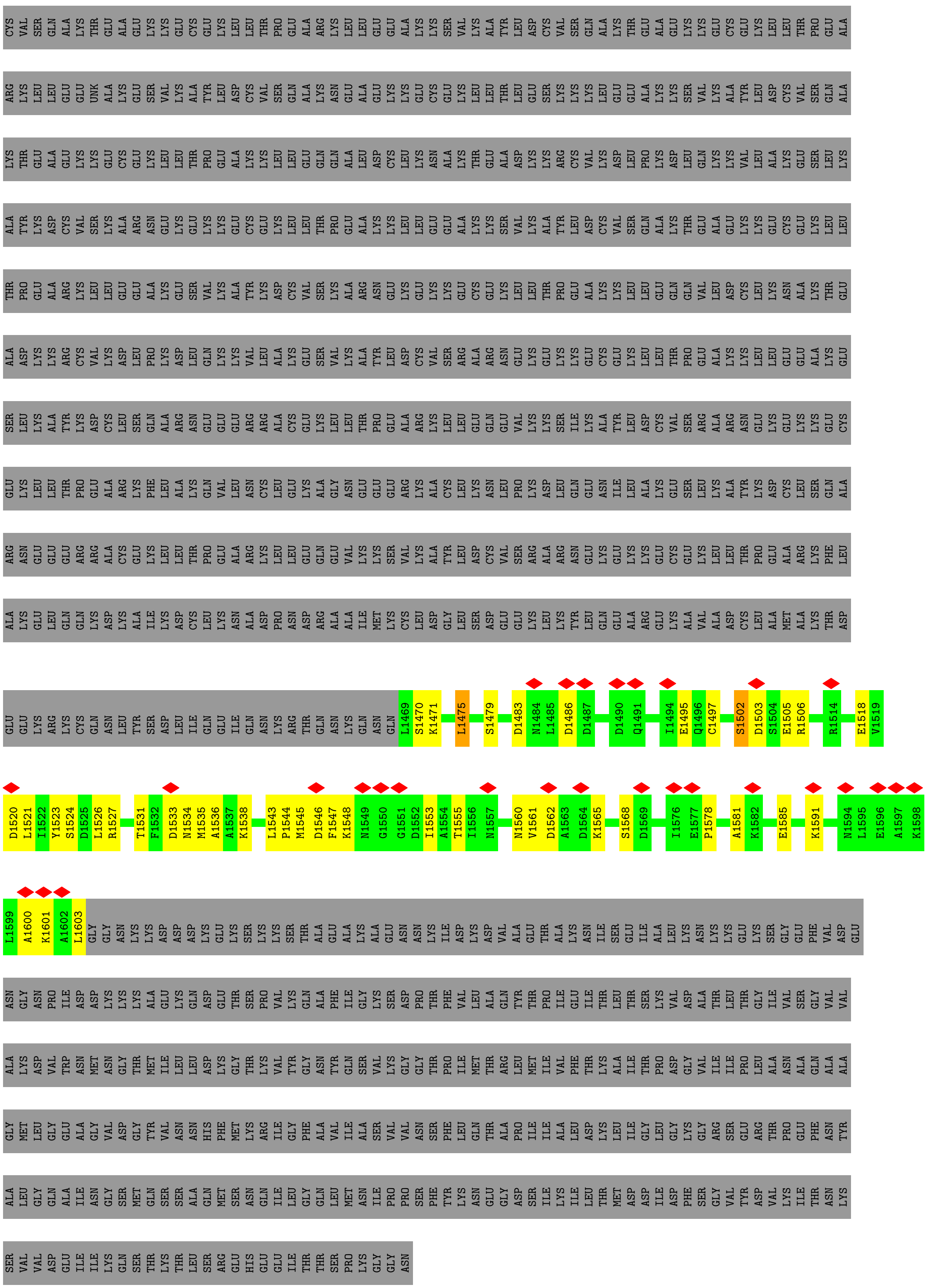
PHE ARG LYS GLU LEU GLU LEU GLN LYS GLU LEU GLN GLU TYR LYS ASP CYS ILE LYS ASN ALA LYS THR GLU ALA GLU LYS ASN LYS CYS LEU LYS GLY LEU SER LYS GLU ALA ILE GLU ARG LEU LYS GLN GLN ALA LEU ASP CYS LEU LYS ASN ALA LYS THR ASP GLU GLU ARG ASN

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

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

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

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



• Molecule 2: Cag pathogenicity island protein (Cag7)

Chain HY:

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

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

ASP GLN GLU ASN ASN GLU TYR GLN GLU GLU THR GLN THR ASP LEU ILE ASP ASP GLU THR SER LYS LYS THR GLN GLN HIS SER PRO GLN ASP LEU SER ASN GLU GLU ALA THR GLU ALA ASN HIS PHE GLU ASN LEU LEU LYS GLU SER LYS GLU SER SER ASP HIS HIS LEU ASP ASN

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

GLU GLU THR GLN GLU LEU ASN GLU GLU ASP ASP GLN GLU ASN ASN GLU TYR GLN GLU GLU THR GLN THR ASP LEU ILE ASP ASP GLU THR SER LYS LYS THR GLN GLN HIS SER PRO GLN ASP LEU SER ASN GLU GLU ALA THR GLU ALA ASN HIS PHE GLU ASN LEU LEU LYS GLU SER

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

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

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

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

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

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

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

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

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

CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA ARG LYS LEU LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA

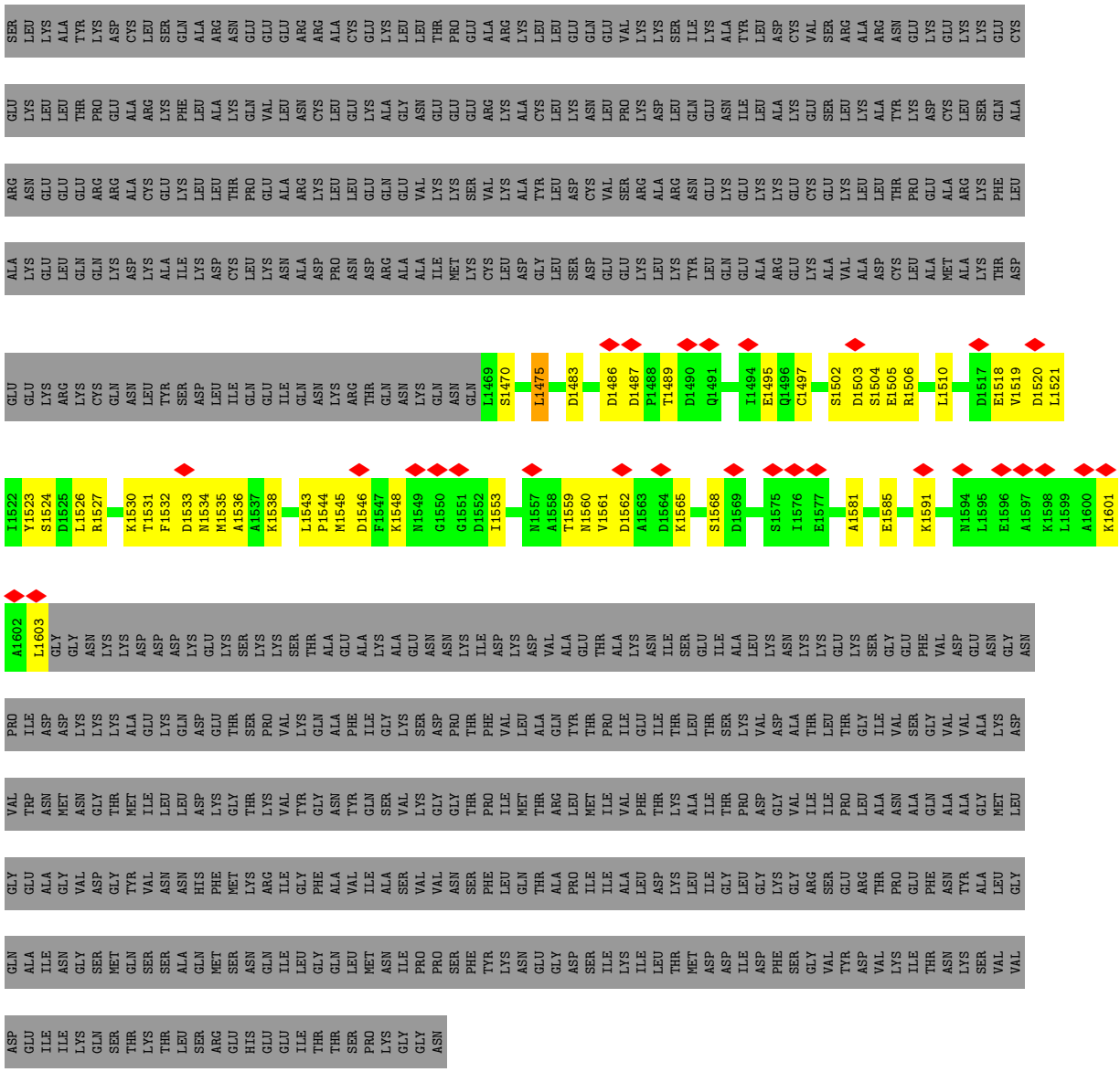
ARG LYS LEU LEU GLU GLU UNK ALA LYS GLU SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS ASN GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR LEU GLU SER LYS LYS LYS LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA

LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LEU LEU GLU GLN GLN ALA LEU ASP CYS LEU LYS ASN ALA LYS THR GLU ALA ASP LYS LYS ARG CYS VAL LYS ASP LEU PRO LYS ASP LEU GLN LYS LYS VAL LEU ALA LYS GLU SER LEU LYS

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

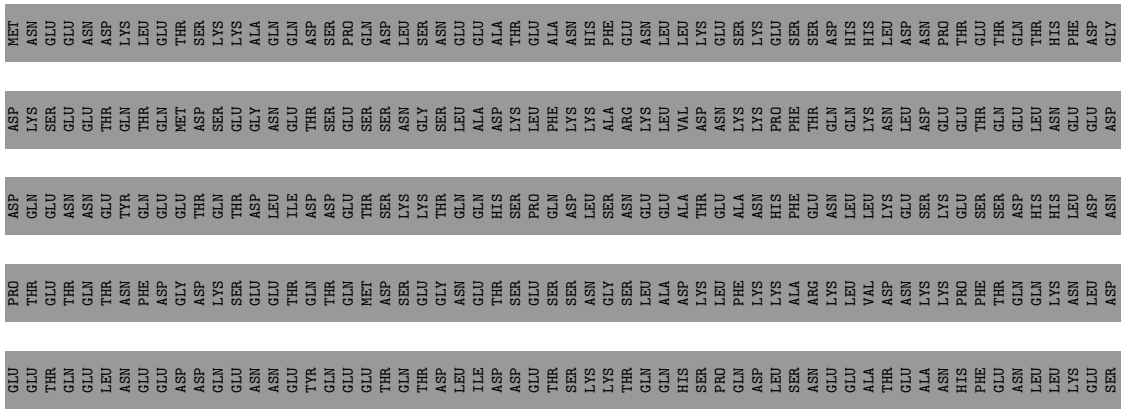
THR PRO GLU ALA ARG LYS LEU LEU GLU GLU ALA LYS GLU SER VAL LYS ALA TYR LYS ASP CYS VAL SER LYS ALA ARG ASN GLU LYS GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LEU LEU GLU GLN GLN VAL LEU ASP CYS LEU LYS ASN ALA LYS THR GLU

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



• Molecule 2: Cag pathogenicity island protein (Cag7)

Chain IY: 5% 93%



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S1470
K1471
L1475
S1479
L1482
D1483
D1486
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P1488
T1489
D1490
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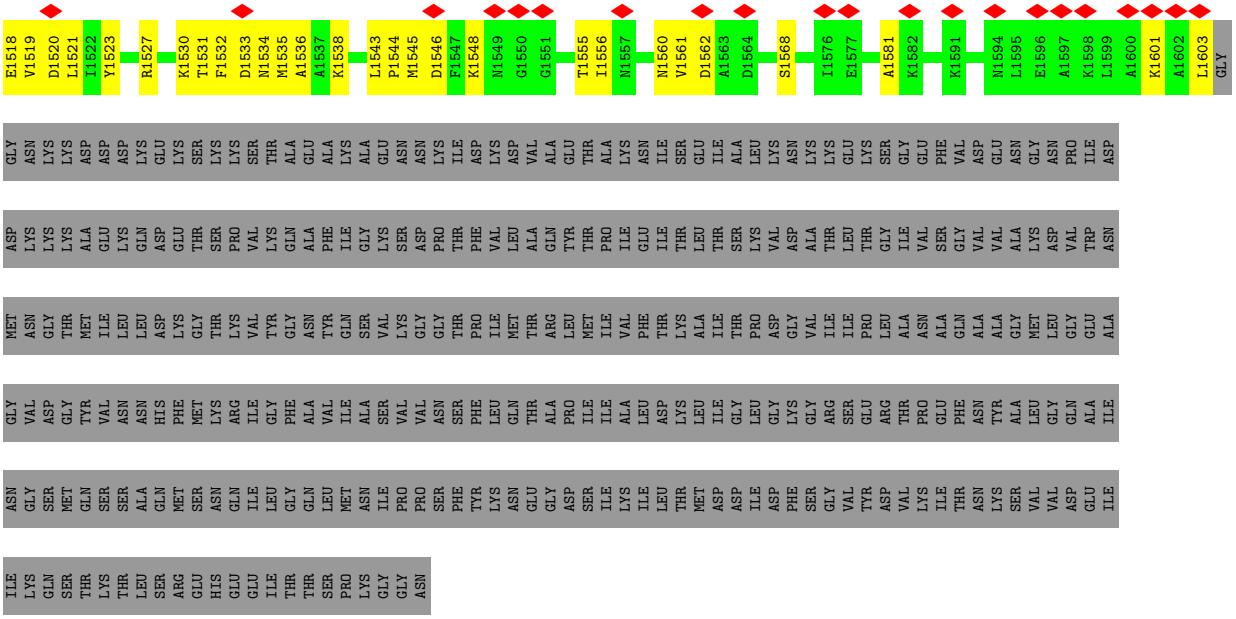
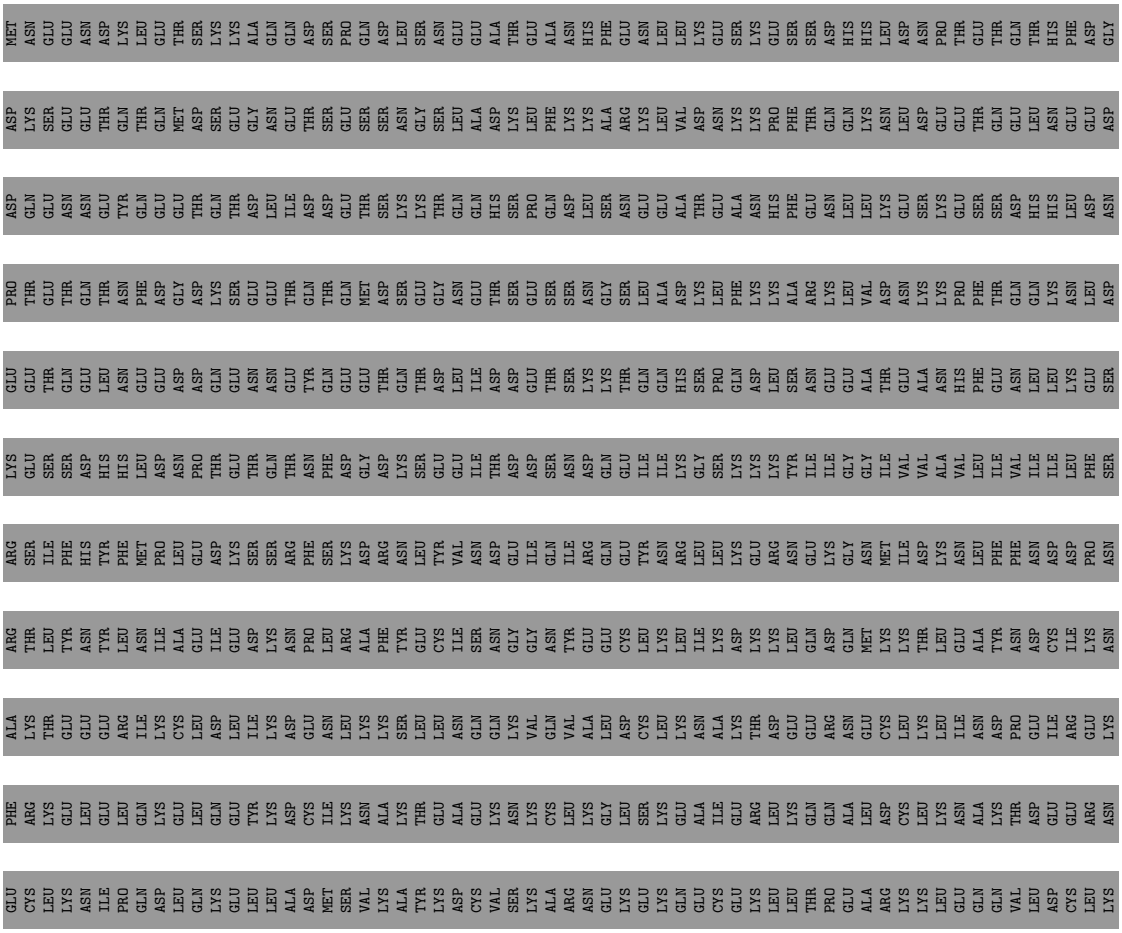
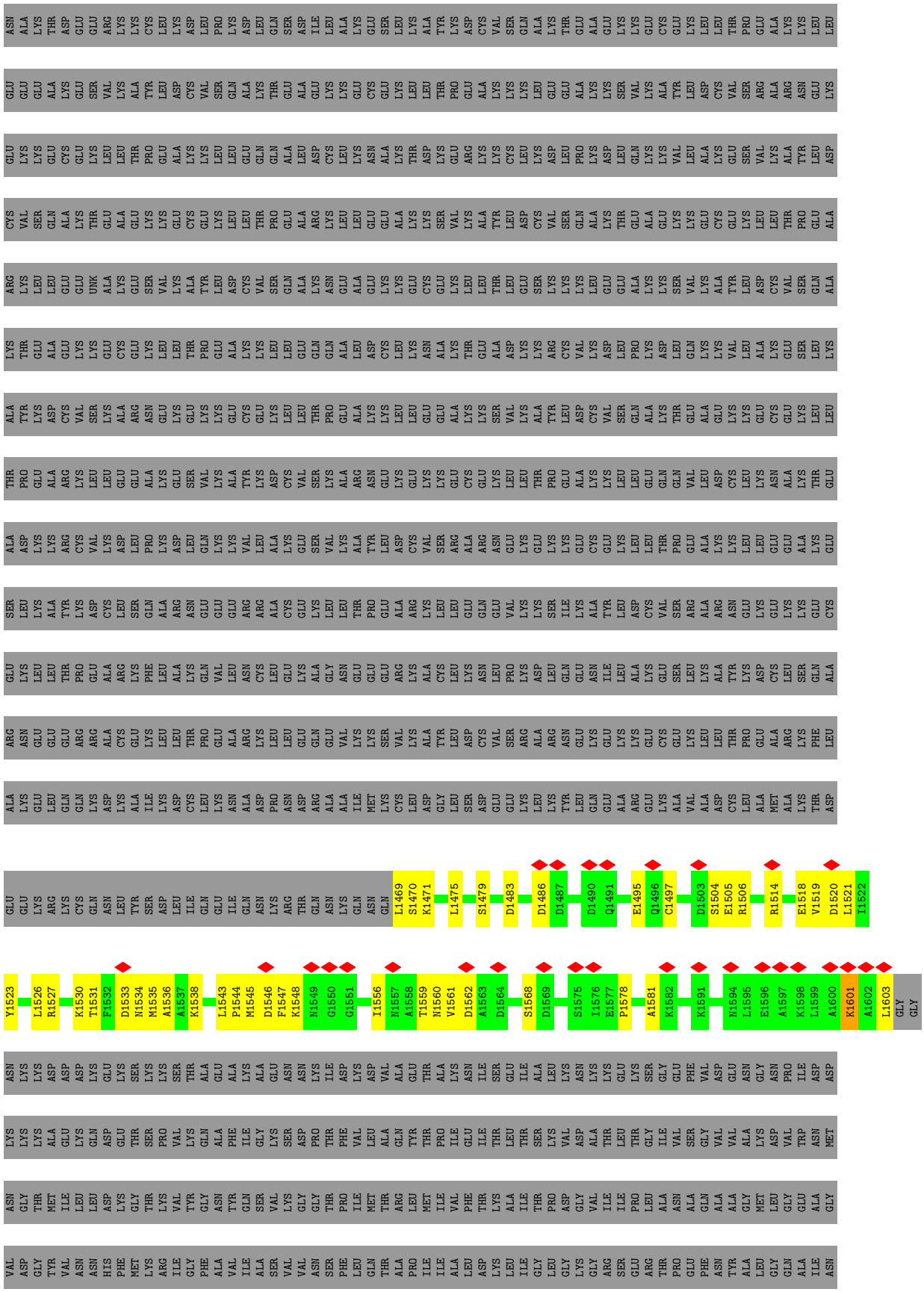


- Molecule 2: Cag pathogenicity island protein (Cag7)

Chain JY: 5% 93%

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GLU GLU GLU ALA LYS GLU SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS THR GLU ALA ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LEU GLU GLU ALA LYS LYS SER VAL LEU ASP CYS LEU LYS ALA ARG ASN GLU LYS
GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LEU GLU GLN ALA LEU ASP CYS LEU LYS ASN ALA LYS THR ASP LYS GLU ARG LYS LYS CYS LEU LYS ASP LEU PRO LYS ASP LEU GLN GLN LYS LYS VAL LEU ALA LYS LYS LEU ASP
CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA ALA ARG LYS LEU LEU THR PRO GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS CYS GLU LYS LEU LEU THR PRO GLU ALA
ARG LYS LEU LEU GLU GLU UNK ALA ALA LYS GLU SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS ASN GLU ALA ALA GLU LYS LYS GLU LYS LEU LEU THR LEU GLU SER LYS LYS LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA
LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LEU GLU GLN GLN ALA LEU ASP CYS LEU LYS ASN ALA LYS THR GLU ALA LYS ASP LYS LYS ARG CYS VAL LYS ASP LEU PRO LYS ASP LEU GLN GLN LYS LYS VAL LEU LYS LYS GLU SER LEU LYS
ALA TYR LYS ASP CYS VAL SER LYS LYS ALA ARG ASN GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA ALA LYS LYS LEU LEU THR PRO GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN GLN LYS LYS LEU GLU ALA LYS LYS GLU CYS GLU LYS LEU LEU
THR PRO GLU ALA ARG LYS LEU LEU GLU GLU ALA ALA LYS GLU SER VAL LYS ALA ALA TYR LYS ASP CYS VAL SER LYS ALA ARG ASN GLU GLU LYS LYS GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS GLU LYS LYS GLU LEU LEU THR PRO GLU ALA LYS LYS GLN GLN VAL LEU ASP CYS LEU LYS ASN ALA LYS THR GLU
ALA ASP LYS LYS ARG CYS VAL LYS ASP LEU PRO LYS ASP LEU LYS VAL LEU ALA LYS GLU SER VAL LYS ALA TYR LEU ASP CYS VAL SER ARG ALA ARG LYS LYS GLU CYS GLU LYS LYS LEU LEU THR PRO GLU ALA LYS LYS LEU LEU GLU GLU ALA LYS LYS GLU
SER LEU LYS ALA TYR LYS ASP CYS LEU SER GLN ALA ARG ASN GLU GLU GLU ARG ARG ALA CYS GLU LYS LYS SER ILE LYS ALA TYR LEU ASP CYS VAL SER ARG ALA ARG ASN GLU LYS LYS GLU LYS LYS GLU CYS
GLU LYS LEU LEU THR PRO GLU ALA ARG LYS PHE LEU ALA LYS GLN VAL LEU ASN CYS LEU GLU LYS ALA GLY ASN GLU GLU GLU GLU LYS LYS LEU GLN GLU ASN ILE LEU ALA ALA LYS GLU SER LEU ALA ALA TYR LEU ASP CYS VAL SER ARG ALA ARG ASN GLU LYS LYS GLN ALA
ARG ASN GLU GLU GLU ARG ARG ALA CYS GLU LYS LEU LYS ALA ARG LYS LEU LEU GLU GLN GLU VAL LYS LYS LYS SER VAL LEU ALA ARG ALA ARG ASN GLU LYS GLU LYS LYS LYS GLU CYS VAL SER ARG ALA LYS LYS GLU LYS LYS LYS LYS PHE LEU
ALA LYS GLU LEU GLN GLN LYS ASP LYS ALA LYS ASP LEU LYS ALA ILE LYS ASP CYS LEU LYS ASP PRO ASN ASP ARG ALA ALA ILE MET LYS CYS LEU ASP GLY LEU SER ASP GLU GLU LYS LEU LYS TYR LEU GLN GLU ALA ARG GLU LYS ALA VAL ALA ALA ASP CYS LEU THR ASP
GLU GLU LYS ARG LYS CYS GLN ASN LEU TYR SER ASP LEU ILE GLN GLU LYS ASN LYS ARG THR GLN ASN GLN L1469 S1470 K1471 L1475 S1479 D1483 D1486 D1487 D1490 Q1491 E1495 Q1496 C1497 D1503 S1504 E1505 R1506 R1514 E1518 V1519 D1520 L1521 I1522
Y1523 L1526 R1527 K1530 T1531 F1532 D1533 N1534 M1535 A1536 A1537 K1538 L1543 P1544 M1545 D1546 F1547 K1548 N1549 G1550 G1551 I1556 N1557 A1558 T1559 N1560 V1561 D1562 A1563 D1564 S1568 D1569 S1575 I1576 E1577 P1578 A1581 K1582 K1591 N1594 L1595 E1596 A1597 K1598 L1599 A1600 K1601 A1602 L1603 GLY GLY
ASN LYS LYS ASP ASP ASP LYS GLU LYS SER LYS SER VAL LYS ILE ASP LYS ASP VAL ALA GLU THR ALA ALA GLN LYS ALA ALA GLN ILE ALA LYS GLU GLN ASN ASN LYS ILE ALA LEU LYS ASN LYS GLU GLY GLU PHE VAL ASP GLU ASN GLY ASN PRO ILE ASP ASP
LYS LYS LYS ALA GLU LYS GLN ASP GLU THR SER PRO VAL LYS GLN ALA PHE ILE GLY LYS SER ASP PRO THR PHE VAL LEU ALA GLN TYR THR PRO ILE GLU ILE THR LEU THR SER LYS VAL ASP ALA THR LEU THR GLY ILE VAL SER GLY VAL ASP VAL ALA LYS ASP VAL TRP ASN MET
ASN GLY THR MET ILE LEU LEU ASP LYS GLY THR LYS VAL TYR GLY ASN TYR GLN SER VAL LYS GLY THR PRO ILE MET THR ARG LEU MET ILE VAL PHE THR LYS ALA ILE THR THR PRO ASP GLY VAL ILE PRO LEU ALA ASN ALA GLN ALA ALA GLY MET LEU GLY GLN ALA GLY
VAL ASP GLY TYR VAL ASN HIS PHE MET LYS ARG ILE GLY PHE ALA VAL ILE ALA SER VAL VAL ASN SER PHE LEU GLN THR ALA PRO ILE ILE ALA LEU ASP LYS LEU ILE GLY LEU GLY LYS GLY ARG SER GLU ARG THR PRO GLU ASP ALA ILE ASN

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

LYS GLN SER THR LYS THR LEU SER ARG GLU HIS GLU GLU ILE THR THR SER PRO LYS GLY GLY ASN

• Molecule 2: Cag pathogenicity island protein (Cag7)

Chain KY: 93%

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

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

ASP GLN GLU ASN ASN GLU TYR GLN GLN GLU GLU THR GLN THR ASP LEU ILE ASP ASP GLU THR SER LYS LYS THR GLN GLN HIS SER PRO GLN ASP LEU SER ASN GLU GLU GLU ALA ASN HIS PHE GLU ASN LEU LEU LYS GLU SER LYS GLU THR SER SER ASP HIS HIS LEU ASN

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

GLU GLU THR GLN GLU LEU ASN GLU GLU ASP ASP GLN GLU ASN ASN GLU TYR GLN GLU GLU THR GLN GLU ILE ASP ASP GLU THR SER LYS LYS THR GLN GLN HIS SER PRO GLN ASP LEU SER ASN GLU GLU ALA THR GLU GLU LYS GLU SER

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

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

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

ALA LYS THR GLU GLU ARG ILE LYS CYS LEU ASP LEU ILE LYS ASP GLU ASN LEU LYS LYS LYS SER LEU LEU ASN GLN GLN LYS VAL GLN VAL ALA LEU ASP CYS LEU LYS ASN ALA LYS THR ASP GLU GLU ARG ASN GLU CYS LEU LYS LEU LYS GLU GLU

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

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

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

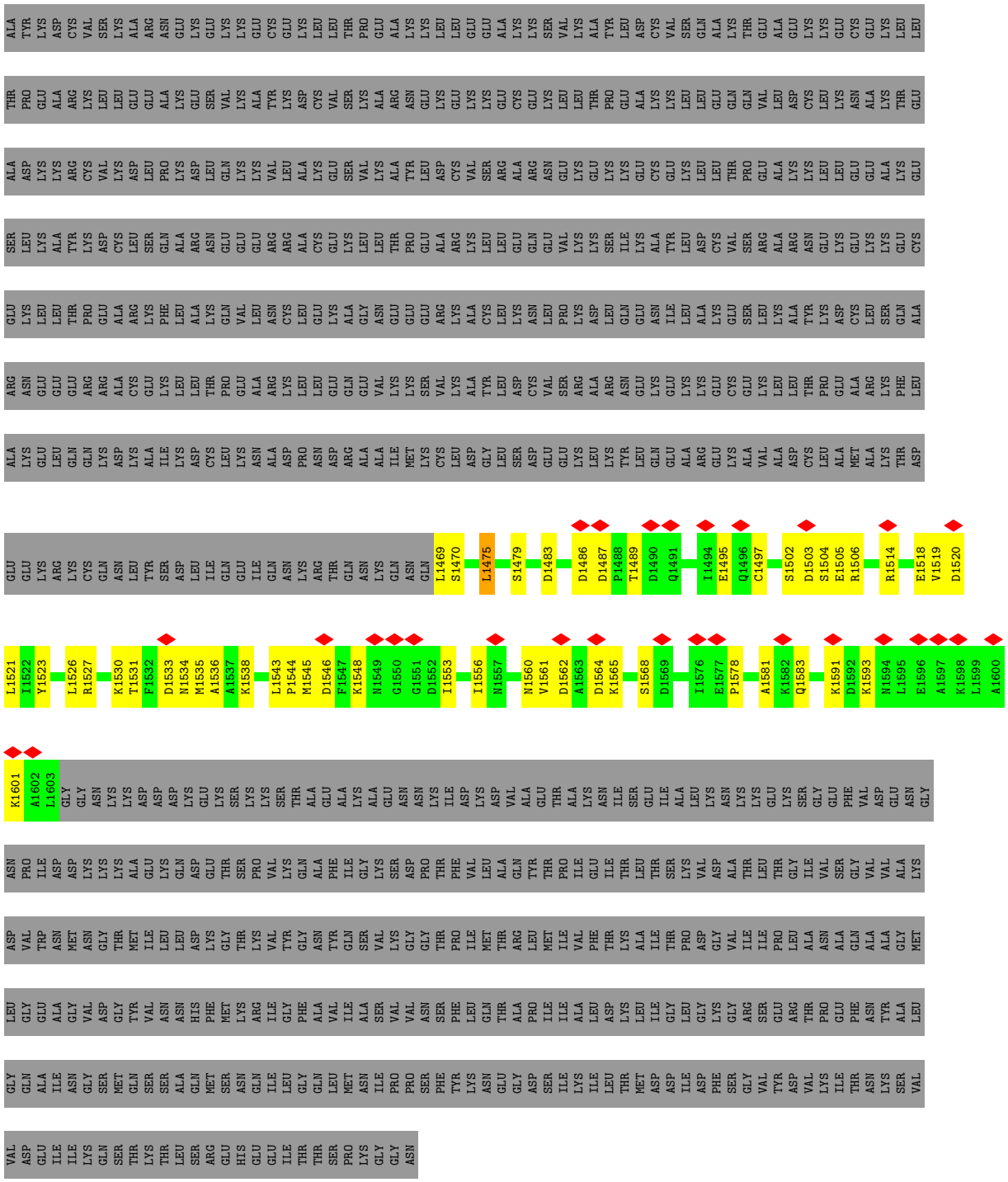
GLU GLU GLU ALA LYS GLU SER VAL LYS ALA TYR LEU ASP VAL SER GLN ALA LYS THR GLU ALA ALA TYR LYS LYS LYS CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LYS LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS LYS GLU LYS

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

CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS GLU LYS LEU LEU THR PRO GLU ALA ARG LYS LEU LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS THR GLU GLU LYS LYS LYS VAL LEU LEU ALA LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA

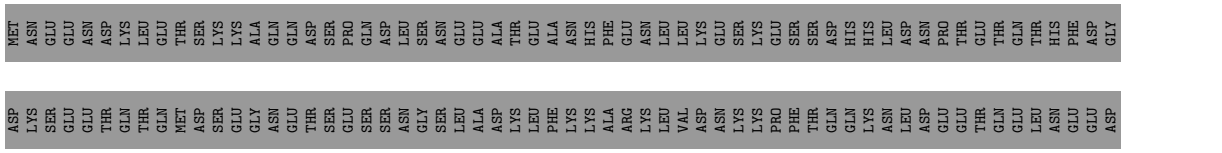
ARG LYS LEU LEU GLU UNK ALA LYS GLU SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS ASN GLU ALA ALA GLU LYS LYS CYS GLU LYS LYS LEU THR LEU GLU GLU SER LYS LYS LYS LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP ASP CYS VAL SER GLN ALA

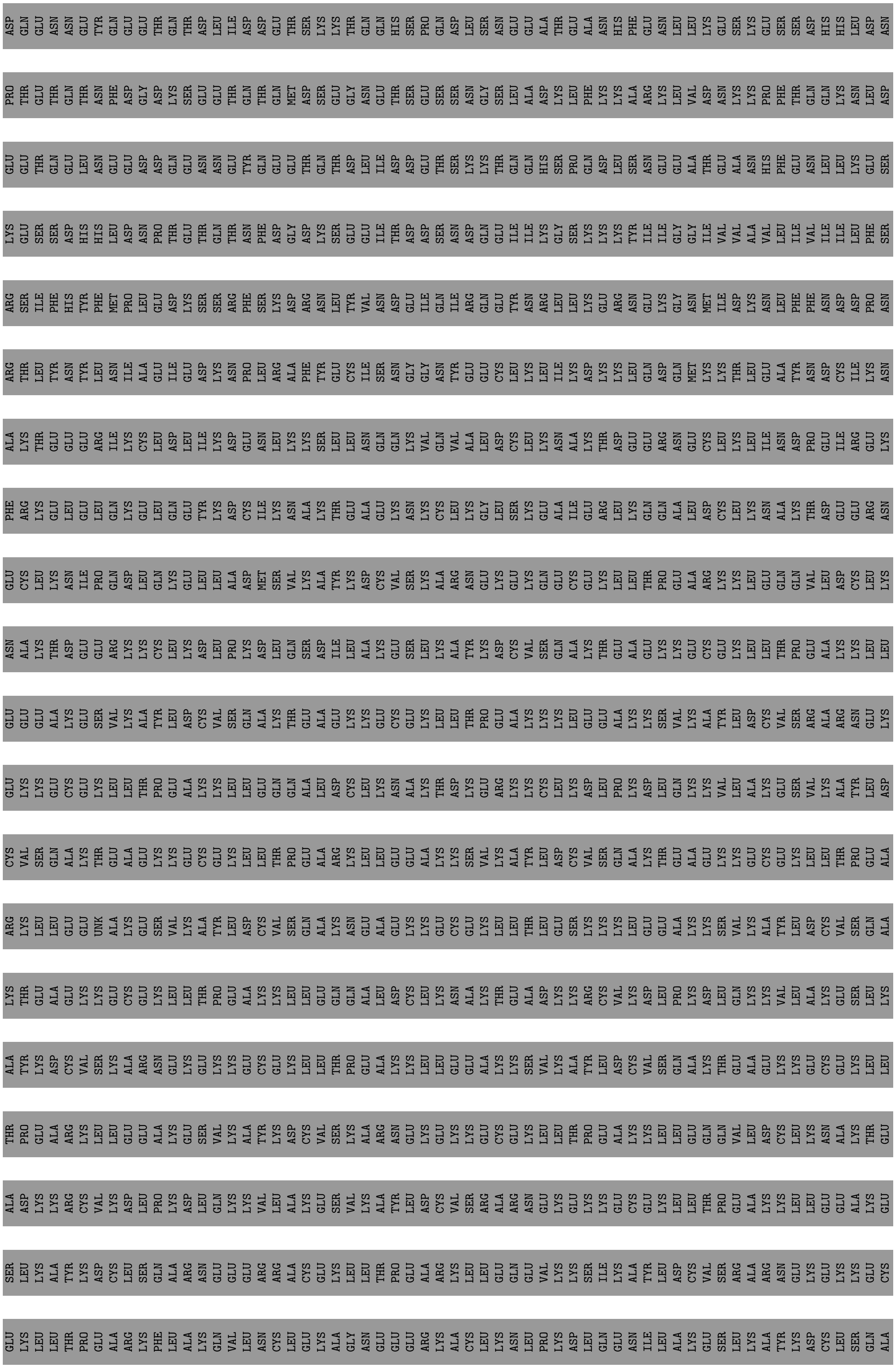
LYS THR GLU ALA GLU LYS LYS GLU ALA LYS LYS LEU LEU THR PRO GLU ALA LYS LYS LEU GLN GLN ALA LEU ASP CYS LEU LYS ASN ALA LYS THR GLU ALA ASP LYS LYS ARG CYS VAL LYS ASP LEU PRO LYS ASP LEU GLN LYS LYS VAL LEU ALA LYS GLU SER LEU LYS



- Molecule 2: Cag pathogenicity island protein (Cag7)

Chain LY: 5% 93%

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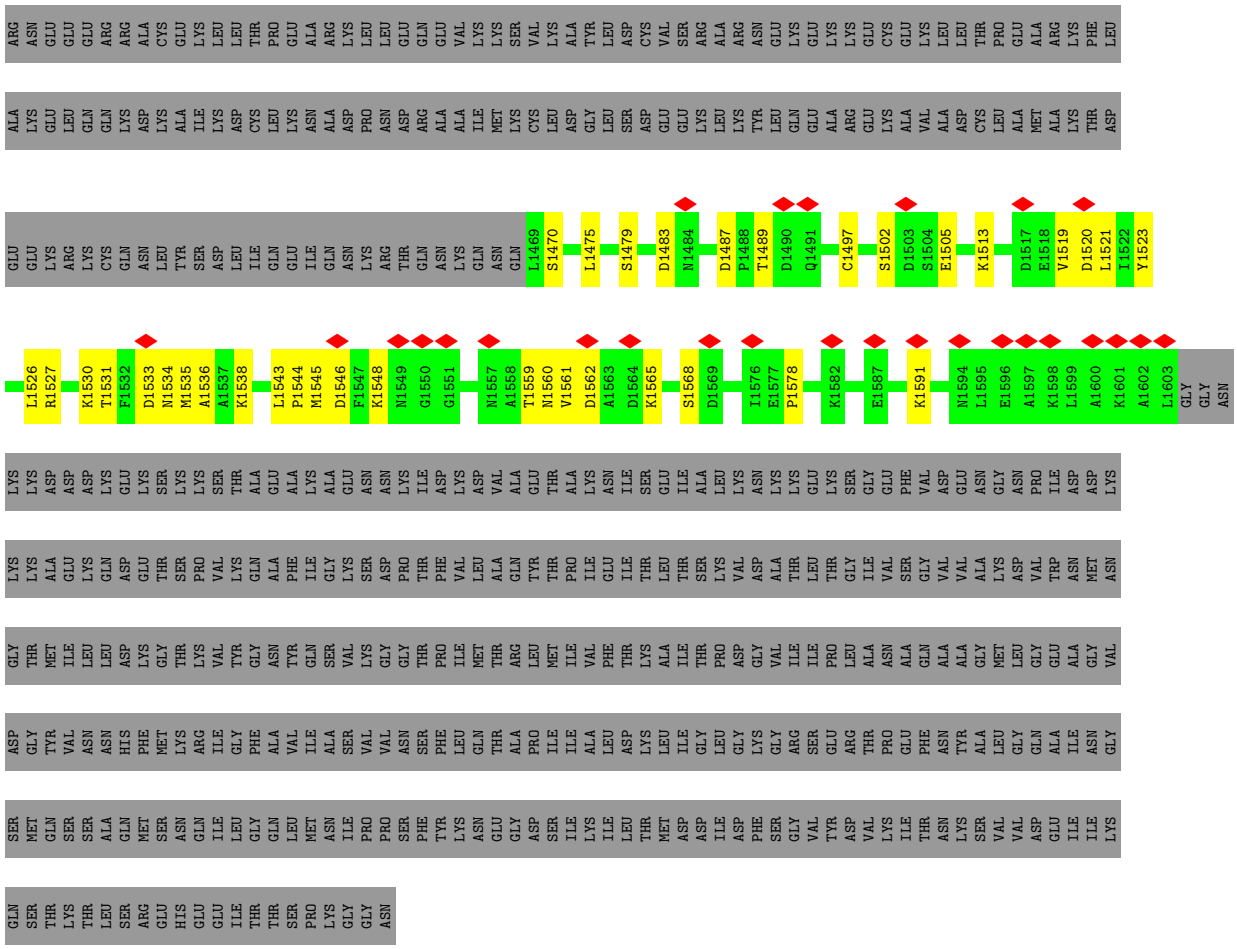
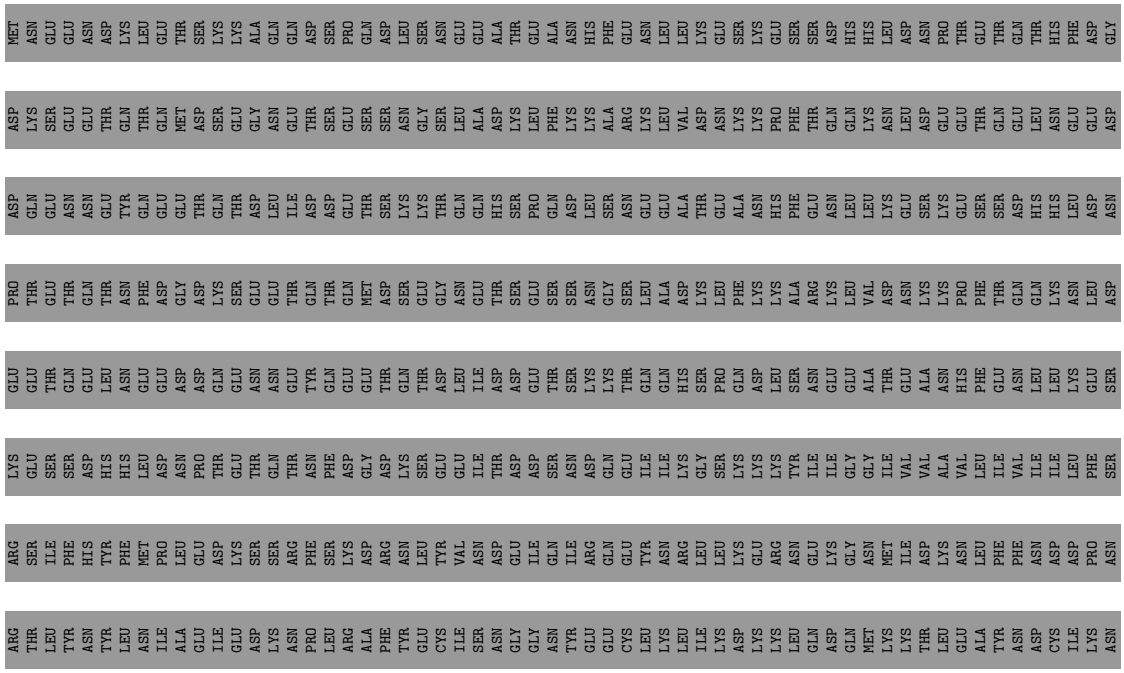
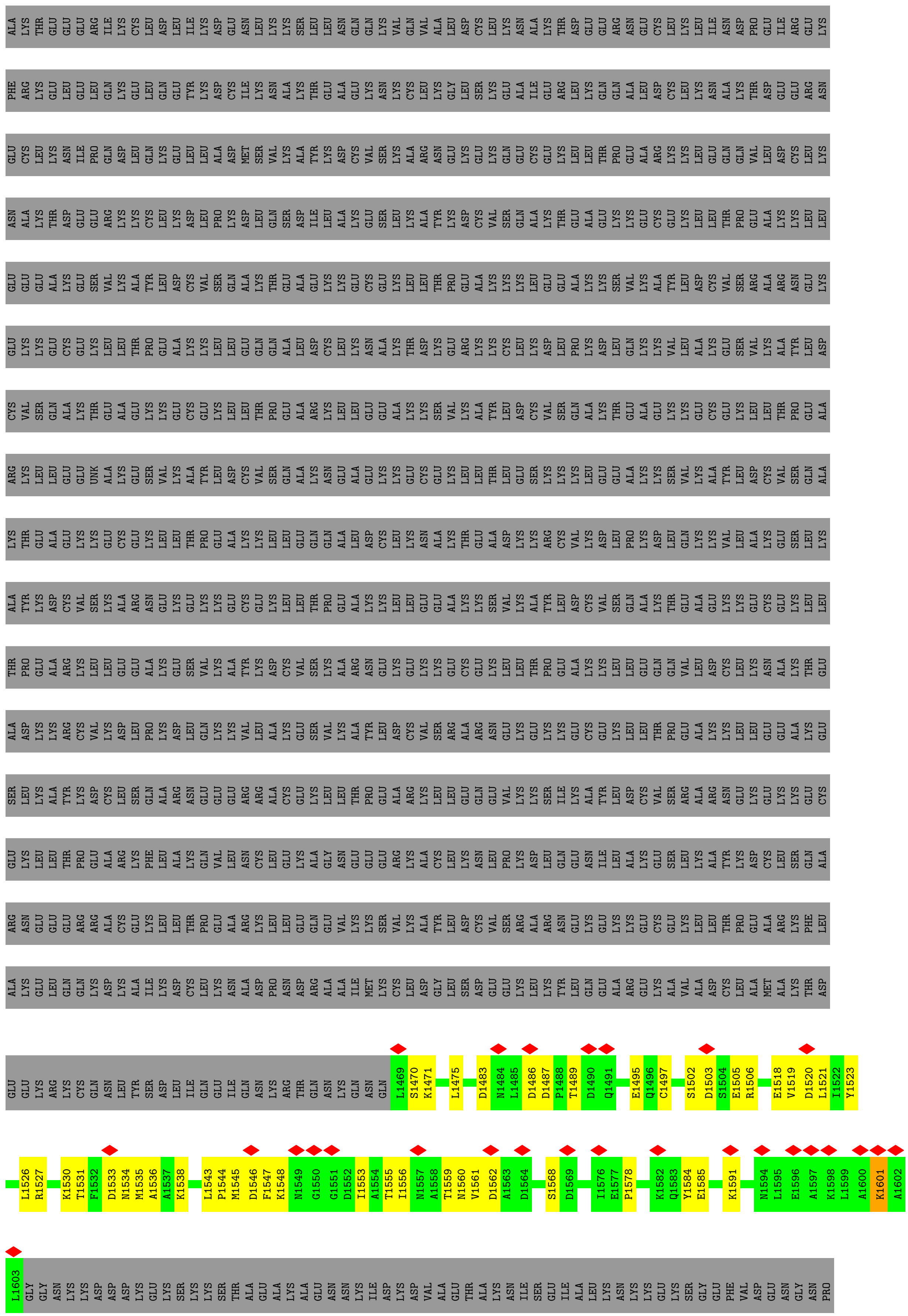
PRO THR GLU THR GLN THR ASN PHE ASP GLY ASP LYS SER GLU GLU THR GLN THR GLN MET ASP SER GLU GLY ASN GLU THR SER GLU SER SER ASN GLY SER LEU ALA ASP LYS LEU PHE LYS LYS ALA ARG LYS LEU VAL ASP ASN LYS LYS PRO PHE THR GLN GLN LYS ASN LEU ASP
GLU GLU THR GLN GLU LEU ASN GLU GLU ASP ASP GLN GLU ASN ASN GLU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



- Molecule 2: Cag pathogenicity island protein (Cag7)

Chain MY: 5% 93%

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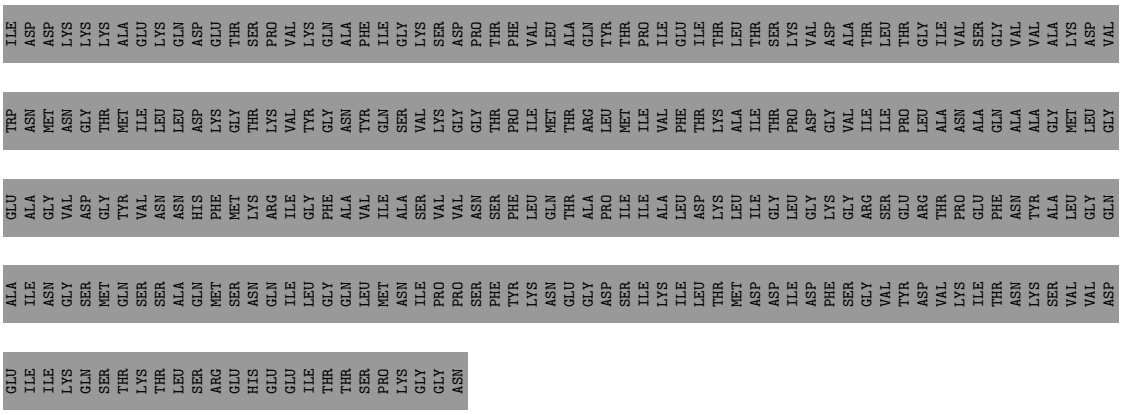
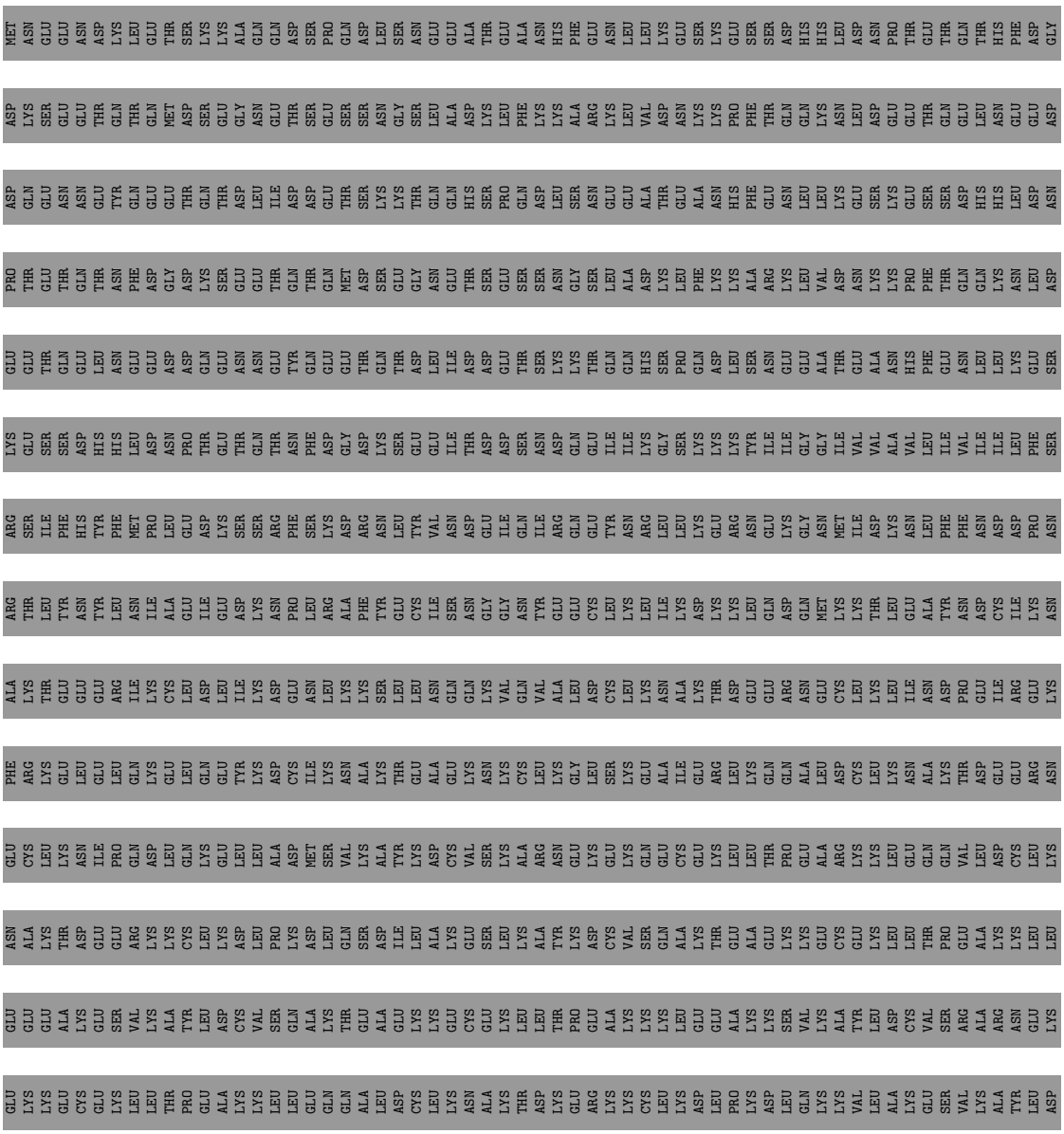
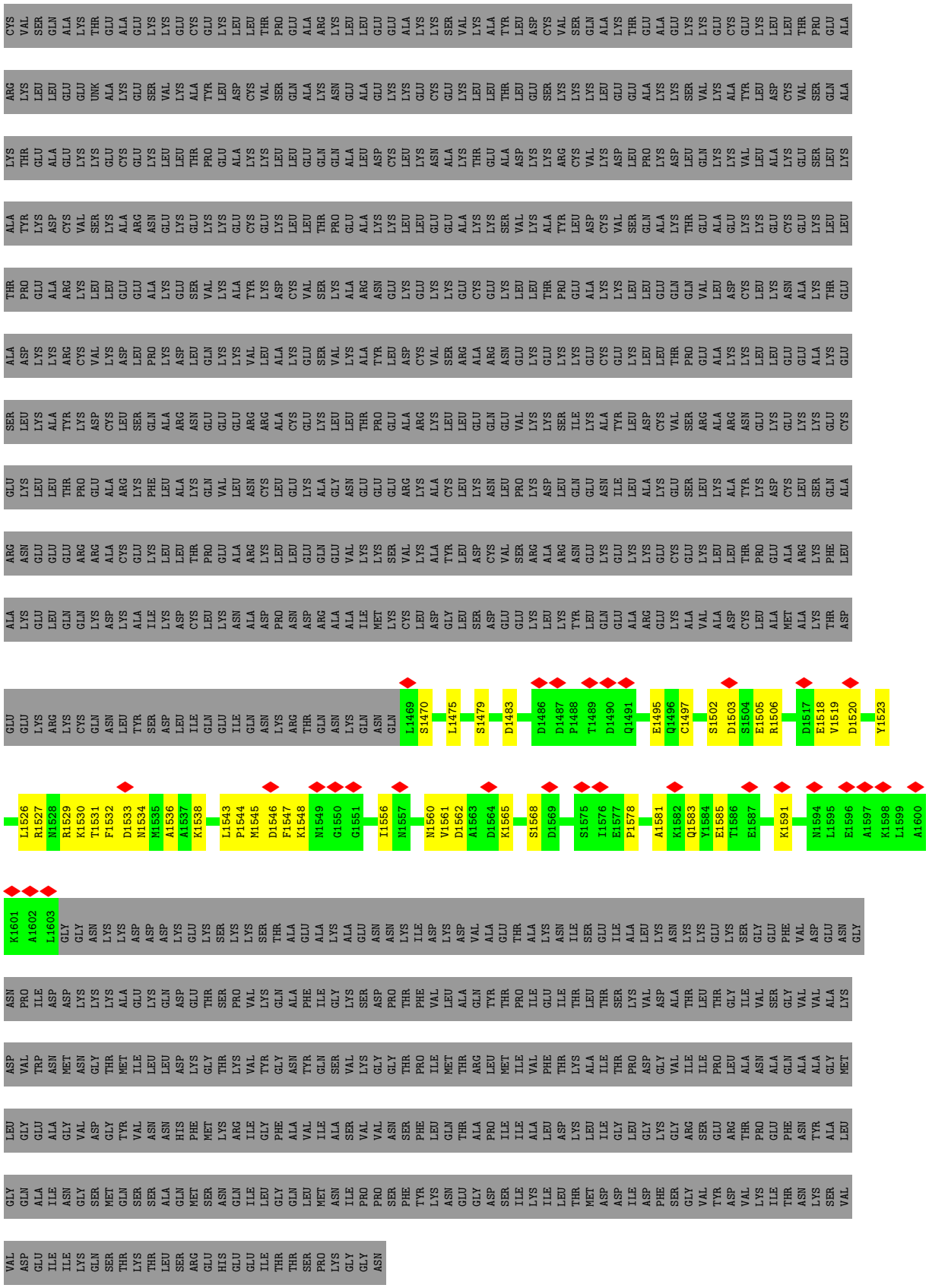
PHE ARG LYS GLU LEU GLU LEU GLN LYS GLU LEU GLN GLU TYR LYS ASP CYS ILE LYS ASN ALA LYS THR GLU ALA GLU LYS ASN LYS CYS LEU LYS GLY LEU SER LYS GLU ALA ILE GLU ARG LEU LYS GLN GLN ALA LEU ASP CYS LEU LYS ASN ALA LYS THR ASP GLU GLU ARG ASN
GLU CYS LEU LYS ASN ILE PRO GLN ASP LEU GLN LYS GLU LEU LEU ALA ASP MET SER VAL LYS ALA TYR LYS ASP CYS VAL SER LYS ALA ARG ASN GLU LYS GLU LYS GLN GLU CYS GLU LYS LEU LEU THR PRO GLU ALA ARG LYS LYS LEU GLU GLN GLN VAL LEU ASP CYS LEU LYS
ASN ALA LYS THR ASP GLU GLU ARG LYS LYS CYS LEU LYS ASP LEU PRO LYS ASP LEU GLN SER ASP ILE LEU ALA LYS GLU SER LEU LYS ALA TYR LYS ASP CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LEU LEU
GLU GLU GLU ALA LYS GLU SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LYS LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER ARG ALA ARG ASN GLU LYS
GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LEU LEU GLU GLN GLN ALA LEU ASP CYS LEU LYS ASN ALA LYS THR ASP LYS GLU ARG LYS LYS CYS LEU LYS ASP LEU PRO LYS ASP LEU GLN LYS LYS VAL LEU ALA LYS GLU SER VAL LYS ALA TYR LEU ASP
CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA ARG LYS LEU LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA
ARG LYS LEU LEU GLU GLU UNK ALA LYS GLU SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS ASN GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR LEU GLU SER LYS LYS LYS LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA
LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LEU LEU GLU GLN GLN ALA LEU ASP CYS LEU LYS ASN ALA LYS THR GLU ALA ASP LYS LYS ARG CYS VAL LYS ASP LEU PRO LYS ASP LEU GLN LYS LYS VAL LEU ALA LYS GLU SER LEU LYS
ALA TYR LYS ASP CYS VAL SER LYS ALA ARG ASN GLU LYS GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LEU LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU
THR PRO GLU ALA ARG LYS LEU LEU GLU GLU ALA LYS GLU SER VAL LYS ALA TYR LYS ASP CYS VAL SER LYS ALA ARG ASN GLU LYS GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LEU LEU GLU GLN GLN VAL LEU ASP CYS LEU LYS ASN ALA LYS THR GLU
ALA ASP LYS LYS ARG CYS VAL LYS ASP LEU PRO LYS ASP LEU GLN LYS LYS VAL LEU ALA LYS GLU SER VAL LYS ALA TYR LEU ASP CYS VAL SER ARG ALA ARG ASN GLU LYS GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LEU LEU GLU GLU ALA LYS GLU
SER LEU LYS ALA TYR LYS ASP CYS LEU SER GLN ALA ARG ASN GLU GLU GLU ARG ARG ALA CYS GLU LYS LEU LEU THR PRO GLU ALA ARG LYS LEU LEU GLU GLN GLU VAL LYS LYS SER ILE LYS ALA TYR LEU ASP CYS VAL SER ARG ALA ARG ASN GLU LYS GLU LYS LYS GLU CYS
GLU LYS LEU LEU THR PRO GLU ALA ARG LYS PHE LEU ALA LYS GLN VAL LEU ASN CYS LEU GLU LYS ALA GLY ASN GLU GLU GLU ARG LYS ALA CYS LEU LYS ASN LEU PRO LYS ASP LEU GLN GLU ASN ILE LEU ALA LYS GLU SER LEU LYS ALA TYR LYS ASP CYS LEU SER GLN ALA
ARG ASN GLU GLU GLU ARG ARG ALA CYS GLU LYS LEU LEU THR PRO GLU ALA ARG LYS LEU LEU GLU GLN GLU VAL LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER ARG ALA ARG ASN GLU LYS GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA ARG LYS PHE LEU
ALA LYS GLU LEU GLN GLN LYS ASP LYS ALA ILE LYS ASP CYS LEU LYS ASN ALA ASP PRO ASN ASP ARG ALA ALA ILE MET LYS CYS LEU ASP GLY LEU SER ASP GLU GLU LYS LEU LYS TYR LEU GLN GLU ALA ARG GLU LYS ALA VAL ALA ASP CYS LEU ALA MET ALA LYS THR ASP
GLU GLU LYS ARG LYS CYS GLN ASN LEU TYR SER ASP LEU ILE GLN GLU ILE GLN ASN LYS ARG THR GLN ASN LYS GLN ASN GLN L1469 S1470 K1471 L1475 D1483 N1484 L1485 D1486 D1487 P1488 T1489 D1490 Q1491 E1495 Q1496 C1497 S1502 D1503 S1504 E1505 R1506 E1518 V1519 D1520 L1521 I1522 Y1523
L1526 R1527 K1530 T1531 F1532 D1533 N1534 M1535 A1536 A1537 K1538 L1543 P1544 M1545 D1546 F1547 K1548 N1549 G1550 G1551 D1552 I1553 A1554 T1555 I1556 N1557 A1558 T1559 N1560 V1561 D1562 A1563 D1564 S1568 D1569 I1576 E1577 P1578 K1582 Q1583 Y1584 E1585 K1591 N1594 L1595 E1596 A1597 K1598 L1599 A1600 K1601 A1602
L1603 GLY GLY ASN LYS LYS ASP ASP ASP LYS GLU LYS SER LYS LYS SER THR ALA GLU ALA LYS ALA GLU ASN ASN LYS ILE ASP LYS ASP VAL ALA GLU THR ALA LYS ASN ILE SER GLU ILE ALA LEU LYS ASN LYS LYS GLU LYS SER GLY GLU PHE VAL ASP GLU ASN GLY ASN PRO



• Molecule 2: Cag pathogenicity island protein (Cag7)

Chain NY: 5% • 93%





• Molecule 2: Cag pathogenicity island protein (Cag7)

Chain OY:

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

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

ASP GLN GLU ASN ASN GLU TYR GLN GLU GLU THR GLN THR ASP LEU ILE ASP ASP GLU THR SER LYS LYS THR GLN GLN HIS SER PRO GLN ASP LEU SER ASN GLU GLU ALA THR GLU ALA ASN HIS PHE GLU ASN LEU LEU LYS GLU SER LYS GLU SER SER ASP HIS HIS LEU ASP ASN

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

GLU GLU THR GLN GLU LEU ASN GLU ASP ASP GLN GLU ASN ASN GLU TYR GLN GLU GLU THR GLN THR ASP LEU ILE ASP ASP GLU THR SER LYS LYS THR GLN GLN HIS SER PRO GLN ASP LEU SER ASN GLU GLU ALA THR GLU ALA ASN HIS PHE GLU ASN LEU LEU LYS GLU SER

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

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

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

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

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

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

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

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

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

CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA ARG LYS LEU LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA

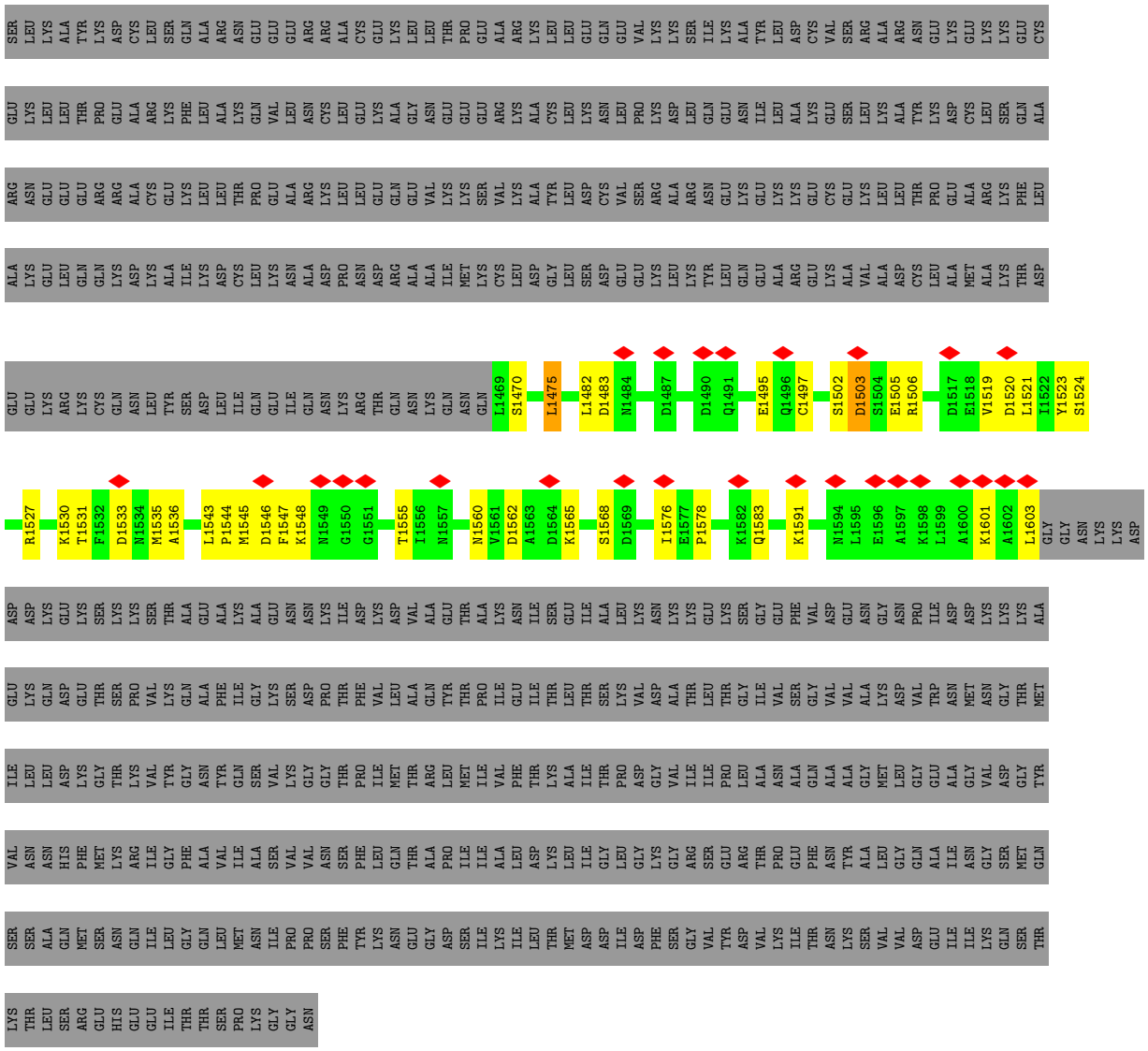
ARG LYS LEU LEU GLU GLU UNK ALA LYS GLU SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS ASN GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR LEU GLU SER LYS LYS LYS LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA

LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LEU LEU GLU GLN GLN ALA LEU ASP CYS LEU LYS ASN ALA LYS THR GLU ALA ASP LYS LYS ARG CYS VAL LYS ASP LEU PRO LYS ASP LEU GLN LYS LYS VAL LEU ALA LYS GLU SER LEU LYS

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

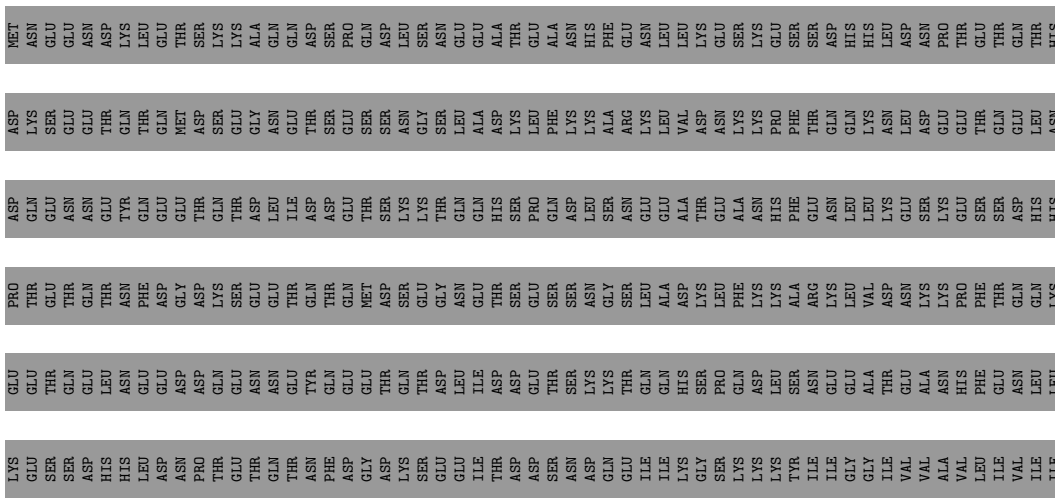
THR PRO GLU ALA ARG LYS LEU LEU GLU GLU ALA LYS GLU SER VAL LYS ALA TYR LYS ASP CYS VAL SER LYS ALA ARG ASN GLU LYS GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LEU LEU GLU GLN GLN VAL LEU ASP CYS LEU LYS ASN ALA LYS THR GLU

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



• Molecule 2: Cag pathogenicity island protein (Cag7)

Chain PY: 5% 93%



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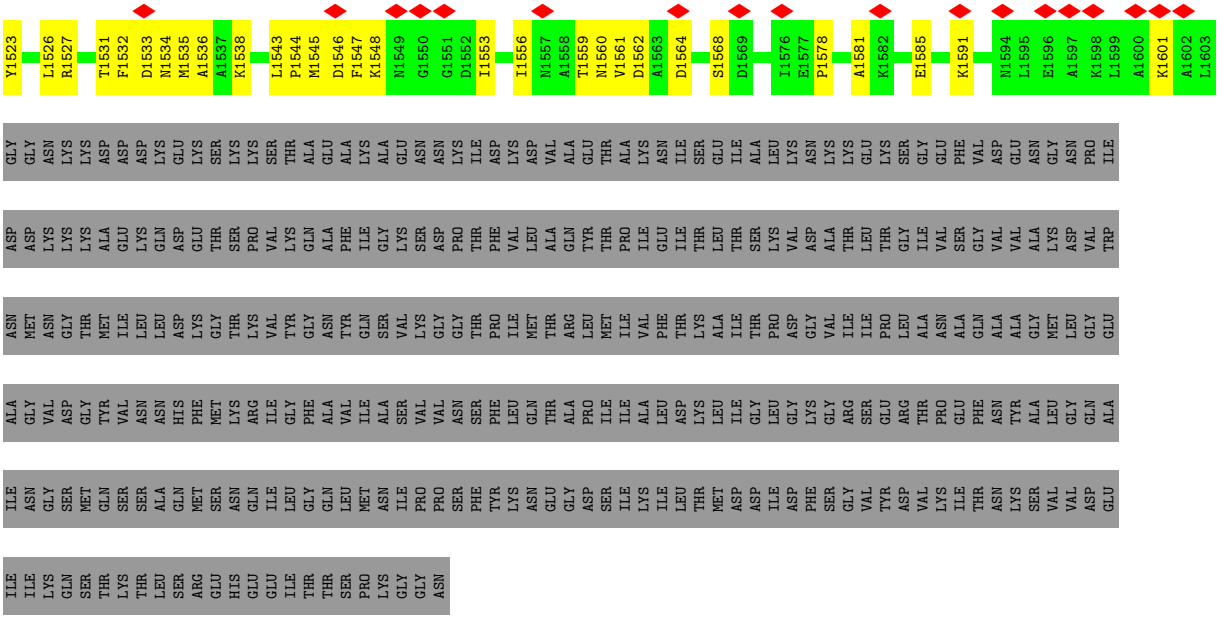
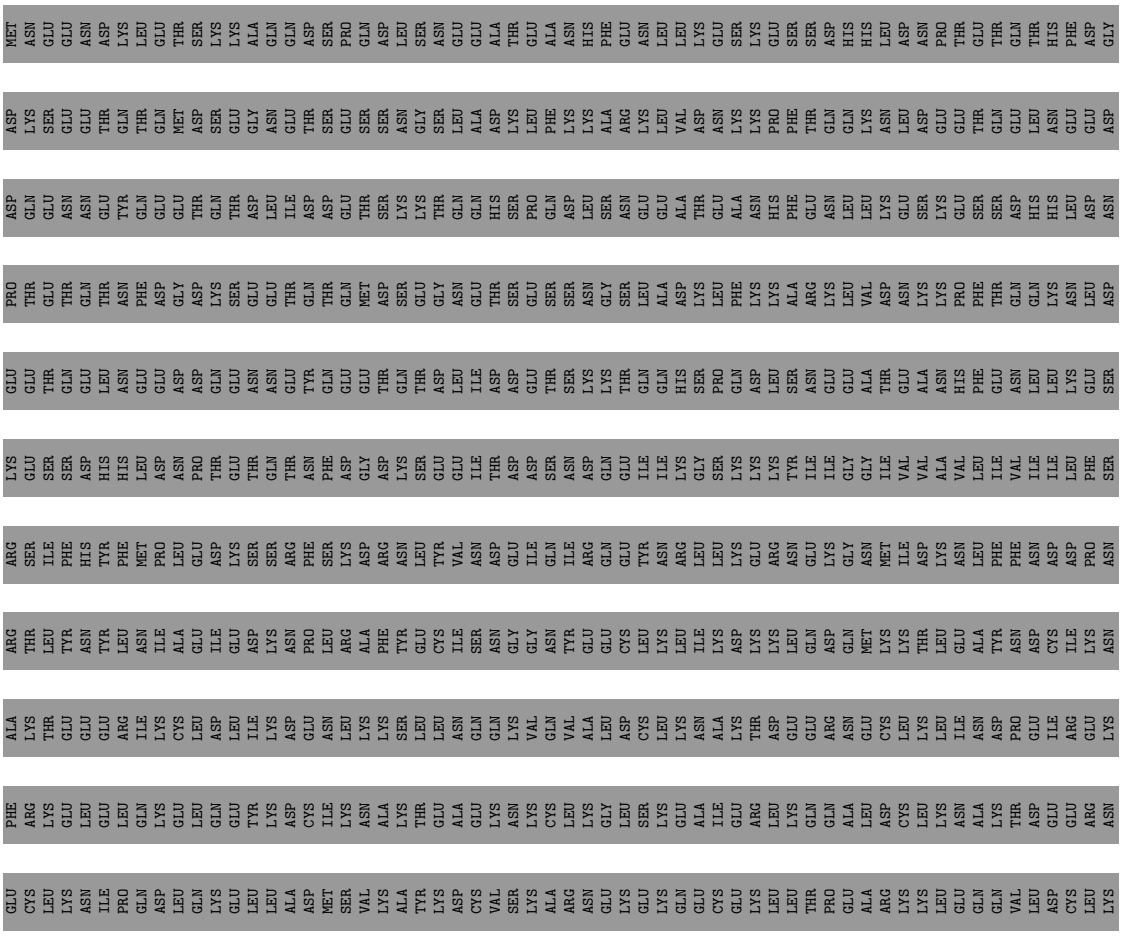
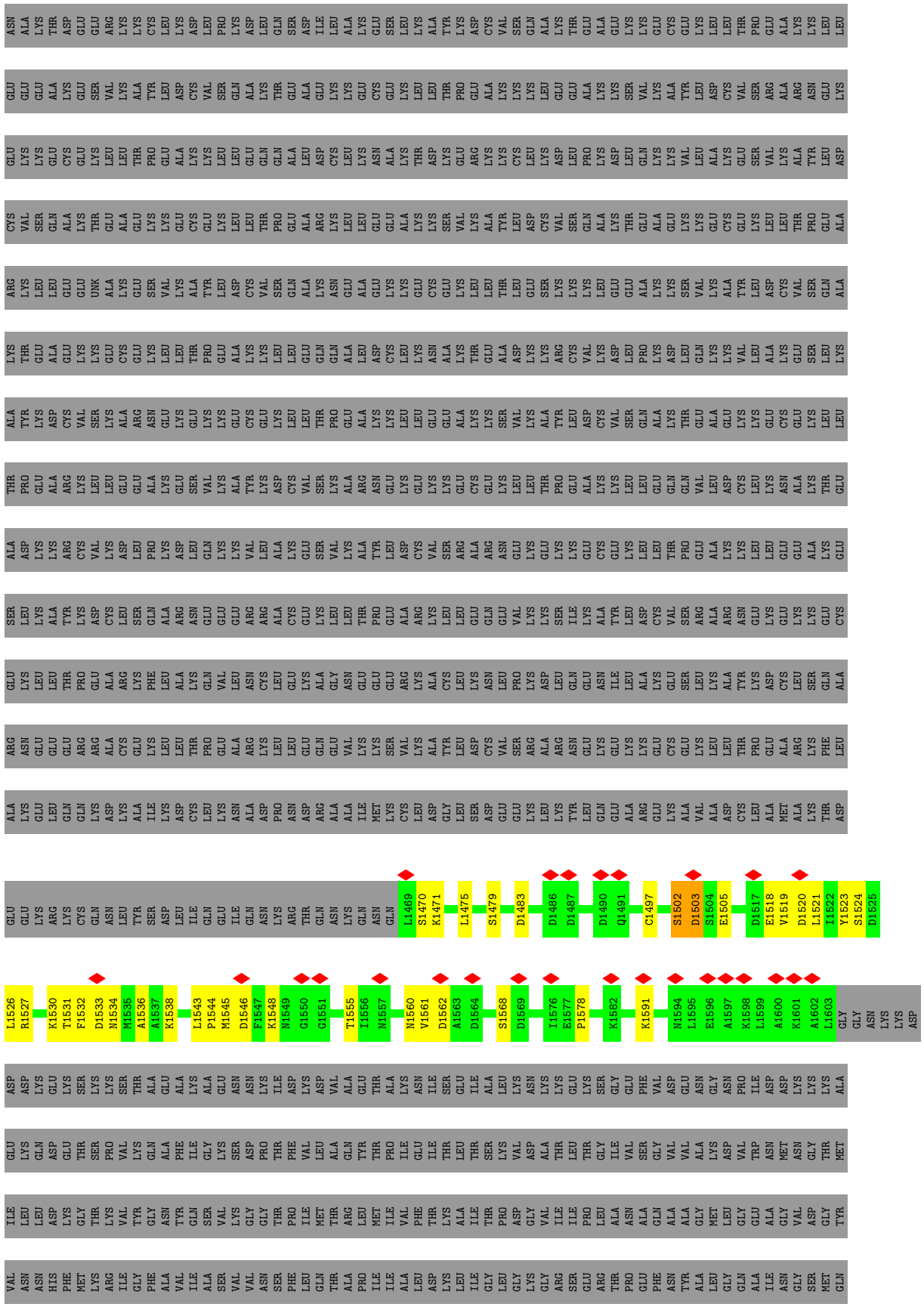


- Molecule 2: Cag pathogenicity island protein (Cag7)

Chain QY: 5% 93%

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K1598
L1599
A1600
K1601
A1602
L1603
GLY
GLY
ASN
LYS
LYS
ASP

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

LYS THR LEU SER ARG GLU HIS GLU GLU ILE THR THR SER PRO LYS GLY GLY ASN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10477	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 ($e^-/Å^2$)	59.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.042	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	510.0, 510.0, 510.0	wwPDB
Map dimensions	510, 510, 510	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	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	AX	0.34	0/1365	0.51	0/1845
1	BX	0.34	0/1365	0.49	0/1845
1	CX	0.34	0/1365	0.49	0/1845
1	DX	0.34	0/1365	0.48	0/1845
1	EX	0.34	0/1365	0.48	0/1845
1	FX	0.34	0/1365	0.49	0/1845
1	GX	0.34	0/1365	0.48	0/1845
1	HX	0.34	0/1365	0.49	0/1845
1	IX	0.33	0/1365	0.47	0/1845
1	JX	0.34	0/1365	0.48	0/1845
1	KX	0.35	0/1365	0.48	0/1845
1	LX	0.34	0/1365	0.50	0/1845
1	MX	0.34	0/1365	0.47	0/1845
1	NX	0.34	0/1365	0.50	0/1845
1	OX	0.34	0/1365	0.49	0/1845
1	PX	0.35	0/1365	0.48	0/1845
1	QX	0.34	0/1365	0.48	0/1845
2	AY	0.25	0/1061	0.48	0/1432
2	BY	0.25	0/1061	0.46	0/1432
2	CY	0.25	0/1061	0.47	0/1432
2	DY	0.25	0/1061	0.48	0/1432
2	EY	0.25	0/1061	0.47	0/1432
2	FY	0.24	0/1061	0.46	0/1432
2	GY	0.25	0/1061	0.50	0/1432
2	HY	0.26	0/1061	0.49	0/1432
2	IY	0.24	0/1061	0.45	0/1432
2	JY	0.25	0/1061	0.48	0/1432
2	KY	0.25	0/1061	0.51	0/1432
2	LY	0.25	0/1061	0.44	0/1432
2	MY	0.25	0/1061	0.45	0/1432
2	NY	0.24	0/1061	0.47	0/1432
2	OY	0.25	0/1061	0.47	0/1432
2	PY	0.25	0/1061	0.50	0/1432
2	QY	0.25	0/1061	0.48	0/1432

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.30	0/41242	0.48	0/55709

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	AX	1339	0	1355	41	0
1	BX	1339	0	1355	44	0
1	CX	1339	0	1355	43	0
1	DX	1339	0	1355	42	0
1	EX	1339	0	1355	45	0
1	FX	1339	0	1355	43	0
1	GX	1339	0	1355	42	0
1	HX	1339	0	1355	44	0
1	IX	1339	0	1355	37	0
1	JX	1339	0	1355	42	0
1	KX	1339	0	1355	51	0
1	LX	1339	0	1355	47	0
1	MX	1339	0	1355	36	0
1	NX	1339	0	1355	43	0
1	OX	1339	0	1355	45	0
1	PX	1339	0	1355	41	0
1	QX	1339	0	1355	44	0
2	AY	1050	0	1038	27	0
2	BY	1050	0	1038	32	0
2	CY	1050	0	1038	31	0
2	DY	1050	0	1038	29	0
2	EY	1050	0	1038	28	0
2	FY	1050	0	1038	23	0
2	GY	1050	0	1038	27	0
2	HY	1050	0	1038	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	IY	1050	0	1038	29	0
2	JY	1050	0	1038	29	0
2	KY	1050	0	1038	33	0
2	LY	1050	0	1038	22	0
2	MY	1050	0	1038	31	0
2	NY	1050	0	1038	30	0
2	OY	1050	0	1038	27	0
2	PY	1050	0	1038	29	0
2	QY	1050	0	1038	22	0
All	All	40613	0	40681	958	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 12.

All (958) 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:BX:126:LEU:O	1:BX:130:LYS:HB2	1.66	0.95
1:AX:126:LEU:O	1:AX:130:LYS:HB2	1.66	0.94
1:KX:126:LEU:O	1:KX:130:LYS:HB2	1.67	0.94
1:IX:126:LEU:O	1:IX:130:LYS:HB2	1.68	0.93
1:HX:126:LEU:O	1:HX:130:LYS:HB2	1.68	0.93
1:DX:126:LEU:O	1:DX:130:LYS:HB2	1.68	0.93
1:GX:126:LEU:O	1:GX:130:LYS:HB2	1.68	0.93
1:QX:126:LEU:O	1:QX:130:LYS:HB2	1.68	0.93
1:NX:126:LEU:O	1:NX:130:LYS:HB2	1.70	0.92
1:MX:126:LEU:O	1:MX:130:LYS:HB2	1.69	0.92
1:PX:126:LEU:O	1:PX:130:LYS:HB2	1.69	0.92
1:FX:126:LEU:O	1:FX:130:LYS:HB2	1.68	0.91
1:OX:126:LEU:O	1:OX:130:LYS:HB2	1.69	0.91
1:JX:126:LEU:O	1:JX:130:LYS:HB2	1.69	0.91
1:LX:126:LEU:O	1:LX:130:LYS:HB2	1.70	0.91
1:EX:126:LEU:O	1:EX:130:LYS:HB2	1.80	0.82
1:PX:272:SER:O	1:PX:276:TRP:HB2	1.92	0.70
1:LX:272:SER:O	1:LX:276:TRP:HB2	1.93	0.68
1:OX:277:ARG:HD2	1:OX:294:ARG:HH11	1.59	0.68
1:DX:272:SER:O	1:DX:276:TRP:HB2	1.93	0.68
2:AY:1533:ASP:HA	2:BY:1519:VAL:HG21	1.76	0.68
1:PX:277:ARG:HD2	1:PX:294:ARG:HH11	1.59	0.67
1:GX:272:SER:O	1:GX:276:TRP:HB2	1.94	0.67
2:OY:1533:ASP:HA	2:PY:1519:VAL:HG21	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NX:277:ARG:HD2	1:NX:294:ARG:HH11	1.60	0.67
1:JX:277:ARG:HD2	1:JX:294:ARG:HH11	1.60	0.67
1:DX:277:ARG:HD2	1:DX:294:ARG:HH11	1.60	0.66
1:HX:277:ARG:HD2	1:HX:294:ARG:HH11	1.60	0.66
1:KX:277:ARG:HD2	1:KX:294:ARG:HH11	1.61	0.66
1:BX:272:SER:O	1:BX:276:TRP:HB2	1.95	0.66
1:QX:277:ARG:HD2	1:QX:294:ARG:HH11	1.59	0.66
2:EY:1533:ASP:HA	2:FY:1519:VAL:HG21	1.77	0.66
1:EX:272:SER:O	1:EX:276:TRP:HB2	1.96	0.66
1:OX:272:SER:O	1:OX:276:TRP:HB2	1.96	0.66
1:FX:277:ARG:HD2	1:FX:294:ARG:HH11	1.60	0.66
2:JY:1533:ASP:HA	2:KY:1519:VAL:HG21	1.78	0.66
2:DY:1533:ASP:HA	2:EY:1519:VAL:HG21	1.77	0.66
1:LX:277:ARG:HD2	1:LX:294:ARG:HH11	1.61	0.66
2:BY:1533:ASP:HA	2:CY:1519:VAL:HG21	1.79	0.65
1:NX:272:SER:O	1:NX:276:TRP:HB2	1.96	0.65
1:MX:277:ARG:HD2	1:MX:294:ARG:HH11	1.60	0.65
1:AX:77:TYR:HB2	1:AX:283:ARG:HH21	1.62	0.65
1:AX:277:ARG:HD2	1:AX:294:ARG:HH11	1.60	0.65
2:KY:1533:ASP:HA	2:LY:1519:VAL:HG21	1.78	0.65
1:MX:77:TYR:HB2	1:MX:283:ARG:HH21	1.61	0.64
2:AY:1519:VAL:HG21	2:QY:1533:ASP:HA	1.78	0.64
1:IX:277:ARG:HD2	1:IX:294:ARG:HH11	1.62	0.64
2:HY:1533:ASP:HA	2:IY:1519:VAL:HG21	1.78	0.64
2:NY:1533:ASP:HA	2:OY:1519:VAL:HG21	1.79	0.64
2:IY:1533:ASP:HA	2:JY:1519:VAL:HG21	1.79	0.64
2:LY:1578:PRO:HD3	2:MY:1591:LYS:HB3	1.79	0.64
2:PY:1533:ASP:HA	2:QY:1519:VAL:HG21	1.80	0.64
1:MX:272:SER:O	1:MX:276:TRP:HB2	1.98	0.63
1:AX:318:VAL:O	1:AX:322:ILE:HB	1.99	0.63
1:FX:272:SER:O	1:FX:276:TRP:HB2	1.98	0.63
2:LY:1533:ASP:HA	2:MY:1519:VAL:HG21	1.79	0.63
2:NY:1578:PRO:HD3	2:OY:1591:LYS:HB3	1.81	0.63
1:CX:277:ARG:HD2	1:CX:294:ARG:HH11	1.62	0.63
1:KX:272:SER:O	1:KX:276:TRP:HB2	1.98	0.63
2:CY:1533:ASP:HA	2:DY:1519:VAL:HG21	1.80	0.63
1:FX:77:TYR:HB2	1:FX:283:ARG:HH21	1.63	0.63
1:AX:272:SER:O	1:AX:276:TRP:HB2	1.99	0.62
1:EX:277:ARG:HD2	1:EX:294:ARG:HH11	1.63	0.62
1:GX:77:TYR:HB2	1:GX:283:ARG:HH21	1.63	0.62
1:NX:283:ARG:NH2	1:OX:91:ASN:OD1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GX:277:ARG:HD2	1:GX:294:ARG:HH11	1.62	0.62
1:PX:77:TYR:HB2	1:PX:283:ARG:HH21	1.64	0.62
1:BX:277:ARG:HD2	1:BX:294:ARG:HH11	1.61	0.62
1:IX:77:TYR:HB2	1:IX:283:ARG:HH21	1.65	0.62
1:QX:77:TYR:HB2	1:QX:283:ARG:HH21	1.64	0.62
2:GY:1533:ASP:HA	2:HY:1519:VAL:HG21	1.82	0.62
1:HX:77:TYR:HB2	1:HX:283:ARG:HH21	1.64	0.62
1:DX:77:TYR:HB2	1:DX:283:ARG:HH21	1.65	0.62
1:JX:272:SER:O	1:JX:276:TRP:HB2	2.00	0.62
1:AX:283:ARG:NH2	1:BX:91:ASN:OD1	2.32	0.62
1:MX:283:ARG:NH2	1:NX:91:ASN:OD1	2.33	0.62
2:FY:1578:PRO:HD3	2:GY:1591:LYS:HB3	1.82	0.62
2:MY:1533:ASP:HA	2:NY:1519:VAL:HG21	1.80	0.61
1:DX:283:ARG:NH2	1:EX:91:ASN:OD1	2.33	0.61
1:FX:283:ARG:NH2	1:GX:91:ASN:OD1	2.33	0.61
1:OX:77:TYR:HB2	1:OX:283:ARG:HH21	1.65	0.61
1:PX:283:ARG:NH2	1:QX:91:ASN:OD1	2.34	0.61
1:IX:272:SER:O	1:IX:276:TRP:HB2	2.00	0.61
1:JX:283:ARG:NH2	1:KX:91:ASN:OD1	2.33	0.61
1:EX:283:ARG:NH2	1:FX:91:ASN:OD1	2.33	0.61
1:NX:77:TYR:HB2	1:NX:283:ARG:HH21	1.65	0.61
1:OX:92:SER:O	1:OX:93:ASN:ND2	2.34	0.61
1:AX:91:ASN:OD1	1:QX:283:ARG:NH2	2.33	0.61
1:BX:283:ARG:NH2	1:CX:91:ASN:OD1	2.33	0.61
1:HX:272:SER:O	1:HX:276:TRP:HB2	2.00	0.61
1:CX:281:VAL:HG21	1:DX:66:VAL:HG21	1.83	0.61
1:LX:283:ARG:NH2	1:MX:91:ASN:OD1	2.34	0.60
1:QX:272:SER:O	1:QX:276:TRP:HB2	2.00	0.60
1:CX:283:ARG:NH2	1:DX:91:ASN:OD1	2.34	0.60
1:HX:283:ARG:NH2	1:IX:91:ASN:OD1	2.34	0.60
1:CX:77:TYR:HB2	1:CX:283:ARG:HH21	1.66	0.60
1:EX:42:VAL:O	1:EX:305:TYR:HA	2.02	0.60
1:FX:92:SER:O	1:FX:93:ASN:ND2	2.35	0.60
1:IX:283:ARG:NH2	1:JX:91:ASN:OD1	2.34	0.60
1:MX:272:SER:HB3	2:LY:1531:THR:HB	1.82	0.60
1:JX:92:SER:O	1:JX:93:ASN:ND2	2.35	0.60
1:KX:283:ARG:NH2	1:LX:91:ASN:OD1	2.35	0.60
1:CX:272:SER:HB3	2:BY:1531:THR:HB	1.84	0.60
1:BX:77:TYR:HB2	1:BX:283:ARG:HH21	1.66	0.59
1:EX:80:THR:O	1:EX:83:ASN:ND2	2.35	0.59
1:EX:92:SER:O	1:EX:93:ASN:ND2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:JY:1536:ALA:HB3	2:KY:1519:VAL:HG23	1.83	0.59
1:AX:92:SER:O	1:AX:93:ASN:ND2	2.36	0.59
1:HX:92:SER:O	1:HX:93:ASN:ND2	2.36	0.59
1:CX:92:SER:O	1:CX:93:ASN:ND2	2.36	0.59
1:JX:281:VAL:HG21	1:KX:66:VAL:HG11	1.84	0.59
1:GX:272:SER:HB3	2:FY:1531:THR:HB	1.84	0.59
1:QX:80:THR:O	1:QX:83:ASN:ND2	2.36	0.59
1:KX:42:VAL:O	1:KX:305:TYR:HA	2.02	0.59
1:KX:268:GLU:OE1	2:JY:1530:LYS:NZ	2.36	0.59
1:MX:92:SER:O	1:MX:93:ASN:ND2	2.36	0.59
1:OX:283:ARG:NH2	1:PX:91:ASN:OD1	2.36	0.59
1:QX:92:SER:O	1:QX:93:ASN:ND2	2.35	0.59
2:MY:1578:PRO:HD3	2:NY:1591:LYS:HB3	1.84	0.59
2:NY:1536:ALA:HB3	2:OY:1519:VAL:HG23	1.83	0.59
1:KX:92:SER:O	1:KX:93:ASN:ND2	2.36	0.59
2:EY:1536:ALA:HB3	2:FY:1519:VAL:HG23	1.85	0.58
2:MY:1536:ALA:HB3	2:NY:1519:VAL:HG23	1.85	0.58
1:DX:92:SER:O	1:DX:93:ASN:ND2	2.36	0.58
2:IY:1536:ALA:HB3	2:JY:1519:VAL:HG23	1.85	0.58
1:EX:272:SER:HB3	2:DY:1531:THR:HB	1.85	0.58
1:JX:80:THR:O	1:JX:83:ASN:ND2	2.37	0.58
1:PX:92:SER:O	1:PX:93:ASN:ND2	2.35	0.58
2:BY:1536:ALA:HB3	2:CY:1519:VAL:HG23	1.84	0.58
2:MY:1535:MET:HE2	2:MY:1544:PRO:HD3	1.85	0.58
1:IX:92:SER:O	1:IX:93:ASN:ND2	2.36	0.58
2:PY:1536:ALA:HB3	2:QY:1519:VAL:HG23	1.85	0.58
1:EX:77:TYR:HB2	1:EX:283:ARG:HH21	1.69	0.58
1:NX:92:SER:O	1:NX:93:ASN:ND2	2.36	0.58
1:BX:92:SER:O	1:BX:93:ASN:ND2	2.35	0.58
1:GX:92:SER:O	1:GX:93:ASN:ND2	2.36	0.58
2:CY:1536:ALA:HB3	2:DY:1519:VAL:HG23	1.84	0.58
2:OY:1536:ALA:HB3	2:PY:1519:VAL:HG23	1.85	0.58
1:CX:272:SER:O	1:CX:276:TRP:HB2	2.03	0.58
1:HX:272:SER:HB3	2:GY:1531:THR:HB	1.85	0.58
1:PX:80:THR:O	1:PX:83:ASN:ND2	2.37	0.58
2:GY:1578:PRO:HD3	2:HY:1591:LYS:HB3	1.84	0.58
1:CX:80:THR:O	1:CX:83:ASN:ND2	2.36	0.57
1:FX:80:THR:O	1:FX:83:ASN:ND2	2.36	0.57
1:IX:80:THR:O	1:IX:83:ASN:ND2	2.36	0.57
1:NX:80:THR:O	1:NX:83:ASN:ND2	2.37	0.57
1:QX:318:VAL:O	1:QX:322:ILE:HB	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AY:1578:PRO:HD3	2:BY:1591:LYS:HB3	1.84	0.57
1:HX:42:VAL:O	1:HX:305:TYR:HA	2.04	0.57
1:JX:77:TYR:HB2	1:JX:283:ARG:HH21	1.69	0.57
1:LX:92:SER:O	1:LX:93:ASN:ND2	2.35	0.57
1:GX:80:THR:O	1:GX:83:ASN:ND2	2.36	0.57
1:FX:78:ILE:HG12	1:FX:90:PRO:HG3	1.85	0.57
2:LY:1536:ALA:HB3	2:MY:1519:VAL:HG23	1.86	0.57
1:KX:318:VAL:O	1:KX:322:ILE:HB	2.04	0.57
2:EY:1578:PRO:HD3	2:FY:1591:LYS:HB3	1.85	0.57
2:JY:1578:PRO:HD3	2:KY:1591:LYS:HB3	1.85	0.57
1:HX:71:LYS:HG3	2:GY:1568:SER:HA	1.87	0.57
1:KX:80:THR:O	1:KX:83:ASN:ND2	2.38	0.57
1:PX:42:VAL:O	1:PX:305:TYR:HA	2.04	0.57
1:AX:80:THR:O	1:AX:83:ASN:ND2	2.37	0.57
2:GY:1536:ALA:HB3	2:HY:1519:VAL:HG23	1.86	0.57
1:HX:80:THR:O	1:HX:83:ASN:ND2	2.37	0.57
1:LX:67:ILE:HA	1:LX:308:VAL:HG23	1.87	0.57
1:LX:77:TYR:HB2	1:LX:283:ARG:HH21	1.69	0.57
2:EY:1523:TYR:OH	2:EY:1527:ARG:NH2	2.38	0.57
2:QY:1523:TYR:OH	2:QY:1527:ARG:NH2	2.38	0.57
2:PY:1578:PRO:HD3	2:QY:1591:LYS:HB3	1.86	0.57
2:IY:1535:MET:HE2	2:IY:1544:PRO:HD3	1.87	0.56
2:MY:1523:TYR:OH	2:MY:1527:ARG:NH2	2.38	0.56
1:NX:272:SER:HB3	2:MY:1531:THR:HB	1.86	0.56
2:AY:1536:ALA:HB3	2:BY:1519:VAL:HG23	1.86	0.56
2:DY:1548:LYS:HG3	2:EY:1527:ARG:HH22	1.70	0.56
2:OY:1535:MET:HE2	2:OY:1544:PRO:HD3	1.87	0.56
1:IX:91:ASN:ND2	2:HY:1559:THR:OG1	2.39	0.56
1:QX:71:LYS:HG3	2:PY:1568:SER:HA	1.87	0.56
2:AY:1519:VAL:HG23	2:QY:1536:ALA:HB3	1.88	0.56
2:IY:1523:TYR:OH	2:IY:1527:ARG:NH2	2.38	0.56
1:MX:80:THR:O	1:MX:83:ASN:ND2	2.38	0.56
2:LY:1535:MET:HE2	2:LY:1544:PRO:HD3	1.88	0.56
2:NY:1523:TYR:OH	2:NY:1527:ARG:NH2	2.38	0.56
2:CY:1523:TYR:OH	2:CY:1527:ARG:NH2	2.39	0.56
2:DY:1536:ALA:HB3	2:EY:1519:VAL:HG23	1.87	0.56
2:HY:1536:ALA:HB3	2:IY:1519:VAL:HG23	1.87	0.56
1:DX:80:THR:O	1:DX:83:ASN:ND2	2.38	0.56
1:GX:67:ILE:HA	1:GX:308:VAL:HG23	1.88	0.56
1:JX:71:LYS:HG3	2:IY:1568:SER:HA	1.87	0.56
2:HY:1523:TYR:OH	2:HY:1527:ARG:NH2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:JY:1523:TYR:OH	2:JY:1527:ARG:NH2	2.39	0.56
1:AX:268:GLU:OE2	2:QY:1530:LYS:NZ	2.39	0.56
1:BX:80:THR:O	1:BX:83:ASN:ND2	2.38	0.56
1:LX:79:THR:OG1	1:LX:83:ASN:ND2	2.39	0.56
1:QX:272:SER:HB3	2:PY:1531:THR:HB	1.87	0.56
1:AX:272:SER:HB3	2:QY:1531:THR:HB	1.88	0.56
1:OX:67:ILE:HA	1:OX:308:VAL:HG23	1.87	0.56
2:KY:1536:ALA:HB3	2:LY:1519:VAL:HG23	1.86	0.56
1:GX:71:LYS:HG3	2:FY:1568:SER:HA	1.88	0.56
1:OX:80:THR:O	1:OX:83:ASN:ND2	2.38	0.56
2:AY:1475:LEU:HD21	2:AY:1505:GLU:HB3	1.88	0.56
2:BY:1523:TYR:OH	2:BY:1527:ARG:NH2	2.39	0.55
2:FY:1523:TYR:OH	2:FY:1527:ARG:NH2	2.39	0.55
2:LY:1523:TYR:OH	2:LY:1527:ARG:NH2	2.39	0.55
1:BX:91:ASN:ND2	2:AY:1559:THR:OG1	2.39	0.55
2:GY:1523:TYR:OH	2:GY:1527:ARG:NH2	2.39	0.55
2:AY:1523:TYR:OH	2:AY:1527:ARG:NH2	2.39	0.55
2:KY:1523:TYR:OH	2:KY:1527:ARG:NH2	2.40	0.55
2:LY:1548:LYS:HG3	2:MY:1527:ARG:HH22	1.72	0.55
2:EY:1535:MET:HE2	2:EY:1544:PRO:HD3	1.87	0.55
2:PY:1523:TYR:OH	2:PY:1527:ARG:NH2	2.40	0.55
1:EX:71:LYS:HG3	2:DY:1568:SER:HA	1.89	0.55
1:KX:71:LYS:HG3	2:JY:1568:SER:HA	1.89	0.55
1:PX:71:LYS:HG3	2:OY:1568:SER:HA	1.89	0.55
1:LX:71:LYS:HG3	2:KY:1568:SER:HA	1.88	0.55
2:CY:1578:PRO:HD3	2:DY:1591:LYS:HB3	1.89	0.55
2:DY:1523:TYR:OH	2:DY:1527:ARG:NH2	2.40	0.55
2:OY:1523:TYR:OH	2:OY:1527:ARG:NH2	2.40	0.55
1:BX:71:LYS:HG3	2:AY:1568:SER:HA	1.89	0.54
1:FX:36:ARG:NH2	2:EY:1483:ASP:O	2.40	0.54
1:KX:62:ASP:OD2	2:JY:1527:ARG:NH2	2.41	0.54
1:QX:42:VAL:O	1:QX:305:TYR:HA	2.08	0.54
1:AX:71:LYS:HG3	2:QY:1568:SER:HA	1.88	0.54
1:DX:42:VAL:O	1:DX:305:TYR:HA	2.07	0.54
1:NX:268:GLU:OE2	2:MY:1530:LYS:NZ	2.40	0.54
2:IY:1548:LYS:HG3	2:JY:1527:ARG:HH22	1.73	0.54
2:LY:1475:LEU:HD21	2:LY:1505:GLU:HB3	1.90	0.54
2:HY:1548:LYS:HG3	2:IY:1527:ARG:HH22	1.72	0.54
1:LX:268:GLU:OE1	2:KY:1530:LYS:NZ	2.40	0.54
2:EY:1486:ASP:OD1	2:EY:1486:ASP:N	2.39	0.54
1:GX:283:ARG:NH2	1:HX:91:ASN:OD1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:JY:1495:GLU:OE1	2:JY:1506:ARG:NH2	2.41	0.54
1:CX:91:ASN:ND2	2:BY:1559:THR:OG1	2.41	0.54
1:GX:299:ASP:OD1	1:GX:299:ASP:N	2.37	0.54
2:HY:1495:GLU:OE2	2:HY:1506:ARG:NH2	2.41	0.54
1:JX:264:ASP:OD1	1:JX:264:ASP:N	2.38	0.54
2:GY:1495:GLU:OE2	2:GY:1506:ARG:NH2	2.41	0.54
2:AY:1527:ARG:HH22	2:QY:1548:LYS:HG3	1.73	0.54
2:PY:1548:LYS:HG3	2:QY:1527:ARG:HH22	1.73	0.54
1:GX:268:GLU:OE1	2:FY:1530:LYS:NZ	2.40	0.53
1:LX:36:ARG:NH2	2:KY:1483:ASP:O	2.41	0.53
1:OX:36:ARG:NH2	2:NY:1483:ASP:O	2.41	0.53
2:EY:1495:GLU:OE2	2:EY:1506:ARG:NH2	2.41	0.53
2:OY:1548:LYS:HG3	2:PY:1527:ARG:HH22	1.73	0.53
1:AX:67:ILE:HA	1:AX:308:VAL:HG23	1.89	0.53
1:IX:36:ARG:NH2	2:HY:1483:ASP:O	2.41	0.53
1:NX:62:ASP:OD2	2:MY:1527:ARG:NH2	2.41	0.53
2:PY:1495:GLU:OE2	2:PY:1506:ARG:NH2	2.42	0.53
1:AX:35:ASN:O	1:AX:298:LYS:NZ	2.39	0.53
1:GX:62:ASP:OD2	2:FY:1527:ARG:NH2	2.41	0.53
1:BX:67:ILE:HA	1:BX:308:VAL:HG23	1.88	0.53
1:IX:42:VAL:O	1:IX:305:TYR:HA	2.09	0.53
2:BY:1564:ASP:OD2	2:BY:1564:ASP:N	2.38	0.53
1:MX:36:ARG:NH2	2:LY:1483:ASP:O	2.41	0.53
1:KX:91:ASN:ND2	2:JY:1559:THR:OG1	2.42	0.53
1:NX:67:ILE:HA	1:NX:308:VAL:HG23	1.89	0.53
1:DX:36:ARG:NH2	2:CY:1483:ASP:O	2.41	0.53
1:JX:62:ASP:OD2	2:IY:1527:ARG:NH2	2.41	0.53
1:KX:77:TYR:HB2	1:KX:283:ARG:HH21	1.73	0.53
1:OX:78:ILE:HG12	2:NY:1556:ILE:HD12	1.91	0.53
1:QX:62:ASP:OD2	2:PY:1527:ARG:NH2	2.42	0.53
2:AY:1495:GLU:OE1	2:AY:1506:ARG:NH2	2.42	0.53
1:LX:282:VAL:HG13	1:LX:289:TYR:HB2	1.90	0.53
2:EY:1548:LYS:HG3	2:FY:1527:ARG:HH22	1.74	0.53
2:KY:1548:LYS:HG3	2:LY:1527:ARG:HH22	1.74	0.53
1:LX:89:VAL:HG13	1:LX:96:PHE:HB2	1.91	0.52
2:MY:1475:LEU:HD21	2:MY:1505:GLU:HB3	1.91	0.52
1:FX:42:VAL:O	1:FX:305:TYR:HA	2.08	0.52
1:KX:36:ARG:NH2	2:JY:1483:ASP:O	2.42	0.52
1:NX:281:VAL:HG21	1:OX:66:VAL:HG21	1.91	0.52
1:OX:318:VAL:O	1:OX:322:ILE:HB	2.09	0.52
2:IY:1495:GLU:OE1	2:IY:1506:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BX:36:ARG:NH2	2:AY:1483:ASP:O	2.42	0.52
1:JX:80:THR:H	1:JX:83:ASN:HD21	1.57	0.52
1:PX:62:ASP:OD2	2:OY:1527:ARG:NH2	2.43	0.52
1:HX:264:ASP:OD1	1:HX:264:ASP:N	2.40	0.52
1:JX:36:ARG:NH2	2:IY:1483:ASP:O	2.42	0.52
1:OX:104:SER:HB2	2:NY:1547:PHE:HB3	1.91	0.52
1:OX:299:ASP:OD1	1:OX:299:ASP:N	2.39	0.52
2:CY:1548:LYS:HG3	2:DY:1527:ARG:HH22	1.75	0.52
2:EY:1475:LEU:HD21	2:EY:1505:GLU:HB3	1.91	0.52
2:NY:1548:LYS:HG3	2:OY:1527:ARG:HH22	1.74	0.52
1:FX:264:ASP:OD1	1:FX:264:ASP:N	2.39	0.52
1:CX:36:ARG:NH2	2:BY:1483:ASP:O	2.42	0.52
1:LX:62:ASP:OD2	2:KY:1527:ARG:NH2	2.43	0.52
1:MX:71:LYS:HG3	2:LY:1568:SER:HA	1.91	0.52
2:FY:1535:MET:HE2	2:FY:1544:PRO:HD3	1.92	0.52
2:GY:1534:ASN:OD1	2:GY:1538:LYS:NZ	2.43	0.52
1:FX:268:GLU:OE1	2:EY:1530:LYS:NZ	2.42	0.52
1:HX:62:ASP:OD2	2:GY:1527:ARG:NH2	2.43	0.52
1:IX:66:VAL:HA	1:IX:95:ILE:O	2.10	0.52
1:LX:68:GLN:HA	1:LX:94:HIS:HB3	1.92	0.52
1:DX:79:THR:OG1	1:DX:83:ASN:ND2	2.43	0.52
1:FX:62:ASP:OD2	2:EY:1527:ARG:NH2	2.43	0.52
1:GX:36:ARG:NH2	2:FY:1483:ASP:O	2.43	0.52
1:IX:282:VAL:HG13	1:IX:289:TYR:HB2	1.92	0.52
1:EX:299:ASP:OD1	1:EX:299:ASP:N	2.40	0.51
1:HX:36:ARG:NH2	2:GY:1483:ASP:O	2.43	0.51
1:KX:104:SER:HB2	2:JY:1547:PHE:HB3	1.91	0.51
1:NX:36:ARG:NH2	2:MY:1483:ASP:O	2.43	0.51
1:FX:107:MET:N	2:EY:1543:LEU:O	2.42	0.51
1:LX:80:THR:O	1:LX:83:ASN:ND2	2.42	0.51
1:PX:104:SER:HB2	2:OY:1547:PHE:HB3	1.92	0.51
2:CY:1475:LEU:HD21	2:CY:1505:GLU:HB3	1.90	0.51
2:PY:1545:MET:HE3	2:PY:1546:ASP:H	1.75	0.51
1:AX:36:ARG:NH2	2:QY:1483:ASP:O	2.44	0.51
1:KX:107:MET:N	2:JY:1543:LEU:O	2.43	0.51
2:BY:1545:MET:HE3	2:BY:1546:ASP:H	1.76	0.51
2:OY:1475:LEU:HD21	2:OY:1505:GLU:HB3	1.92	0.51
1:AX:42:VAL:O	1:AX:305:TYR:HA	2.11	0.51
1:LX:66:VAL:HA	1:LX:95:ILE:O	2.11	0.51
2:FY:1486:ASP:OD1	2:FY:1486:ASP:N	2.41	0.51
1:AX:62:ASP:OD2	2:QY:1527:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EX:104:SER:HB2	2:DY:1547:PHE:HB3	1.92	0.51
1:IX:35:ASN:O	1:IX:298:LYS:NZ	2.40	0.51
1:JX:42:VAL:O	1:JX:305:TYR:HA	2.10	0.51
2:DY:1545:MET:HE3	2:DY:1546:ASP:H	1.76	0.51
2:KY:1534:ASN:OD1	2:KY:1538:LYS:NZ	2.44	0.51
2:LY:1545:MET:HE3	2:LY:1546:ASP:H	1.75	0.51
1:BX:104:SER:HB2	2:AY:1547:PHE:HB3	1.92	0.51
1:EX:282:VAL:HG13	1:EX:289:TYR:HB2	1.92	0.51
1:GX:280:LEU:N	1:GX:291:PHE:O	2.37	0.51
1:HX:280:LEU:N	1:HX:291:PHE:O	2.37	0.51
1:NX:104:SER:HB2	2:MY:1547:PHE:HB3	1.93	0.51
1:PX:318:VAL:O	1:PX:322:ILE:HB	2.10	0.51
1:QX:89:VAL:HG13	1:QX:96:PHE:HB2	1.93	0.51
2:JY:1548:LYS:HG3	2:KY:1527:ARG:HH22	1.75	0.51
1:KX:282:VAL:HG13	1:KX:289:TYR:HB2	1.91	0.51
1:CX:62:ASP:OD2	2:BY:1527:ARG:NH2	2.43	0.51
1:IX:62:ASP:OD2	2:HY:1527:ARG:NH2	2.44	0.51
1:NX:79:THR:OG1	1:NX:83:ASN:ND2	2.42	0.51
2:KY:1495:GLU:OE1	2:KY:1506:ARG:NH2	2.42	0.51
1:FX:280:LEU:N	1:FX:291:PHE:O	2.38	0.51
1:FX:299:ASP:OD1	1:FX:299:ASP:N	2.39	0.51
1:LX:68:GLN:HG2	1:LX:309:LYS:HG3	1.93	0.51
1:NX:35:ASN:O	1:NX:298:LYS:NZ	2.40	0.51
1:PX:36:ARG:NH2	2:OY:1483:ASP:O	2.44	0.51
1:QX:80:THR:H	1:QX:83:ASN:HD21	1.58	0.51
2:BY:1475:LEU:HD21	2:BY:1505:GLU:HB3	1.93	0.51
1:GX:42:VAL:O	1:GX:305:TYR:HA	2.11	0.50
1:GX:282:VAL:HG13	1:GX:289:TYR:HB2	1.93	0.50
1:OX:42:VAL:O	1:OX:305:TYR:HA	2.10	0.50
1:PX:68:GLN:HA	1:PX:94:HIS:HB3	1.93	0.50
2:JY:1545:MET:HE3	2:JY:1546:ASP:H	1.76	0.50
1:CX:42:VAL:O	1:CX:305:TYR:HA	2.11	0.50
1:DX:62:ASP:OD2	2:CY:1527:ARG:NH2	2.43	0.50
2:FY:1475:LEU:HD21	2:FY:1505:GLU:HB3	1.92	0.50
1:CX:104:SER:HB2	2:BY:1547:PHE:HB3	1.93	0.50
1:JX:78:ILE:HG12	2:IY:1556:ILE:HD12	1.93	0.50
2:FY:1545:MET:HE3	2:FY:1546:ASP:H	1.76	0.50
1:JX:299:ASP:OD1	1:JX:299:ASP:N	2.38	0.50
1:OX:78:ILE:HG21	1:OX:90:PRO:HG3	1.93	0.50
2:MY:1548:LYS:HG3	2:NY:1527:ARG:HH22	1.76	0.50
2:QY:1545:MET:HE3	2:QY:1546:ASP:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NX:42:VAL:O	1:NX:305:TYR:HA	2.11	0.50
1:NX:280:LEU:N	1:NX:291:PHE:O	2.37	0.50
2:BY:1578:PRO:HD3	2:CY:1591:LYS:HB3	1.92	0.50
1:DX:68:GLN:HA	1:DX:94:HIS:HB3	1.94	0.50
1:HX:80:THR:HG22	1:HX:280:LEU:HA	1.94	0.50
1:MX:66:VAL:HA	1:MX:95:ILE:O	2.12	0.50
1:NX:91:ASN:ND2	2:MY:1559:THR:OG1	2.45	0.50
1:QX:78:ILE:HG21	1:QX:90:PRO:HG3	1.93	0.50
2:AY:1548:LYS:HG3	2:BY:1527:ARG:HH22	1.77	0.50
1:MX:42:VAL:O	1:MX:305:TYR:HA	2.11	0.50
2:BY:1548:LYS:HG3	2:CY:1527:ARG:HH22	1.77	0.50
2:GY:1548:LYS:HG3	2:HY:1527:ARG:HH22	1.77	0.50
2:JY:1475:LEU:HD21	2:JY:1505:GLU:HB3	1.93	0.50
1:MX:92:SER:HB3	2:LY:1560:ASN:HA	1.93	0.50
2:KY:1475:LEU:HD21	2:KY:1505:GLU:HB3	1.93	0.50
2:MY:1545:MET:HE3	2:MY:1546:ASP:H	1.76	0.50
2:OY:1545:MET:HE3	2:OY:1546:ASP:H	1.76	0.50
1:AX:67:ILE:O	1:AX:94:HIS:HA	2.12	0.50
1:EX:36:ARG:NH2	2:DY:1483:ASP:O	2.45	0.50
1:HX:89:VAL:HG13	1:HX:96:PHE:HB2	1.94	0.50
1:MX:61:LEU:HD22	1:MX:271:PRO:HG2	1.94	0.50
1:MX:268:GLU:OE1	2:LY:1530:LYS:NZ	2.43	0.50
1:OX:71:LYS:HG3	2:NY:1568:SER:HA	1.93	0.50
1:QX:36:ARG:NH2	2:PY:1483:ASP:O	2.45	0.50
2:PY:1475:LEU:HD21	2:PY:1505:GLU:HB3	1.94	0.50
2:QY:1475:LEU:HD21	2:QY:1505:GLU:HB3	1.93	0.50
1:LX:107:MET:N	2:KY:1543:LEU:O	2.44	0.49
1:OX:68:GLN:HG2	1:OX:309:LYS:HG3	1.94	0.49
1:EX:90:PRO:HB3	1:EX:95:ILE:HG23	1.94	0.49
1:GX:35:ASN:O	1:GX:298:LYS:NZ	2.40	0.49
1:OX:61:LEU:HD22	1:OX:271:PRO:HG2	1.94	0.49
2:HY:1475:LEU:HD21	2:HY:1505:GLU:HB3	1.94	0.49
1:LX:297:GLN:HB2	1:LX:300:ASN:HB2	1.94	0.49
2:NY:1495:GLU:OE2	2:NY:1506:ARG:NH2	2.43	0.49
2:NY:1545:MET:HE3	2:NY:1546:ASP:H	1.77	0.49
2:OY:1495:GLU:OE1	2:OY:1506:ARG:NH2	2.45	0.49
1:BX:272:SER:HB3	2:AY:1531:THR:HB	1.95	0.49
1:FX:89:VAL:HG13	1:FX:96:PHE:HB2	1.94	0.49
1:GX:104:SER:HB2	2:FY:1547:PHE:HB3	1.94	0.49
1:HX:297:GLN:HB2	1:HX:300:ASN:HB2	1.95	0.49
1:NX:71:LYS:HG3	2:MY:1568:SER:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QX:80:THR:HG22	1:QX:280:LEU:HA	1.94	0.49
1:AX:80:THR:HG22	1:AX:280:LEU:HA	1.94	0.49
1:AX:282:VAL:HG13	1:AX:289:TYR:HB2	1.94	0.49
1:FX:282:VAL:HG13	1:FX:289:TYR:HB2	1.95	0.49
1:HX:107:MET:N	2:GY:1543:LEU:O	2.44	0.49
1:IX:80:THR:H	1:IX:83:ASN:HD21	1.60	0.49
1:QX:280:LEU:N	1:QX:291:PHE:O	2.37	0.49
1:QX:91:ASN:ND2	2:PY:1559:THR:OG1	2.45	0.49
2:CY:1545:MET:HE3	2:CY:1546:ASP:H	1.76	0.49
1:EX:107:MET:N	2:DY:1543:LEU:O	2.44	0.49
1:HX:282:VAL:HG13	1:HX:289:TYR:HB2	1.95	0.49
1:JX:68:GLN:HA	1:JX:94:HIS:HB3	1.95	0.49
1:OX:89:VAL:HG13	1:OX:96:PHE:HB2	1.94	0.49
1:PX:66:VAL:HA	1:PX:95:ILE:O	2.12	0.49
1:FX:68:GLN:HA	1:FX:94:HIS:HB3	1.95	0.49
1:IX:280:LEU:N	1:IX:291:PHE:O	2.37	0.49
1:LX:280:LEU:N	1:LX:291:PHE:O	2.37	0.49
1:BX:282:VAL:HG13	1:BX:289:TYR:HB2	1.93	0.49
1:CX:79:THR:OG1	1:CX:83:ASN:ND2	2.46	0.49
1:EX:61:LEU:HD22	1:EX:271:PRO:HG2	1.95	0.49
1:GX:79:THR:OG1	1:GX:83:ASN:ND2	2.42	0.49
1:KX:67:ILE:O	1:KX:94:HIS:HA	2.13	0.49
1:LX:80:THR:HG22	1:LX:280:LEU:HA	1.94	0.49
1:PX:107:MET:N	2:OY:1543:LEU:O	2.43	0.49
1:EX:80:THR:HG22	1:EX:280:LEU:HA	1.95	0.48
1:MX:107:MET:N	2:LY:1543:LEU:O	2.44	0.48
1:NX:66:VAL:HA	1:NX:95:ILE:O	2.13	0.48
1:QX:68:GLN:HA	1:QX:94:HIS:HB3	1.94	0.48
2:DY:1475:LEU:HD21	2:DY:1505:GLU:HB3	1.94	0.48
1:DX:107:MET:N	2:CY:1543:LEU:O	2.43	0.48
1:IX:272:SER:HB3	2:HY:1531:THR:HB	1.96	0.48
1:JX:280:LEU:N	1:JX:291:PHE:O	2.38	0.48
2:DY:1495:GLU:OE2	2:DY:1506:ARG:NH2	2.41	0.48
2:FY:1548:LYS:HG3	2:GY:1527:ARG:HH22	1.78	0.48
2:KY:1545:MET:HE3	2:KY:1546:ASP:H	1.78	0.48
1:AX:107:MET:N	2:QY:1543:LEU:O	2.43	0.48
1:EX:62:ASP:OD2	2:DY:1527:ARG:NH2	2.46	0.48
1:MX:68:GLN:HA	1:MX:94:HIS:HB3	1.95	0.48
1:AX:280:LEU:N	1:AX:291:PHE:O	2.38	0.48
1:DX:282:VAL:HG13	1:DX:289:TYR:HB2	1.94	0.48
1:MX:280:LEU:N	1:MX:291:PHE:O	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NX:107:MET:N	2:MY:1543:LEU:O	2.45	0.48
2:GY:1475:LEU:HD21	2:GY:1505:GLU:HB3	1.93	0.48
1:CX:107:MET:N	2:BY:1543:LEU:O	2.43	0.48
1:GX:92:SER:HB3	2:FY:1560:ASN:HA	1.94	0.48
1:HX:92:SER:HB3	2:GY:1560:ASN:HA	1.96	0.48
1:KX:57:ILE:HD12	1:KX:308:VAL:HG21	1.96	0.48
1:KX:264:ASP:OD1	1:KX:264:ASP:N	2.39	0.48
1:OX:272:SER:HB3	2:NY:1531:THR:HB	1.94	0.48
1:OX:280:LEU:N	1:OX:291:PHE:O	2.38	0.48
1:PX:35:ASN:O	1:PX:298:LYS:NZ	2.38	0.48
1:PX:280:LEU:N	1:PX:291:PHE:O	2.38	0.48
2:AY:1534:ASN:OD1	2:AY:1538:LYS:NZ	2.45	0.48
1:CX:280:LEU:N	1:CX:291:PHE:O	2.37	0.48
1:EX:68:GLN:HA	1:EX:94:HIS:HB3	1.95	0.48
1:GX:107:MET:N	2:FY:1543:LEU:O	2.45	0.48
1:KX:280:LEU:N	1:KX:291:PHE:O	2.37	0.48
1:LX:42:VAL:O	1:LX:305:TYR:HA	2.14	0.48
1:MX:282:VAL:HG13	1:MX:289:TYR:HB2	1.94	0.48
1:QX:104:SER:HB2	2:PY:1547:PHE:HB3	1.94	0.48
2:HY:1545:MET:HE3	2:HY:1546:ASP:H	1.78	0.48
1:KX:80:THR:H	1:KX:83:ASN:HD21	1.61	0.48
1:NX:80:THR:HG22	1:NX:280:LEU:HA	1.95	0.48
1:AX:79:THR:OG1	1:AX:83:ASN:ND2	2.41	0.48
1:HX:78:ILE:HG21	1:HX:90:PRO:HG3	1.95	0.48
1:JX:268:GLU:OE1	2:IY:1530:LYS:NZ	2.47	0.48
1:NX:80:THR:H	1:NX:83:ASN:HD21	1.61	0.48
2:HY:1535:MET:HE2	2:HY:1544:PRO:HD3	1.95	0.48
2:PY:1535:MET:HE2	2:PY:1544:PRO:HD3	1.95	0.48
1:AX:61:LEU:HD22	1:AX:271:PRO:HG2	1.96	0.48
1:DX:104:SER:HB2	2:CY:1547:PHE:HB3	1.96	0.48
1:GX:80:THR:HG22	1:GX:280:LEU:HA	1.95	0.48
2:OY:1578:PRO:HD3	2:PY:1591:LYS:HB3	1.95	0.48
2:QY:1534:ASN:OD1	2:QY:1538:LYS:NZ	2.44	0.48
1:AX:66:VAL:HA	1:AX:95:ILE:O	2.14	0.48
1:BX:80:THR:HG22	1:BX:280:LEU:HA	1.94	0.48
1:BX:92:SER:HB3	2:AY:1560:ASN:HA	1.95	0.48
1:BX:280:LEU:HB3	1:BX:291:PHE:HB2	1.95	0.48
1:HX:66:VAL:HA	1:HX:95:ILE:O	2.14	0.48
1:KX:299:ASP:OD1	1:KX:299:ASP:N	2.40	0.48
1:CX:297:GLN:HB2	1:CX:300:ASN:HB2	1.96	0.47
1:GX:264:ASP:OD1	1:GX:264:ASP:N	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PX:61:LEU:HD22	1:PX:271:PRO:HG2	1.95	0.47
1:QX:78:ILE:HG12	2:PY:1556:ILE:HD12	1.96	0.47
2:AY:1545:MET:HE3	2:AY:1546:ASP:H	1.78	0.47
2:GY:1545:MET:HE3	2:GY:1546:ASP:H	1.79	0.47
1:BX:66:VAL:HA	1:BX:95:ILE:O	2.13	0.47
1:CX:66:VAL:HA	1:CX:95:ILE:O	2.14	0.47
1:HX:322:ILE:HG23	2:IY:1581:ALA:HA	1.96	0.47
1:KX:80:THR:HG22	1:KX:280:LEU:HA	1.97	0.47
1:MX:79:THR:OG1	1:MX:83:ASN:ND2	2.45	0.47
1:BX:280:LEU:N	1:BX:291:PHE:O	2.38	0.47
1:DX:71:LYS:HG3	2:CY:1568:SER:HA	1.94	0.47
1:EX:268:GLU:OE2	2:DY:1530:LYS:NZ	2.47	0.47
1:HX:79:THR:OG1	1:HX:83:ASN:ND2	2.41	0.47
1:LX:35:ASN:O	1:LX:298:LYS:NZ	2.39	0.47
1:PX:92:SER:HB3	2:OY:1560:ASN:HA	1.95	0.47
1:QX:280:LEU:HB3	1:QX:291:PHE:HB2	1.95	0.47
2:EY:1545:MET:HE3	2:EY:1546:ASP:H	1.79	0.47
2:KY:1593:LYS:HB3	2:KY:1593:LYS:HE3	1.65	0.47
2:NY:1475:LEU:HD21	2:NY:1505:GLU:HB3	1.96	0.47
1:CX:68:GLN:HA	1:CX:94:HIS:HB3	1.95	0.47
1:GX:66:VAL:HA	1:GX:95:ILE:O	2.15	0.47
1:GX:80:THR:H	1:GX:83:ASN:HD21	1.63	0.47
1:OX:107:MET:N	2:NY:1543:LEU:O	2.45	0.47
1:OX:322:ILE:HG23	2:PY:1581:ALA:HA	1.97	0.47
1:QX:282:VAL:HG13	1:QX:289:TYR:HB2	1.94	0.47
2:IY:1470:SER:OG	2:IY:1471:LYS:N	2.47	0.47
1:HX:57:ILE:HD12	1:HX:308:VAL:HG21	1.96	0.47
1:KX:78:ILE:HG12	2:JY:1556:ILE:HD12	1.96	0.47
1:NX:92:SER:HB3	2:MY:1560:ASN:HA	1.96	0.47
1:MX:80:THR:HG22	1:MX:280:LEU:HA	1.95	0.47
1:MX:80:THR:H	1:MX:83:ASN:HD21	1.61	0.47
1:PX:70:GLU:HB3	1:PX:73:GLU:HG3	1.95	0.47
1:PX:282:VAL:HG13	1:PX:289:TYR:HB2	1.95	0.47
2:HY:1534:ASN:OD1	2:HY:1538:LYS:NZ	2.44	0.47
1:DX:280:LEU:N	1:DX:291:PHE:O	2.37	0.47
1:EX:66:VAL:HA	1:EX:95:ILE:O	2.14	0.47
1:FX:61:LEU:HD22	1:FX:271:PRO:HG2	1.96	0.47
2:JY:1535:MET:HE2	2:JY:1544:PRO:HD3	1.96	0.47
2:LY:1534:ASN:OD1	2:LY:1538:LYS:NZ	2.45	0.47
1:BX:42:VAL:O	1:BX:305:TYR:HA	2.15	0.47
1:CX:80:THR:H	1:CX:83:ASN:HD21	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CX:268:GLU:OE2	2:BY:1530:LYS:NZ	2.46	0.47
1:IX:322:ILE:HG23	2:JY:1581:ALA:HA	1.96	0.47
1:JX:92:SER:HB3	2:IY:1560:ASN:HA	1.96	0.47
1:QX:66:VAL:HA	1:QX:95:ILE:O	2.15	0.47
1:KX:67:ILE:HA	1:KX:308:VAL:HG23	1.97	0.47
2:PY:1534:ASN:OD1	2:PY:1538:LYS:NZ	2.47	0.47
1:BX:80:THR:H	1:BX:83:ASN:HD21	1.62	0.47
1:IX:92:SER:HB3	2:HY:1560:ASN:HA	1.97	0.47
1:IX:297:GLN:HB2	1:IX:300:ASN:HB2	1.98	0.47
1:AX:280:LEU:HB3	1:AX:291:PHE:HB2	1.97	0.46
1:FX:80:THR:H	1:FX:83:ASN:HD21	1.62	0.46
1:OX:282:VAL:HG13	1:OX:289:TYR:HB2	1.96	0.46
2:IY:1475:LEU:HD21	2:IY:1505:GLU:HB3	1.96	0.46
2:NY:1534:ASN:OD1	2:NY:1538:LYS:NZ	2.46	0.46
1:CX:71:LYS:HG3	2:BY:1568:SER:HA	1.96	0.46
1:IX:80:THR:HG22	1:IX:280:LEU:HA	1.97	0.46
1:JX:66:VAL:HA	1:JX:95:ILE:O	2.14	0.46
2:MY:1495:GLU:OE2	2:MY:1506:ARG:NH2	2.43	0.46
1:BX:79:THR:OG1	1:BX:83:ASN:ND2	2.42	0.46
1:DX:92:SER:HB3	2:CY:1560:ASN:HA	1.96	0.46
1:JX:282:VAL:HG13	1:JX:289:TYR:HB2	1.98	0.46
1:KX:272:SER:HB3	2:JY:1531:THR:HB	1.98	0.46
1:LX:280:LEU:HB3	1:LX:291:PHE:HB2	1.97	0.46
2:IY:1534:ASN:OD1	2:IY:1538:LYS:NZ	2.45	0.46
1:GX:87:SER:OG	1:GX:98:GLN:O	2.33	0.46
1:JX:61:LEU:HD22	1:JX:271:PRO:HG2	1.97	0.46
1:NX:67:ILE:HD11	1:NX:97:ILE:HD13	1.98	0.46
1:NX:282:VAL:HG13	1:NX:289:TYR:HB2	1.96	0.46
1:OX:92:SER:HB3	2:NY:1560:ASN:HA	1.96	0.46
1:IX:90:PRO:HB3	1:IX:95:ILE:HG23	1.97	0.46
1:QX:107:MET:N	2:PY:1543:LEU:O	2.45	0.46
1:AX:92:SER:HB3	2:QY:1560:ASN:HA	1.96	0.46
1:CX:282:VAL:HG13	1:CX:289:TYR:HB2	1.97	0.46
1:HX:62:ASP:OD2	2:FY:1548:LYS:NZ	2.44	0.46
1:HX:70:GLU:OE1	1:HX:286:LYS:NZ	2.41	0.46
1:JX:107:MET:N	2:IY:1543:LEU:O	2.43	0.46
1:QX:79:THR:OG1	1:QX:83:ASN:ND2	2.44	0.46
2:CY:1534:ASN:OD1	2:CY:1538:LYS:NZ	2.45	0.46
1:BX:268:GLU:OE1	2:AY:1530:LYS:NZ	2.49	0.46
1:OX:68:GLN:HA	1:OX:94:HIS:HB3	1.98	0.46
1:DX:272:SER:HB3	2:CY:1531:THR:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KX:297:GLN:HB2	1:KX:300:ASN:HB2	1.98	0.46
1:FX:80:THR:HG22	1:FX:280:LEU:HA	1.98	0.46
1:IX:71:LYS:HG3	2:HY:1568:SER:HA	1.97	0.46
1:NX:70:GLU:HB3	1:NX:73:GLU:HG3	1.98	0.46
2:BY:1534:ASN:OD1	2:BY:1538:LYS:NZ	2.47	0.46
2:JY:1534:ASN:OD1	2:JY:1538:LYS:NZ	2.45	0.46
1:EX:92:SER:HB3	2:DY:1560:ASN:HA	1.96	0.46
1:IX:61:LEU:HD22	1:IX:271:PRO:HG2	1.97	0.46
1:IX:79:THR:OG1	1:IX:83:ASN:ND2	2.45	0.46
1:LX:70:GLU:HB3	1:LX:73:GLU:HG3	1.98	0.46
1:PX:80:THR:H	1:PX:83:ASN:HD21	1.61	0.46
2:BY:1535:MET:HE2	2:BY:1544:PRO:HD3	1.97	0.46
1:AX:264:ASP:OD1	1:AX:264:ASP:N	2.37	0.45
1:EX:79:THR:OG1	1:EX:83:ASN:ND2	2.43	0.45
1:HX:80:THR:H	1:HX:83:ASN:HD21	1.63	0.45
2:NY:1502:SER:OG	2:NY:1503:ASP:N	2.49	0.45
1:BX:62:ASP:OD2	2:AY:1527:ARG:NH2	2.49	0.45
1:DX:297:GLN:HB2	1:DX:300:ASN:HB2	1.98	0.45
1:IX:68:GLN:HA	1:IX:94:HIS:HB3	1.98	0.45
1:KX:273:ASP:OD2	1:KX:300:ASN:ND2	2.49	0.45
1:LX:291:PHE:HZ	1:LX:310:LEU:HD11	1.82	0.45
1:NX:61:LEU:HD22	1:NX:271:PRO:HG2	1.97	0.45
1:NX:78:ILE:HG21	1:NX:90:PRO:HG3	1.97	0.45
1:OX:291:PHE:HZ	1:OX:310:LEU:HD11	1.81	0.45
1:PX:268:GLU:OE2	2:OY:1530:LYS:NZ	2.49	0.45
1:BX:107:MET:N	2:AY:1543:LEU:O	2.44	0.45
1:QX:35:ASN:O	1:QX:298:LYS:NZ	2.40	0.45
1:DX:80:THR:HG22	1:DX:280:LEU:HA	1.98	0.45
1:EX:280:LEU:N	1:EX:291:PHE:O	2.38	0.45
1:LX:92:SER:HB3	2:KY:1560:ASN:HA	1.98	0.45
1:OX:80:THR:HG22	1:OX:280:LEU:HA	1.99	0.45
1:QX:92:SER:HB3	2:PY:1560:ASN:HA	1.98	0.45
1:QX:297:GLN:HB2	1:QX:300:ASN:HB2	1.98	0.45
1:DX:49:LEU:H	1:DX:49:LEU:HG	1.66	0.45
1:FX:280:LEU:HB3	1:FX:291:PHE:HB2	1.97	0.45
1:GX:280:LEU:HB3	1:GX:291:PHE:HB2	1.98	0.45
1:HX:61:LEU:HD22	1:HX:271:PRO:HG2	1.98	0.45
1:KX:79:THR:OG1	1:KX:83:ASN:ND2	2.46	0.45
1:PX:57:ILE:HD12	1:PX:308:VAL:HG21	1.99	0.45
1:EX:280:LEU:HB3	1:EX:291:PHE:HB2	1.97	0.45
1:HX:35:ASN:O	1:HX:298:LYS:NZ	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JX:35:ASN:O	1:JX:298:LYS:NZ	2.39	0.45
1:NX:67:ILE:O	1:NX:94:HIS:HA	2.17	0.45
1:OX:62:ASP:OD2	2:NY:1527:ARG:NH2	2.49	0.45
1:QX:291:PHE:HZ	1:QX:310:LEU:HD11	1.82	0.45
2:IY:1486:ASP:OD1	2:IY:1486:ASP:N	2.39	0.45
1:GX:68:GLN:HA	1:GX:94:HIS:HB3	1.99	0.45
1:GX:297:GLN:HB2	1:GX:300:ASN:HB2	1.99	0.45
1:JX:272:SER:HB3	2:IY:1531:THR:HB	1.99	0.45
2:GY:1470:SER:OG	2:GY:1471:LYS:N	2.50	0.45
1:FX:79:THR:OG1	1:FX:83:ASN:ND2	2.45	0.45
2:MY:1470:SER:OG	2:MY:1471:LYS:N	2.47	0.45
1:BX:57:ILE:HD12	1:BX:308:VAL:HG21	1.99	0.45
1:FX:71:LYS:HG3	2:EY:1568:SER:HA	1.99	0.45
1:LX:78:ILE:HG21	1:LX:90:PRO:HG3	1.98	0.45
1:QX:61:LEU:HD22	1:QX:271:PRO:HG2	1.98	0.45
2:IY:1545:MET:HE3	2:IY:1546:ASP:H	1.82	0.45
1:EX:264:ASP:OD1	1:EX:264:ASP:N	2.37	0.45
1:MX:78:ILE:HG21	1:MX:90:PRO:HG3	1.99	0.45
2:EY:1470:SER:OG	2:EY:1471:LYS:N	2.50	0.45
2:GY:1600:ALA:HA	2:GY:1603:LEU:HD12	1.99	0.45
2:QY:1532:PHE:HD2	2:QY:1544:PRO:HG2	1.82	0.45
1:BX:299:ASP:OD1	1:BX:299:ASP:N	2.37	0.44
1:CX:60:SER:OG	1:CX:61:LEU:N	2.51	0.44
1:DX:68:GLN:HG2	1:DX:309:LYS:HG3	1.99	0.44
1:EX:80:THR:H	1:EX:83:ASN:HD21	1.65	0.44
1:EX:297:GLN:HB2	1:EX:300:ASN:HB2	1.99	0.44
1:FX:318:VAL:O	1:FX:322:ILE:HB	2.17	0.44
1:HX:104:SER:HB2	2:GY:1547:PHE:HB3	1.99	0.44
1:IX:273:ASP:OD2	1:IX:300:ASN:ND2	2.50	0.44
1:JX:126:LEU:HD23	1:JX:126:LEU:HA	1.87	0.44
1:BX:127:LYS:HA	1:BX:127:LYS:HD3	1.77	0.44
2:CY:1486:ASP:OD2	2:DY:1470:SER:OG	2.35	0.44
2:DY:1502:SER:OG	2:DY:1503:ASP:N	2.50	0.44
2:FY:1564:ASP:OD1	2:FY:1564:ASP:N	2.47	0.44
2:PY:1486:ASP:OD1	2:PY:1486:ASP:N	2.41	0.44
1:AX:297:GLN:HB2	1:AX:300:ASN:HB2	2.00	0.44
1:EX:70:GLU:HB3	1:EX:73:GLU:HG3	1.99	0.44
1:EX:75:ILE:HG23	1:EX:282:VAL:HG23	1.99	0.44
1:JX:78:ILE:HG21	1:JX:90:PRO:HG3	1.99	0.44
1:KX:61:LEU:HD22	1:KX:271:PRO:HG2	2.00	0.44
1:KX:92:SER:HB3	2:JY:1560:ASN:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LX:80:THR:H	1:LX:83:ASN:HD21	1.65	0.44
1:NX:127:LYS:HD3	1:NX:127:LYS:HA	1.78	0.44
1:BX:78:ILE:HG21	1:BX:90:PRO:HG3	1.99	0.44
1:BX:297:GLN:HB2	1:BX:300:ASN:HB2	1.99	0.44
1:CX:67:ILE:O	1:CX:94:HIS:HA	2.18	0.44
1:CX:80:THR:HG22	1:CX:280:LEU:HA	1.99	0.44
1:EX:88:ILE:HG22	1:EX:90:PRO:HD3	2.00	0.44
1:HX:126:LEU:HD23	1:HX:126:LEU:HA	1.86	0.44
1:LX:127:LYS:HA	1:LX:127:LYS:HD3	1.80	0.44
1:PX:291:PHE:HZ	1:PX:310:LEU:HD11	1.82	0.44
2:EY:1565:LYS:HB3	2:EY:1565:LYS:HE2	1.85	0.44
1:DX:80:THR:H	1:DX:83:ASN:HD21	1.65	0.44
1:HX:74:THR:OG1	2:GY:1560:ASN:ND2	2.49	0.44
1:LX:107:MET:HE2	1:LX:107:MET:HB3	1.91	0.44
1:PX:49:LEU:H	1:PX:49:LEU:HG	1.66	0.44
1:CX:126:LEU:HD23	1:CX:126:LEU:HA	1.85	0.44
1:DX:107:MET:HE2	1:DX:107:MET:HB3	1.91	0.44
1:FX:66:VAL:HA	1:FX:95:ILE:O	2.18	0.44
2:AY:1565:LYS:HB3	2:AY:1565:LYS:HE2	1.87	0.44
1:EX:127:LYS:HD3	1:EX:127:LYS:HA	1.79	0.44
1:IX:107:MET:N	2:HY:1543:LEU:O	2.43	0.44
1:LX:79:THR:OG1	1:LX:80:THR:N	2.51	0.44
1:NX:291:PHE:HZ	1:NX:310:LEU:HD11	1.83	0.44
1:QX:41:VAL:HB	1:QX:306:LEU:HD11	2.00	0.44
2:MY:1534:ASN:OD1	2:MY:1538:LYS:NZ	2.47	0.44
1:BX:61:LEU:HD22	1:BX:271:PRO:HG2	1.99	0.44
1:CX:65:THR:OG1	1:CX:305:TYR:O	2.28	0.44
1:HX:68:GLN:HA	1:HX:94:HIS:HB3	2.00	0.44
2:IY:1487:ASP:OD1	2:IY:1489:THR:OG1	2.33	0.44
2:JY:1486:ASP:OD1	2:JY:1486:ASP:N	2.41	0.44
1:DX:273:ASP:OD2	1:DX:300:ASN:ND2	2.50	0.44
1:HX:127:LYS:HD3	1:HX:127:LYS:HA	1.78	0.44
1:JX:80:THR:HG22	1:JX:280:LEU:HA	1.99	0.44
1:LX:40:LYS:HD3	1:LX:40:LYS:HA	1.72	0.44
1:LX:61:LEU:HD22	1:LX:271:PRO:HG2	2.00	0.44
2:PY:1564:ASP:N	2:PY:1564:ASP:OD2	2.47	0.44
1:CX:126:LEU:O	1:CX:130:LYS:HB2	2.18	0.43
1:JX:322:ILE:HG23	2:KY:1581:ALA:HA	1.99	0.43
1:KX:67:ILE:HD11	1:KX:97:ILE:HD13	1.99	0.43
1:NX:75:ILE:HG23	1:NX:282:VAL:HG23	2.00	0.43
1:PX:80:THR:HG22	1:PX:280:LEU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PX:107:MET:HE2	1:PX:107:MET:HB3	1.91	0.43
2:AY:1514:ARG:O	2:AY:1518:GLU:HG2	2.18	0.43
2:DY:1486:ASP:OD2	2:EY:1470:SER:OG	2.36	0.43
1:AX:126:LEU:HD23	1:AX:126:LEU:HA	1.88	0.43
1:FX:67:ILE:O	1:FX:94:HIS:HA	2.18	0.43
1:IX:280:LEU:HB3	1:IX:291:PHE:HB2	1.99	0.43
2:KY:1486:ASP:OD1	2:KY:1486:ASP:N	2.39	0.43
1:AX:299:ASP:OD1	1:AX:299:ASP:N	2.37	0.43
1:DX:322:ILE:HG23	2:EY:1581:ALA:HA	2.00	0.43
1:FX:322:ILE:HG23	2:GY:1581:ALA:HA	2.00	0.43
1:IX:70:GLU:HB3	1:IX:73:GLU:HG3	2.01	0.43
1:JX:40:LYS:HA	1:JX:40:LYS:HD3	1.79	0.43
1:JX:75:ILE:HG23	1:JX:282:VAL:HG23	2.00	0.43
1:OX:40:LYS:HA	1:OX:40:LYS:HD3	1.75	0.43
2:DY:1534:ASN:OD1	2:DY:1538:LYS:NZ	2.48	0.43
2:JY:1470:SER:OG	2:JY:1471:LYS:N	2.52	0.43
1:DX:78:ILE:HG21	1:DX:90:PRO:HG3	2.00	0.43
1:GX:70:GLU:HB3	1:GX:73:GLU:HG3	2.00	0.43
1:IX:48:TYR:HD1	1:IX:55:ILE:HD11	1.84	0.43
1:JX:67:ILE:O	1:JX:94:HIS:HA	2.18	0.43
1:JX:70:GLU:HB3	1:JX:73:GLU:HG3	2.01	0.43
1:LX:126:LEU:HD23	1:LX:126:LEU:HA	1.87	0.43
1:QX:48:TYR:HD1	1:QX:55:ILE:HD11	1.84	0.43
1:AX:127:LYS:HA	1:AX:127:LYS:HD3	1.80	0.43
1:BX:75:ILE:HG23	1:BX:282:VAL:HG23	2.00	0.43
1:LX:48:TYR:HD1	1:LX:55:ILE:HD11	1.83	0.43
1:LX:272:SER:HB3	2:KY:1531:THR:HB	2.00	0.43
1:OX:107:MET:O	2:NY:1543:LEU:N	2.49	0.43
1:PX:75:ILE:HG23	1:PX:282:VAL:HG23	2.00	0.43
2:KY:1487:ASP:OD1	2:KY:1489:THR:OG1	2.36	0.43
2:OY:1565:LYS:HB3	2:OY:1565:LYS:HE2	1.84	0.43
1:IX:127:LYS:HA	1:IX:127:LYS:HD3	1.80	0.43
1:MX:297:GLN:HB2	1:MX:300:ASN:HB2	2.01	0.43
1:NX:126:LEU:HD23	1:NX:126:LEU:HA	1.87	0.43
1:PX:48:TYR:HD1	1:PX:55:ILE:HD11	1.84	0.43
2:EY:1543:LEU:HD23	2:EY:1543:LEU:HA	1.91	0.43
1:JX:291:PHE:HZ	1:JX:310:LEU:HD11	1.83	0.43
1:KX:127:LYS:HA	1:KX:127:LYS:HD3	1.78	0.43
1:LX:78:ILE:HG12	2:KY:1556:ILE:HD12	1.99	0.43
1:OX:80:THR:H	1:OX:83:ASN:HD21	1.67	0.43
1:AX:60:SER:OG	1:AX:61:LEU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GX:52:GLU:HG2	1:GX:53:LYS:HG2	2.01	0.43
1:IX:268:GLU:OE2	2:HY:1530:LYS:NZ	2.52	0.43
1:KX:78:ILE:HG21	1:KX:90:PRO:HG3	2.01	0.43
1:MX:280:LEU:HB3	1:MX:291:PHE:HB2	2.00	0.43
1:NX:60:SER:OG	1:NX:61:LEU:N	2.50	0.43
1:NX:297:GLN:HB2	1:NX:300:ASN:HB2	2.01	0.43
2:AY:1486:ASP:OD1	2:AY:1486:ASP:N	2.41	0.43
2:OY:1601:LYS:HE3	2:OY:1601:LYS:HB3	1.85	0.43
1:GX:61:LEU:HD22	1:GX:271:PRO:HG2	2.01	0.43
1:HX:280:LEU:HB3	1:HX:291:PHE:HB2	2.00	0.43
1:KX:66:VAL:HG22	1:KX:307:THR:HA	2.01	0.43
2:GY:1486:ASP:OD1	2:HY:1470:SER:OG	2.36	0.43
1:BX:40:LYS:HA	1:BX:40:LYS:HD3	1.90	0.43
1:HX:107:MET:HE2	1:HX:107:MET:HB3	1.91	0.43
1:KX:70:GLU:HB3	1:KX:73:GLU:HG3	2.01	0.43
2:DY:1535:MET:HE2	2:DY:1544:PRO:HD3	2.01	0.43
2:KY:1535:MET:HE2	2:KY:1544:PRO:HD3	2.00	0.43
2:KY:1565:LYS:HE2	2:KY:1565:LYS:HB3	1.86	0.43
2:PY:1487:ASP:OD1	2:PY:1489:THR:OG1	2.34	0.43
1:AX:48:TYR:HD1	1:AX:55:ILE:HD11	1.83	0.42
1:DX:280:LEU:HB3	1:DX:291:PHE:HB2	2.00	0.42
1:GX:60:SER:OG	1:GX:61:LEU:N	2.52	0.42
1:IX:75:ILE:HG23	1:IX:282:VAL:HG23	2.00	0.42
1:KX:75:ILE:HG23	1:KX:282:VAL:HG23	2.00	0.42
1:LX:264:ASP:OD1	1:LX:264:ASP:N	2.37	0.42
1:PX:126:LEU:HD23	1:PX:126:LEU:HA	1.87	0.42
1:PX:127:LYS:HD3	1:PX:127:LYS:HA	1.79	0.42
1:QX:60:SER:OG	1:QX:61:LEU:N	2.52	0.42
2:BY:1470:SER:OG	2:BY:1471:LYS:N	2.52	0.42
2:EY:1514:ARG:O	2:EY:1518:GLU:HG2	2.19	0.42
1:AX:67:ILE:HD11	1:AX:97:ILE:HD13	2.01	0.42
1:AX:107:MET:HE2	1:AX:107:MET:HB3	1.91	0.42
1:BX:35:ASN:O	1:BX:298:LYS:NZ	2.40	0.42
1:BX:67:ILE:O	1:BX:94:HIS:HA	2.19	0.42
1:CX:92:SER:HB3	2:BY:1560:ASN:HA	2.01	0.42
1:DX:40:LYS:HA	1:DX:40:LYS:HD3	1.76	0.42
1:DX:60:SER:OG	1:DX:61:LEU:N	2.52	0.42
1:EX:322:ILE:HD13	1:EX:322:ILE:HA	1.87	0.42
1:HX:67:ILE:HA	1:HX:308:VAL:HG23	2.02	0.42
1:QX:107:MET:O	2:PY:1543:LEU:N	2.49	0.42
2:CY:1470:SER:OG	2:CY:1471:LYS:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IY:1514:ARG:O	2:IY:1518:GLU:HG2	2.19	0.42
1:HX:67:ILE:O	1:HX:94:HIS:HA	2.19	0.42
1:HX:322:ILE:HD13	1:HX:322:ILE:HA	1.89	0.42
1:LX:273:ASP:OD2	1:LX:300:ASN:ND2	2.52	0.42
1:OX:48:TYR:HD1	1:OX:55:ILE:HD11	1.84	0.42
2:LY:1565:LYS:HB3	2:LY:1565:LYS:HE2	1.85	0.42
1:CX:35:ASN:O	1:CX:298:LYS:NZ	2.40	0.42
1:EX:48:TYR:HD1	1:EX:55:ILE:HD11	1.84	0.42
1:EX:60:SER:OG	1:EX:61:LEU:N	2.52	0.42
1:EX:74:THR:OG1	2:DY:1560:ASN:ND2	2.51	0.42
1:GX:75:ILE:HG23	1:GX:282:VAL:HG23	2.01	0.42
1:KX:291:PHE:HZ	1:KX:310:LEU:HD11	1.84	0.42
1:NX:48:TYR:HD1	1:NX:55:ILE:HD11	1.84	0.42
1:OX:127:LYS:HA	1:OX:127:LYS:HD3	1.79	0.42
2:IY:1502:SER:OG	2:IY:1503:ASP:N	2.52	0.42
1:BX:70:GLU:HB3	1:BX:73:GLU:HG3	2.01	0.42
1:BX:107:MET:O	2:AY:1543:LEU:N	2.49	0.42
1:CX:75:ILE:HG23	1:CX:282:VAL:HG23	2.01	0.42
1:EX:322:ILE:HG23	2:FY:1581:ALA:HA	2.00	0.42
1:FX:60:SER:OG	1:FX:61:LEU:N	2.53	0.42
1:FX:126:LEU:HD23	1:FX:126:LEU:HA	1.86	0.42
1:KX:68:GLN:HA	1:KX:94:HIS:HB3	2.01	0.42
1:KX:107:MET:HE2	1:KX:107:MET:HB3	1.87	0.42
1:MX:60:SER:OG	1:MX:61:LEU:N	2.52	0.42
1:MX:318:VAL:O	1:MX:322:ILE:HB	2.20	0.42
1:MX:322:ILE:HG23	2:NY:1581:ALA:HA	2.01	0.42
1:OX:297:GLN:HB2	1:OX:300:ASN:HB2	2.00	0.42
1:QX:126:LEU:HD23	1:QX:126:LEU:HA	1.87	0.42
2:AY:1591:LYS:HB3	2:QY:1578:PRO:HD3	2.01	0.42
2:CY:1495:GLU:OE2	2:CY:1506:ARG:NH2	2.45	0.42
1:FX:272:SER:HB3	2:EY:1531:THR:HB	2.01	0.42
1:GX:322:ILE:HG23	2:HY:1581:ALA:HA	2.02	0.42
1:JX:297:GLN:HB2	1:JX:300:ASN:HB2	2.02	0.42
1:MX:48:TYR:HD1	1:MX:55:ILE:HD11	1.85	0.42
1:PX:272:SER:HB3	2:OY:1531:THR:HB	2.00	0.42
2:BY:1487:ASP:HB2	2:CY:1471:LYS:HD3	2.02	0.42
2:HY:1487:ASP:OD1	2:HY:1489:THR:OG1	2.37	0.42
2:JY:1514:ARG:O	2:JY:1518:GLU:HG2	2.19	0.42
2:MY:1486:ASP:OD1	2:MY:1486:ASP:N	2.39	0.42
1:CX:61:LEU:HD22	1:CX:271:PRO:HG2	2.01	0.42
1:EX:40:LYS:HA	1:EX:40:LYS:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EX:291:PHE:HZ	1:EX:310:LEU:HD11	1.84	0.42
1:GX:70:GLU:OE2	1:GX:71:LYS:N	2.52	0.42
1:NX:90:PRO:HB3	1:NX:95:ILE:HG23	2.02	0.42
2:MY:1486:ASP:OD2	2:NY:1470:SER:OG	2.37	0.42
1:BX:68:GLN:HA	1:BX:94:HIS:HB3	2.02	0.42
1:CX:48:TYR:HD1	1:CX:55:ILE:HD11	1.85	0.42
1:EX:78:ILE:HD12	1:EX:282:VAL:HB	2.01	0.42
1:FX:75:ILE:HG23	1:FX:282:VAL:HG23	2.00	0.42
1:FX:92:SER:HB3	2:EY:1560:ASN:HA	2.01	0.42
1:FX:127:LYS:HA	1:FX:127:LYS:HD3	1.80	0.42
1:IX:60:SER:OG	1:IX:61:LEU:N	2.52	0.42
2:CY:1486:ASP:OD1	2:CY:1486:ASP:N	2.39	0.42
2:MY:1502:SER:OG	2:MY:1503:ASP:N	2.53	0.42
2:QY:1502:SER:OG	2:QY:1503:ASP:N	2.53	0.42
1:AX:68:GLN:HG2	1:AX:309:LYS:HG3	2.02	0.42
1:BX:48:TYR:HD1	1:BX:55:ILE:HD11	1.85	0.42
1:CX:40:LYS:HA	1:CX:40:LYS:HD3	1.94	0.42
1:FX:48:TYR:HD1	1:FX:55:ILE:HD11	1.85	0.42
1:FX:52:GLU:HG2	1:FX:53:LYS:HG2	2.02	0.42
1:OX:268:GLU:OE2	2:NY:1530:LYS:NZ	2.53	0.42
1:OX:273:ASP:OD2	1:OX:300:ASN:ND2	2.52	0.42
1:OX:277:ARG:HD3	1:PX:38:ARG:HD3	2.01	0.42
2:CY:1502:SER:OG	2:CY:1503:ASP:N	2.52	0.42
2:DY:1564:ASP:OD2	2:DY:1564:ASP:N	2.43	0.42
2:KY:1486:ASP:OD2	2:LY:1470:SER:OG	2.37	0.42
1:AX:80:THR:H	1:AX:83:ASN:HD21	1.67	0.42
1:EX:67:ILE:O	1:EX:94:HIS:HA	2.20	0.42
1:HX:60:SER:OG	1:HX:61:LEU:N	2.53	0.42
1:KX:126:LEU:HD23	1:KX:126:LEU:HA	1.87	0.42
1:LX:49:LEU:H	1:LX:49:LEU:HG	1.68	0.42
1:LX:67:ILE:HD12	1:LX:95:ILE:HD12	2.01	0.42
1:MX:107:MET:HE2	1:MX:107:MET:HB3	1.89	0.42
1:QX:65:THR:OG1	1:QX:305:TYR:O	2.27	0.42
2:CY:1565:LYS:HB3	2:CY:1565:LYS:HE2	1.85	0.42
2:GY:1502:SER:OG	2:GY:1503:ASP:N	2.53	0.42
2:HY:1532:PHE:HD2	2:HY:1544:PRO:HG2	1.84	0.42
2:QY:1470:SER:OG	2:QY:1471:LYS:N	2.52	0.42
1:AX:70:GLU:HB3	1:AX:73:GLU:HG3	2.01	0.41
1:CX:273:ASP:OD2	1:CX:300:ASN:ND2	2.52	0.41
1:FX:297:GLN:HB2	1:FX:300:ASN:HB2	2.02	0.41
1:MX:70:GLU:HB3	1:MX:73:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BY:1502:SER:OG	2:BY:1503:ASP:N	2.53	0.41
2:HY:1486:ASP:OD1	2:HY:1486:ASP:N	2.47	0.41
2:HY:1510:LEU:HD23	2:HY:1510:LEU:HA	1.94	0.41
2:KY:1502:SER:OG	2:KY:1503:ASP:N	2.53	0.41
2:NY:1556:ILE:H	2:NY:1556:ILE:HG13	1.67	0.41
1:CX:74:THR:OG1	2:BY:1560:ASN:ND2	2.53	0.41
1:LX:60:SER:OG	1:LX:61:LEU:N	2.53	0.41
1:OX:67:ILE:O	1:OX:94:HIS:HA	2.20	0.41
1:CX:291:PHE:HZ	1:CX:310:LEU:HD11	1.85	0.41
1:DX:75:ILE:HG23	1:DX:282:VAL:HG23	2.01	0.41
1:DX:90:PRO:HB3	1:DX:95:ILE:HG23	2.02	0.41
1:FX:35:ASN:O	1:FX:298:LYS:NZ	2.41	0.41
1:JX:88:ILE:HG22	1:JX:90:PRO:HD3	2.02	0.41
1:NX:68:GLN:HA	1:NX:94:HIS:HB3	2.02	0.41
1:QX:264:ASP:OD1	1:QX:264:ASP:N	2.40	0.41
2:EY:1487:ASP:OD1	2:EY:1489:THR:OG1	2.36	0.41
2:EY:1532:PHE:HD2	2:EY:1544:PRO:HG2	1.85	0.41
2:IY:1601:LYS:HE3	2:IY:1601:LYS:HB3	1.83	0.41
1:DX:65:THR:OG1	1:DX:305:TYR:O	2.32	0.41
1:JX:48:TYR:HD1	1:JX:55:ILE:HD11	1.85	0.41
1:KX:48:TYR:HD1	1:KX:55:ILE:HD11	1.84	0.41
1:KX:77:TYR:HB2	1:KX:283:ARG:NH2	2.35	0.41
1:KX:280:LEU:HB3	1:KX:291:PHE:HB2	2.02	0.41
1:OX:75:ILE:HG23	1:OX:282:VAL:HG23	2.01	0.41
1:OX:79:THR:OG1	1:OX:83:ASN:ND2	2.49	0.41
2:BY:1556:ILE:H	2:BY:1556:ILE:HG13	1.72	0.41
2:FY:1502:SER:OG	2:FY:1503:ASP:N	2.53	0.41
2:MY:1601:LYS:HE2	2:MY:1601:LYS:HB3	1.87	0.41
1:CX:107:MET:HE2	1:CX:107:MET:HB3	1.89	0.41
1:DX:48:TYR:HD1	1:DX:55:ILE:HD11	1.85	0.41
1:FX:273:ASP:OD2	1:FX:300:ASN:ND2	2.52	0.41
2:KY:1564:ASP:OD2	2:KY:1564:ASP:N	2.48	0.41
1:BX:90:PRO:HB3	1:BX:95:ILE:HG23	2.02	0.41
1:DX:299:ASP:OD1	1:DX:299:ASP:N	2.38	0.41
1:FX:291:PHE:HZ	1:FX:310:LEU:HD11	1.85	0.41
1:GX:126:LEU:HD23	1:GX:126:LEU:HA	1.87	0.41
1:IX:291:PHE:HZ	1:IX:310:LEU:HD11	1.86	0.41
1:LX:323:GLU:OE1	2:MY:1584:TYR:OH	2.33	0.41
1:QX:80:THR:H	1:QX:83:ASN:ND2	2.18	0.41
2:CY:1510:LEU:HD23	2:CY:1510:LEU:HA	1.95	0.41
2:HY:1502:SER:OG	2:HY:1503:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BX:107:MET:HE2	1:BX:107:MET:HB3	1.90	0.41
1:JX:288:LEU:HD21	1:KX:66:VAL:HG21	2.03	0.41
1:KX:35:ASN:O	1:KX:298:LYS:NZ	2.42	0.41
1:NX:49:LEU:H	1:NX:49:LEU:HG	1.74	0.41
1:OX:60:SER:OG	1:OX:61:LEU:N	2.52	0.41
1:QX:315:ARG:O	1:QX:319:SER:OG	2.35	0.41
2:HY:1565:LYS:HE2	2:HY:1565:LYS:HB3	1.92	0.41
2:IY:1482:LEU:HD23	2:IY:1482:LEU:HA	1.94	0.41
1:DX:61:LEU:HD22	1:DX:271:PRO:HG2	2.02	0.41
1:KX:60:SER:OG	1:KX:61:LEU:N	2.53	0.41
1:LX:75:ILE:HG23	1:LX:282:VAL:HG23	2.02	0.41
1:MX:291:PHE:HZ	1:MX:310:LEU:HD11	1.86	0.41
2:CY:1535:MET:HE2	2:CY:1544:PRO:HD3	2.03	0.41
2:IY:1532:PHE:HD2	2:IY:1544:PRO:HG2	1.85	0.41
2:KY:1578:PRO:HD3	2:LY:1591:LYS:HB3	2.03	0.41
1:AX:75:ILE:HG23	1:AX:282:VAL:HG23	2.02	0.41
1:BX:65:THR:OG1	1:BX:305:TYR:O	2.28	0.41
1:CX:299:ASP:OD1	1:CX:299:ASP:N	2.39	0.41
1:EX:52:GLU:HG2	1:EX:53:LYS:HG2	2.03	0.41
1:GX:48:TYR:HD1	1:GX:55:ILE:HD11	1.85	0.41
1:PX:297:GLN:HB2	1:PX:300:ASN:HB2	2.02	0.41
2:AY:1535:MET:HE2	2:AY:1544:PRO:HD3	2.02	0.41
2:CY:1601:LYS:HE3	2:CY:1601:LYS:HB3	1.94	0.41
2:GY:1565:LYS:HE2	2:GY:1565:LYS:HB3	1.87	0.41
2:MY:1487:ASP:OD1	2:MY:1489:THR:OG1	2.35	0.41
2:NY:1565:LYS:HB3	2:NY:1565:LYS:HE2	1.89	0.41
2:OY:1502:SER:OG	2:OY:1503:ASP:N	2.54	0.41
2:OY:1543:LEU:HD23	2:OY:1543:LEU:HA	1.95	0.41
1:DX:88:ILE:HG22	1:DX:90:PRO:HD3	2.02	0.40
1:GX:78:ILE:HG21	1:GX:90:PRO:HG3	2.03	0.40
2:BY:1601:LYS:HE2	2:BY:1601:LYS:HB3	1.88	0.40
2:CY:1487:ASP:OD1	2:CY:1489:THR:OG1	2.36	0.40
2:CY:1593:LYS:HD3	2:DY:1603:LEU:HD23	2.03	0.40
2:JY:1486:ASP:OD2	2:KY:1470:SER:OG	2.37	0.40
2:JY:1601:LYS:HE2	2:JY:1601:LYS:HB3	1.89	0.40
2:KY:1514:ARG:O	2:KY:1518:GLU:HG2	2.20	0.40
1:BX:52:GLU:HG2	1:BX:53:LYS:HG2	2.03	0.40
1:CX:78:ILE:HG12	2:BY:1556:ILE:HD12	2.03	0.40
1:JX:49:LEU:H	1:JX:49:LEU:HG	1.68	0.40
1:KX:68:GLN:HG2	1:KX:309:LYS:HG3	2.02	0.40
1:MX:273:ASP:OD2	1:MX:300:ASN:ND2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NX:108:PHE:O	2:NY:1529:ARG:NH1	2.47	0.40
1:OX:54:PRO:HB2	1:OX:292:ILE:HG12	2.03	0.40
1:PX:65:THR:OG1	1:PX:305:TYR:O	2.27	0.40
1:PX:107:MET:O	2:OY:1543:LEU:N	2.49	0.40
2:DY:1532:PHE:HD2	2:DY:1544:PRO:HG2	1.86	0.40
2:LY:1487:ASP:OD1	2:LY:1489:THR:OG1	2.39	0.40
2:OY:1482:LEU:HD23	2:OY:1482:LEU:HA	1.97	0.40
1:DX:52:GLU:HG2	1:DX:53:LYS:HG2	2.04	0.40
1:HX:48:TYR:HD1	1:HX:55:ILE:HD11	1.86	0.40
1:MX:75:ILE:HG23	1:MX:282:VAL:HG23	2.03	0.40
2:BY:1495:GLU:OE1	2:BY:1506:ARG:NH2	2.53	0.40
2:DY:1565:LYS:HE2	2:DY:1565:LYS:HB3	1.85	0.40
2:GY:1535:MET:HE2	2:GY:1544:PRO:HD3	2.03	0.40
2:KY:1556:ILE:H	2:KY:1556:ILE:HG13	1.69	0.40
1:AX:52:GLU:HG2	1:AX:53:LYS:HG2	2.04	0.40
1:DX:126:LEU:HA	1:DX:126:LEU:HD23	1.87	0.40
1:GX:43:ASN:OD1	1:GX:43:ASN:N	2.54	0.40
1:JX:60:SER:OG	1:JX:61:LEU:N	2.53	0.40
1:PX:90:PRO:HB3	1:PX:95:ILE:HG23	2.03	0.40
1:PX:280:LEU:HB3	1:PX:291:PHE:HB2	2.03	0.40
2:GY:1486:ASP:OD2	2:GY:1486:ASP:N	2.47	0.40
2:MY:1556:ILE:H	2:MY:1556:ILE:HG13	1.74	0.40
2:NY:1532:PHE:HD2	2:NY:1544:PRO:HG2	1.86	0.40
2:PY:1532:PHE:HD2	2:PY:1544:PRO:HG2	1.85	0.40
1:CX:52:GLU:HG2	1:CX:53:LYS:HG2	2.04	0.40
1:EX:107:MET:HE2	1:EX:107:MET:HB3	1.88	0.40
1:FX:322:ILE:HD13	1:FX:322:ILE:HA	1.86	0.40
1:HX:49:LEU:H	1:HX:49:LEU:HG	1.66	0.40
1:MX:40:LYS:HA	1:MX:40:LYS:HD3	1.89	0.40
1:QX:54:PRO:HB2	1:QX:292:ILE:HG12	2.03	0.40
1:QX:299:ASP:N	1:QX:299:ASP:OD1	2.38	0.40
2:BY:1532:PHE:HD2	2:BY:1544:PRO:HG2	1.87	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	AX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	BX	160/521 (31%)	156 (98%)	4 (2%)	0	100	100
1	CX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	DX	160/521 (31%)	155 (97%)	5 (3%)	0	100	100
1	EX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	FX	160/521 (31%)	153 (96%)	7 (4%)	0	100	100
1	GX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	HX	160/521 (31%)	155 (97%)	5 (3%)	0	100	100
1	IX	160/521 (31%)	153 (96%)	7 (4%)	0	100	100
1	JX	160/521 (31%)	155 (97%)	5 (3%)	0	100	100
1	KX	160/521 (31%)	155 (97%)	5 (3%)	0	100	100
1	LX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	MX	160/521 (31%)	155 (97%)	5 (3%)	0	100	100
1	NX	160/521 (31%)	155 (97%)	5 (3%)	0	100	100
1	OX	160/521 (31%)	153 (96%)	7 (4%)	0	100	100
1	PX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	QX	160/521 (31%)	153 (96%)	7 (4%)	0	100	100
2	AY	133/1927 (7%)	127 (96%)	6 (4%)	0	100	100
2	BY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	CY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	DY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	EY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	FY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	GY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	HY	133/1927 (7%)	127 (96%)	6 (4%)	0	100	100
2	IY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	JY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	KY	133/1927 (7%)	129 (97%)	4 (3%)	0	100	100
2	LY	133/1927 (7%)	129 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	MY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	NY	133/1927 (7%)	129 (97%)	4 (3%)	0	100	100
2	OY	133/1927 (7%)	129 (97%)	4 (3%)	0	100	100
2	PY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	QY	133/1927 (7%)	129 (97%)	4 (3%)	0	100	100
All	All	4981/41616 (12%)	4801 (96%)	180 (4%)	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	AX	152/469 (32%)	135 (89%)	17 (11%)	6	24
1	BX	152/469 (32%)	139 (91%)	13 (9%)	10	36
1	CX	152/469 (32%)	137 (90%)	15 (10%)	7	30
1	DX	152/469 (32%)	137 (90%)	15 (10%)	7	30
1	EX	152/469 (32%)	137 (90%)	15 (10%)	7	30
1	FX	152/469 (32%)	134 (88%)	18 (12%)	5	22
1	GX	152/469 (32%)	134 (88%)	18 (12%)	5	22
1	HX	152/469 (32%)	132 (87%)	20 (13%)	4	18
1	IX	152/469 (32%)	137 (90%)	15 (10%)	7	30
1	JX	152/469 (32%)	138 (91%)	14 (9%)	8	33
1	KX	152/469 (32%)	136 (90%)	16 (10%)	6	27
1	LX	152/469 (32%)	134 (88%)	18 (12%)	5	22
1	MX	152/469 (32%)	139 (91%)	13 (9%)	10	36
1	NX	152/469 (32%)	137 (90%)	15 (10%)	7	30
1	OX	152/469 (32%)	133 (88%)	19 (12%)	4	20
1	PX	152/469 (32%)	135 (89%)	17 (11%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	QX	152/469 (32%)	137 (90%)	15 (10%)	7	30
2	AY	115/1724 (7%)	106 (92%)	9 (8%)	11	39
2	BY	115/1724 (7%)	100 (87%)	15 (13%)	4	19
2	CY	115/1724 (7%)	105 (91%)	10 (9%)	9	35
2	DY	115/1724 (7%)	104 (90%)	11 (10%)	8	31
2	EY	115/1724 (7%)	105 (91%)	10 (9%)	9	35
2	FY	115/1724 (7%)	101 (88%)	14 (12%)	5	21
2	GY	115/1724 (7%)	100 (87%)	15 (13%)	4	19
2	HY	115/1724 (7%)	101 (88%)	14 (12%)	5	21
2	IY	115/1724 (7%)	106 (92%)	9 (8%)	11	39
2	JY	115/1724 (7%)	104 (90%)	11 (10%)	8	31
2	KY	115/1724 (7%)	102 (89%)	13 (11%)	5	24
2	LY	115/1724 (7%)	105 (91%)	10 (9%)	9	35
2	MY	115/1724 (7%)	104 (90%)	11 (10%)	8	31
2	NY	115/1724 (7%)	106 (92%)	9 (8%)	11	39
2	OY	115/1724 (7%)	103 (90%)	12 (10%)	7	28
2	PY	115/1724 (7%)	105 (91%)	10 (9%)	9	35
2	QY	115/1724 (7%)	103 (90%)	12 (10%)	7	28
All	All	4539/37281 (12%)	4071 (90%)	468 (10%)	9	28

All (468) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AX	39	VAL
1	AX	42	VAL
1	AX	43	ASN
1	AX	49	LEU
1	AX	56	THR
1	AX	78	ILE
1	AX	83	ASN
1	AX	87	SER
1	AX	91	ASN
1	AX	93	ASN
1	AX	113	VAL
1	AX	264	ASP
1	AX	282	VAL

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Mol	Chain	Res	Type
1	AX	308	VAL
1	AX	320	SER
1	AX	322	ILE
1	AX	324	GLU
1	BX	39	VAL
1	BX	40	LYS
1	BX	42	VAL
1	BX	43	ASN
1	BX	49	LEU
1	BX	91	ASN
1	BX	93	ASN
1	BX	113	VAL
1	BX	130	LYS
1	BX	266	SER
1	BX	270	SER
1	BX	282	VAL
1	BX	308	VAL
1	CX	39	VAL
1	CX	42	VAL
1	CX	43	ASN
1	CX	49	LEU
1	CX	56	THR
1	CX	62	ASP
1	CX	69	LEU
1	CX	78	ILE
1	CX	83	ASN
1	CX	91	ASN
1	CX	93	ASN
1	CX	113	VAL
1	CX	270	SER
1	CX	282	VAL
1	CX	320	SER
1	DX	39	VAL
1	DX	42	VAL
1	DX	43	ASN
1	DX	49	LEU
1	DX	83	ASN
1	DX	87	SER
1	DX	91	ASN
1	DX	93	ASN
1	DX	113	VAL
1	DX	130	LYS

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Mol	Chain	Res	Type
1	DX	270	SER
1	DX	282	VAL
1	DX	319	SER
1	DX	320	SER
1	DX	322	ILE
1	EX	39	VAL
1	EX	40	LYS
1	EX	42	VAL
1	EX	49	LEU
1	EX	56	THR
1	EX	62	ASP
1	EX	87	SER
1	EX	91	ASN
1	EX	93	ASN
1	EX	113	VAL
1	EX	264	ASP
1	EX	282	VAL
1	EX	319	SER
1	EX	320	SER
1	EX	322	ILE
1	FX	39	VAL
1	FX	42	VAL
1	FX	43	ASN
1	FX	49	LEU
1	FX	56	THR
1	FX	62	ASP
1	FX	78	ILE
1	FX	83	ASN
1	FX	87	SER
1	FX	89	VAL
1	FX	91	ASN
1	FX	93	ASN
1	FX	113	VAL
1	FX	274	SER
1	FX	281	VAL
1	FX	282	VAL
1	FX	320	SER
1	FX	322	ILE
1	GX	39	VAL
1	GX	42	VAL
1	GX	43	ASN
1	GX	49	LEU

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Mol	Chain	Res	Type
1	GX	56	THR
1	GX	64	VAL
1	GX	70	GLU
1	GX	91	ASN
1	GX	93	ASN
1	GX	113	VAL
1	GX	130	LYS
1	GX	266	SER
1	GX	270	SER
1	GX	282	VAL
1	GX	308	VAL
1	GX	319	SER
1	GX	320	SER
1	GX	322	ILE
1	HX	39	VAL
1	HX	40	LYS
1	HX	41	VAL
1	HX	42	VAL
1	HX	43	ASN
1	HX	49	LEU
1	HX	56	THR
1	HX	83	ASN
1	HX	89	VAL
1	HX	91	ASN
1	HX	93	ASN
1	HX	113	VAL
1	HX	130	LYS
1	HX	270	SER
1	HX	274	SER
1	HX	282	VAL
1	HX	319	SER
1	HX	320	SER
1	HX	321	VAL
1	HX	322	ILE
1	IX	39	VAL
1	IX	42	VAL
1	IX	43	ASN
1	IX	49	LEU
1	IX	56	THR
1	IX	83	ASN
1	IX	87	SER
1	IX	91	ASN

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Mol	Chain	Res	Type
1	IX	93	ASN
1	IX	113	VAL
1	IX	282	VAL
1	IX	303	SER
1	IX	319	SER
1	IX	320	SER
1	IX	322	ILE
1	JX	39	VAL
1	JX	42	VAL
1	JX	43	ASN
1	JX	49	LEU
1	JX	78	ILE
1	JX	83	ASN
1	JX	87	SER
1	JX	91	ASN
1	JX	93	ASN
1	JX	113	VAL
1	JX	282	VAL
1	JX	319	SER
1	JX	320	SER
1	JX	322	ILE
1	KX	39	VAL
1	KX	42	VAL
1	KX	43	ASN
1	KX	49	LEU
1	KX	56	THR
1	KX	62	ASP
1	KX	66	VAL
1	KX	91	ASN
1	KX	93	ASN
1	KX	113	VAL
1	KX	268	GLU
1	KX	270	SER
1	KX	272	SER
1	KX	274	SER
1	KX	282	VAL
1	KX	322	ILE
1	LX	39	VAL
1	LX	42	VAL
1	LX	43	ASN
1	LX	49	LEU
1	LX	56	THR

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Mol	Chain	Res	Type
1	LX	62	ASP
1	LX	66	VAL
1	LX	87	SER
1	LX	89	VAL
1	LX	91	ASN
1	LX	93	ASN
1	LX	113	VAL
1	LX	270	SER
1	LX	274	SER
1	LX	282	VAL
1	LX	308	VAL
1	LX	319	SER
1	LX	320	SER
1	MX	39	VAL
1	MX	42	VAL
1	MX	43	ASN
1	MX	49	LEU
1	MX	56	THR
1	MX	83	ASN
1	MX	87	SER
1	MX	91	ASN
1	MX	93	ASN
1	MX	113	VAL
1	MX	282	VAL
1	MX	320	SER
1	MX	322	ILE
1	NX	39	VAL
1	NX	42	VAL
1	NX	49	LEU
1	NX	56	THR
1	NX	62	ASP
1	NX	83	ASN
1	NX	91	ASN
1	NX	93	ASN
1	NX	113	VAL
1	NX	130	LYS
1	NX	282	VAL
1	NX	303	SER
1	NX	308	VAL
1	NX	319	SER
1	NX	320	SER
1	OX	39	VAL

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Mol	Chain	Res	Type
1	OX	42	VAL
1	OX	43	ASN
1	OX	49	LEU
1	OX	56	THR
1	OX	62	ASP
1	OX	83	ASN
1	OX	87	SER
1	OX	89	VAL
1	OX	91	ASN
1	OX	93	ASN
1	OX	113	VAL
1	OX	130	LYS
1	OX	281	VAL
1	OX	282	VAL
1	OX	308	VAL
1	OX	319	SER
1	OX	320	SER
1	OX	322	ILE
1	PX	39	VAL
1	PX	42	VAL
1	PX	43	ASN
1	PX	49	LEU
1	PX	62	ASP
1	PX	78	ILE
1	PX	87	SER
1	PX	91	ASN
1	PX	93	ASN
1	PX	113	VAL
1	PX	266	SER
1	PX	270	SER
1	PX	274	SER
1	PX	282	VAL
1	PX	319	SER
1	PX	320	SER
1	PX	322	ILE
1	QX	39	VAL
1	QX	40	LYS
1	QX	42	VAL
1	QX	43	ASN
1	QX	49	LEU
1	QX	56	THR
1	QX	87	SER

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Mol	Chain	Res	Type
1	QX	89	VAL
1	QX	91	ASN
1	QX	93	ASN
1	QX	113	VAL
1	QX	282	VAL
1	QX	319	SER
1	QX	320	SER
1	QX	322	ILE
2	AY	1470	SER
2	AY	1497	CYS
2	AY	1504	SER
2	AY	1520	ASP
2	AY	1521	LEU
2	AY	1526	LEU
2	AY	1561	VAL
2	AY	1562	ASP
2	AY	1585	GLU
2	BY	1475	LEU
2	BY	1479	SER
2	BY	1497	CYS
2	BY	1503	ASP
2	BY	1518	GLU
2	BY	1520	ASP
2	BY	1521	LEU
2	BY	1524	SER
2	BY	1526	LEU
2	BY	1553	ILE
2	BY	1555	THR
2	BY	1561	VAL
2	BY	1562	ASP
2	BY	1601	LYS
2	BY	1603	LEU
2	CY	1497	CYS
2	CY	1502	SER
2	CY	1518	GLU
2	CY	1520	ASP
2	CY	1521	LEU
2	CY	1526	LEU
2	CY	1555	THR
2	CY	1559	THR
2	CY	1561	VAL
2	CY	1562	ASP

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Mol	Chain	Res	Type
2	DY	1497	CYS
2	DY	1502	SER
2	DY	1503	ASP
2	DY	1517	ASP
2	DY	1520	ASP
2	DY	1521	LEU
2	DY	1526	LEU
2	DY	1555	THR
2	DY	1562	ASP
2	DY	1585	GLU
2	DY	1601	LYS
2	EY	1475	LEU
2	EY	1479	SER
2	EY	1497	CYS
2	EY	1520	ASP
2	EY	1521	LEU
2	EY	1526	LEU
2	EY	1528	ASN
2	EY	1562	ASP
2	EY	1585	GLU
2	EY	1601	LYS
2	FY	1469	LEU
2	FY	1479	SER
2	FY	1497	CYS
2	FY	1517	ASP
2	FY	1518	GLU
2	FY	1520	ASP
2	FY	1521	LEU
2	FY	1524	SER
2	FY	1526	LEU
2	FY	1561	VAL
2	FY	1562	ASP
2	FY	1585	GLU
2	FY	1601	LYS
2	FY	1603	LEU
2	GY	1475	LEU
2	GY	1479	SER
2	GY	1497	CYS
2	GY	1502	SER
2	GY	1518	GLU
2	GY	1520	ASP
2	GY	1521	LEU

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Mol	Chain	Res	Type
2	GY	1524	SER
2	GY	1526	LEU
2	GY	1553	ILE
2	GY	1555	THR
2	GY	1561	VAL
2	GY	1562	ASP
2	GY	1585	GLU
2	GY	1601	LYS
2	HY	1475	LEU
2	HY	1497	CYS
2	HY	1504	SER
2	HY	1518	GLU
2	HY	1520	ASP
2	HY	1521	LEU
2	HY	1524	SER
2	HY	1526	LEU
2	HY	1553	ILE
2	HY	1561	VAL
2	HY	1562	ASP
2	HY	1585	GLU
2	HY	1601	LYS
2	HY	1603	LEU
2	IY	1475	LEU
2	IY	1479	SER
2	IY	1497	CYS
2	IY	1520	ASP
2	IY	1521	LEU
2	IY	1555	THR
2	IY	1561	VAL
2	IY	1562	ASP
2	IY	1603	LEU
2	JY	1469	LEU
2	JY	1479	SER
2	JY	1497	CYS
2	JY	1504	SER
2	JY	1520	ASP
2	JY	1521	LEU
2	JY	1526	LEU
2	JY	1561	VAL
2	JY	1562	ASP
2	JY	1601	LYS
2	JY	1603	LEU

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Mol	Chain	Res	Type
2	KY	1469	LEU
2	KY	1475	LEU
2	KY	1479	SER
2	KY	1497	CYS
2	KY	1504	SER
2	KY	1520	ASP
2	KY	1521	LEU
2	KY	1526	LEU
2	KY	1553	ILE
2	KY	1561	VAL
2	KY	1562	ASP
2	KY	1583	GLN
2	KY	1601	LYS
2	LY	1479	SER
2	LY	1497	CYS
2	LY	1502	SER
2	LY	1513	LYS
2	LY	1520	ASP
2	LY	1521	LEU
2	LY	1526	LEU
2	LY	1559	THR
2	LY	1561	VAL
2	LY	1562	ASP
2	MY	1497	CYS
2	MY	1518	GLU
2	MY	1520	ASP
2	MY	1521	LEU
2	MY	1526	LEU
2	MY	1553	ILE
2	MY	1555	THR
2	MY	1561	VAL
2	MY	1562	ASP
2	MY	1585	GLU
2	MY	1601	LYS
2	NY	1479	SER
2	NY	1497	CYS
2	NY	1518	GLU
2	NY	1520	ASP
2	NY	1526	LEU
2	NY	1561	VAL
2	NY	1562	ASP
2	NY	1583	GLN

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Mol	Chain	Res	Type
2	NY	1585	GLU
2	OY	1470	SER
2	OY	1475	LEU
2	OY	1497	CYS
2	OY	1503	ASP
2	OY	1520	ASP
2	OY	1521	LEU
2	OY	1524	SER
2	OY	1555	THR
2	OY	1562	ASP
2	OY	1576	ILE
2	OY	1583	GLN
2	OY	1603	LEU
2	PY	1470	SER
2	PY	1497	CYS
2	PY	1502	SER
2	PY	1520	ASP
2	PY	1526	LEU
2	PY	1553	ILE
2	PY	1561	VAL
2	PY	1562	ASP
2	PY	1585	GLU
2	PY	1601	LYS
2	QY	1479	SER
2	QY	1497	CYS
2	QY	1502	SER
2	QY	1503	ASP
2	QY	1518	GLU
2	QY	1520	ASP
2	QY	1521	LEU
2	QY	1524	SER
2	QY	1526	LEU
2	QY	1555	THR
2	QY	1561	VAL
2	QY	1562	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	AX	265	ASN
1	BX	83	ASN
1	BX	265	ASN

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Mol	Chain	Res	Type
1	CX	83	ASN
1	CX	91	ASN
1	CX	265	ASN
1	DX	265	ASN
1	EX	63	ASN
1	EX	83	ASN
1	EX	265	ASN
1	FX	83	ASN
1	FX	265	ASN
1	GX	265	ASN
1	HX	63	ASN
1	HX	83	ASN
1	HX	265	ASN
1	IX	265	ASN
1	JX	83	ASN
1	KX	83	ASN
1	KX	265	ASN
1	LX	83	ASN
1	MX	83	ASN
1	MX	265	ASN
1	NX	83	ASN
1	OX	265	ASN
1	PX	83	ASN
1	PX	265	ASN
1	QX	83	ASN
1	QX	265	ASN
2	AY	1476	HIS
2	AY	1549	ASN
2	BY	1476	HIS
2	BY	1549	ASN
2	BY	1570	ASN
2	CY	1476	HIS
2	CY	1549	ASN
2	CY	1570	ASN
2	CY	1583	GLN
2	DY	1476	HIS
2	DY	1477	GLN
2	DY	1528	ASN
2	DY	1570	ASN
2	EY	1476	HIS
2	EY	1477	GLN
2	EY	1549	ASN

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Mol	Chain	Res	Type
2	EY	1583	GLN
2	FY	1476	HIS
2	FY	1528	ASN
2	FY	1549	ASN
2	GY	1476	HIS
2	GY	1570	ASN
2	HY	1476	HIS
2	HY	1549	ASN
2	HY	1570	ASN
2	HY	1583	GLN
2	HY	1594	ASN
2	IY	1476	HIS
2	IY	1549	ASN
2	JY	1476	HIS
2	JY	1570	ASN
2	KY	1476	HIS
2	KY	1583	GLN
2	KY	1594	ASN
2	LY	1476	HIS
2	LY	1549	ASN
2	LY	1570	ASN
2	MY	1476	HIS
2	MY	1491	GLN
2	MY	1570	ASN
2	NY	1476	HIS
2	NY	1570	ASN
2	NY	1583	GLN
2	OY	1476	HIS
2	OY	1549	ASN
2	OY	1570	ASN
2	OY	1583	GLN
2	OY	1594	ASN
2	PY	1476	HIS
2	PY	1570	ASN
2	QY	1476	HIS
2	QY	1570	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.

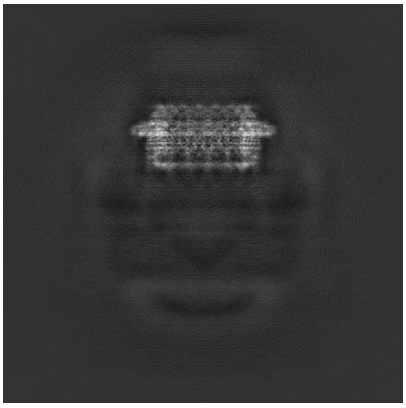
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22077. These allow visual inspection of the internal detail of the map and identification of artifacts.

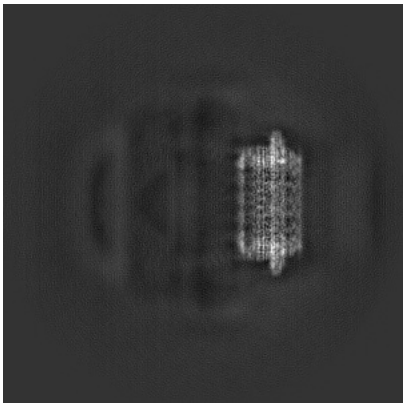
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

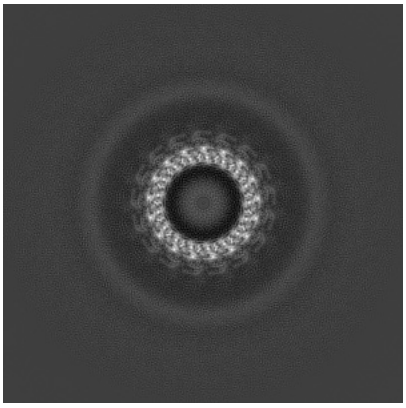
6.1.1 Primary map



X



Y

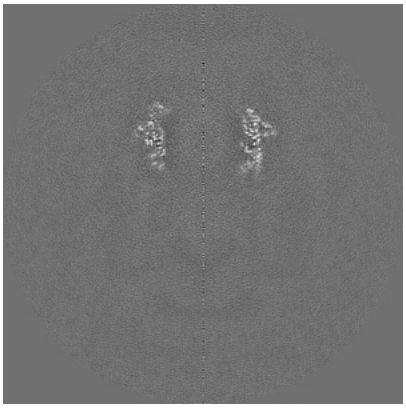


Z

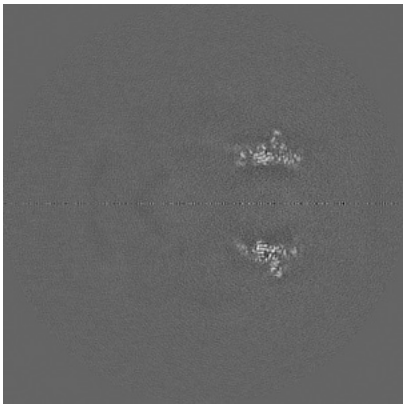
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

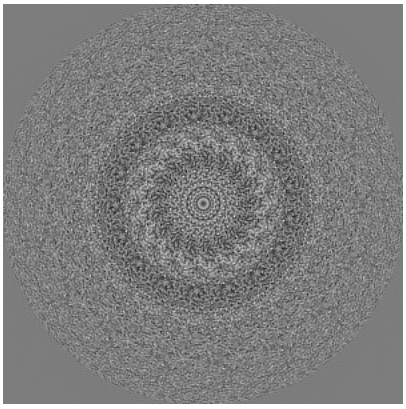
6.2.1 Primary map



X Index: 255



Y Index: 255



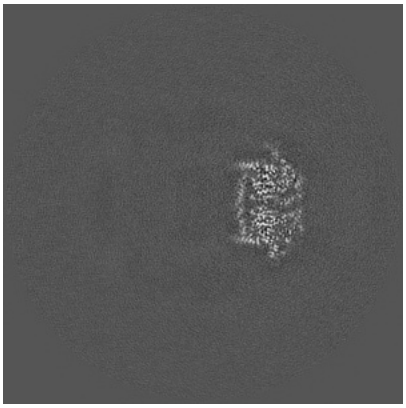
Z Index: 255

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

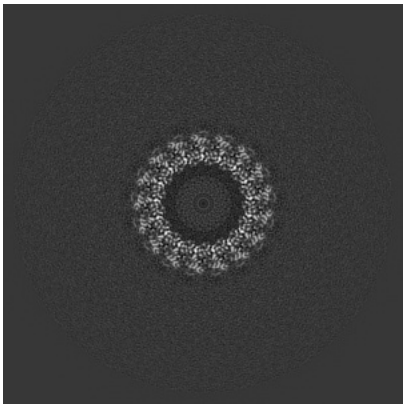
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 309



Y Index: 307

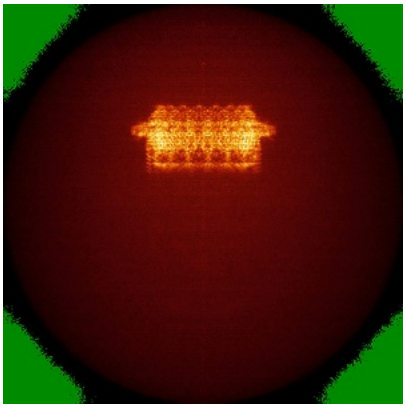


Z Index: 342

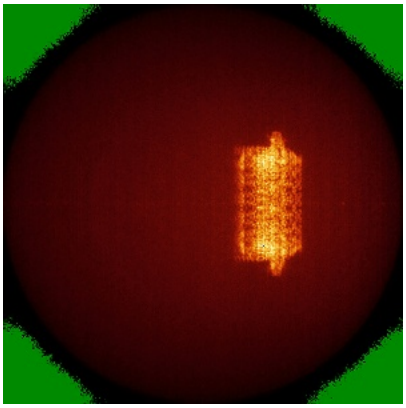
The images above show the largest variance slices of the map in three orthogonal directions.

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

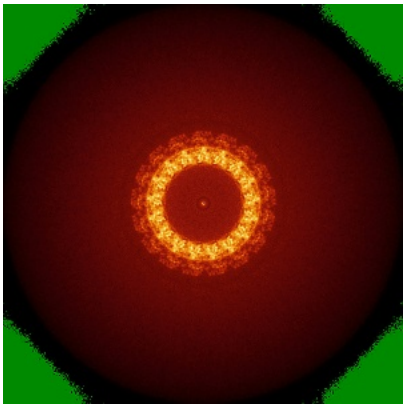
6.4.1 Primary map



X



Y

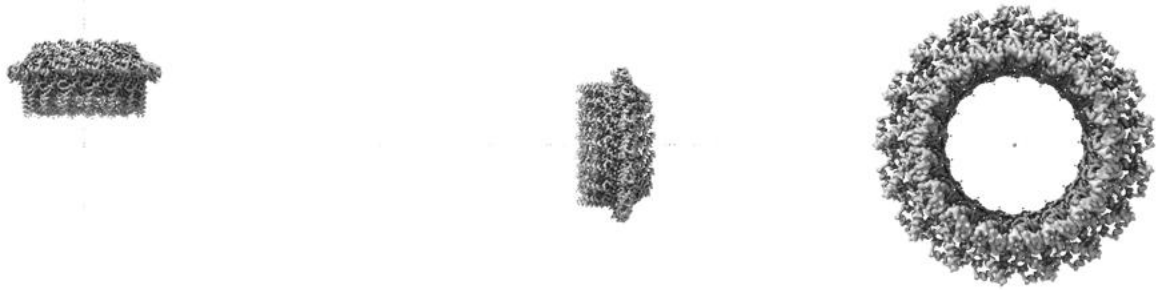


Z

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 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

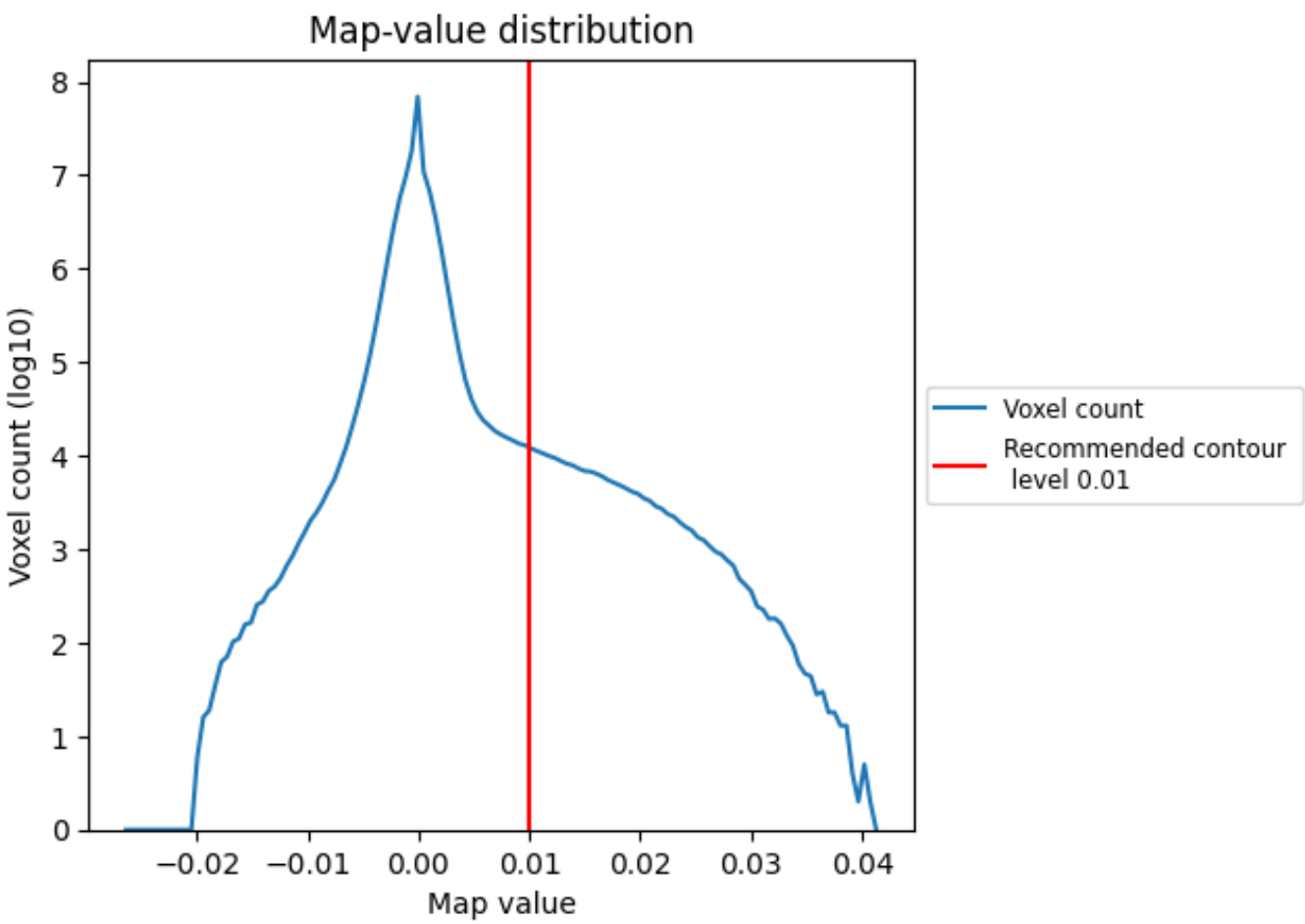
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

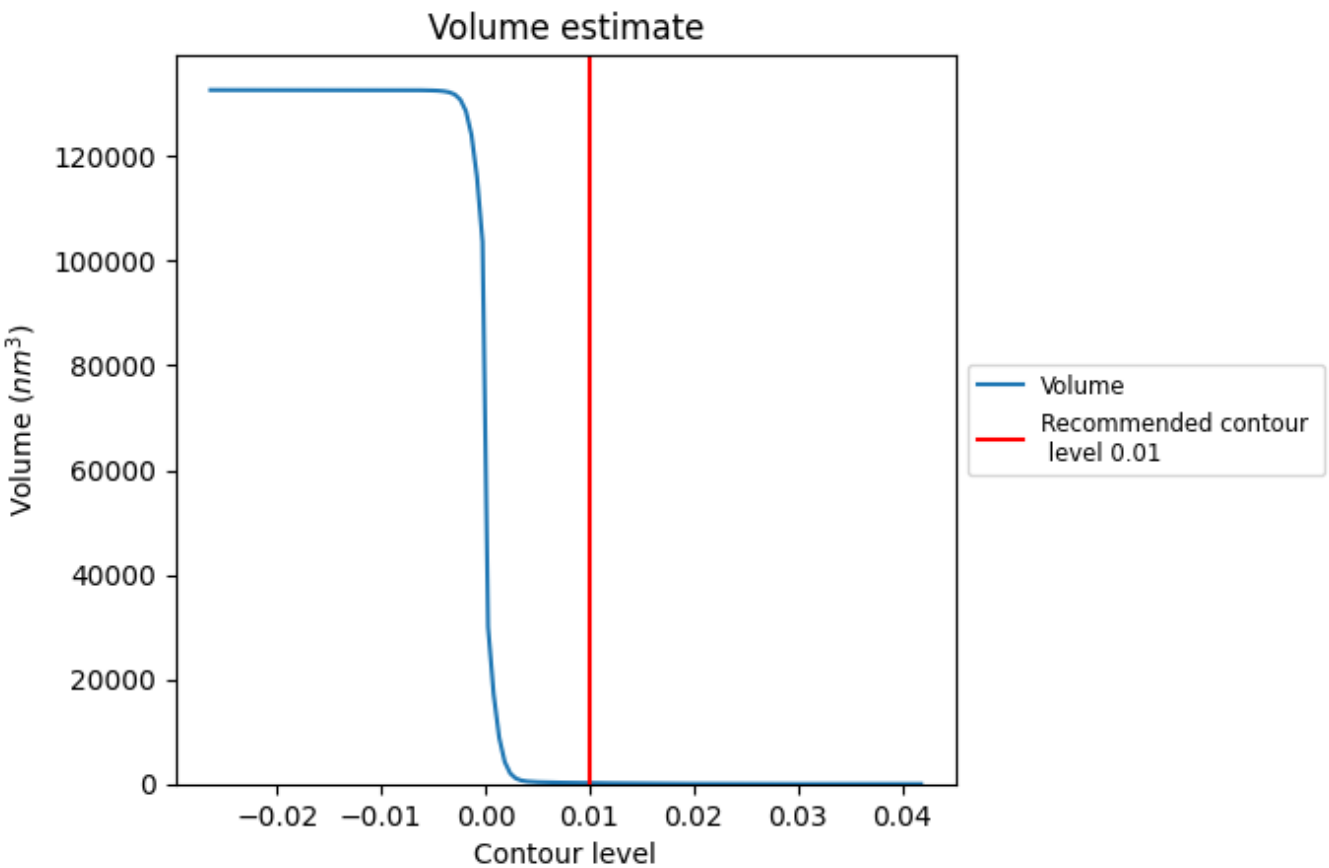
This section contains the results of statistical analysis of the map.

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.

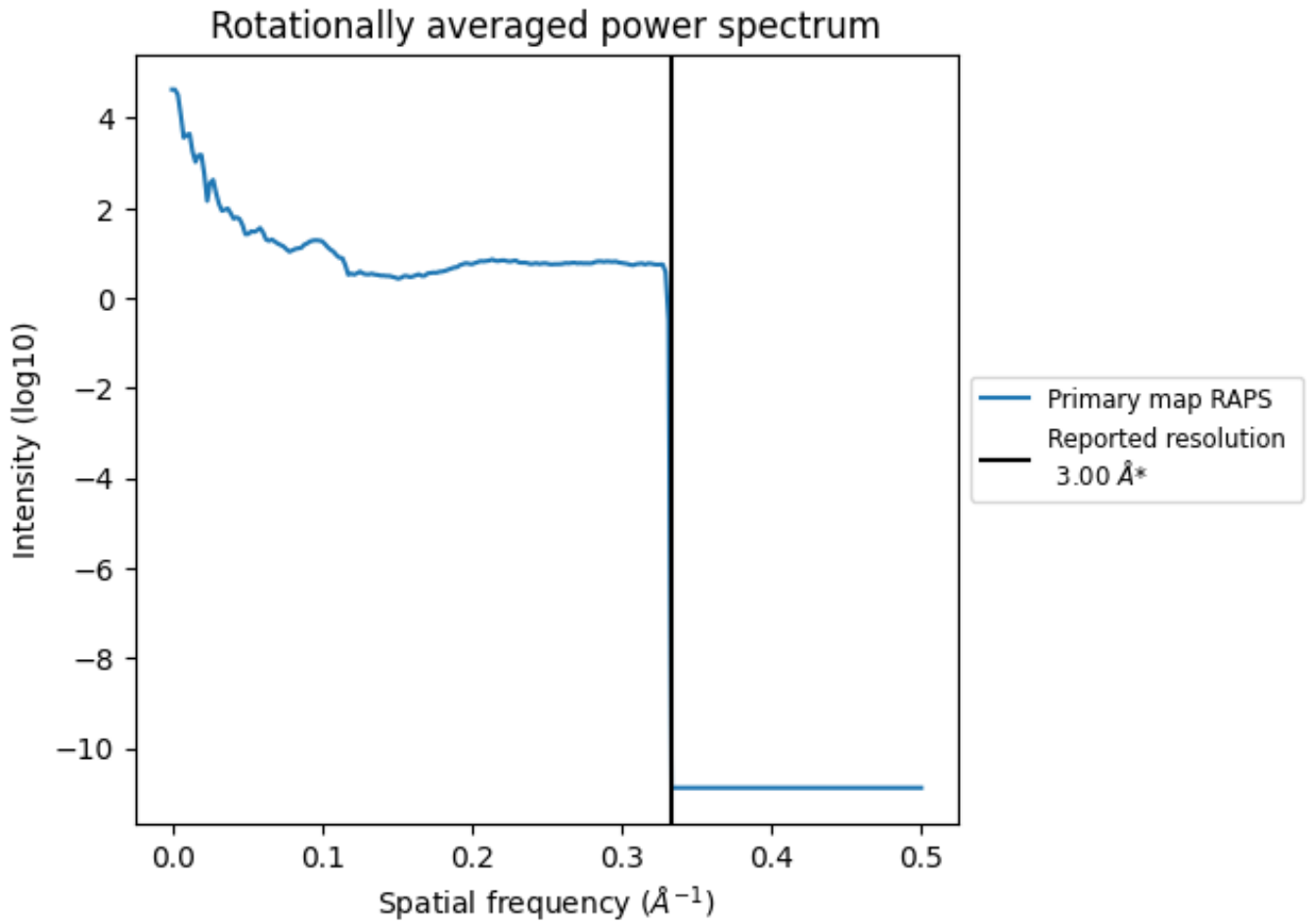
7.2 Volume estimate (i)



The volume at the recommended contour level is 175 nm^3; this corresponds to an approximate mass of 158 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)

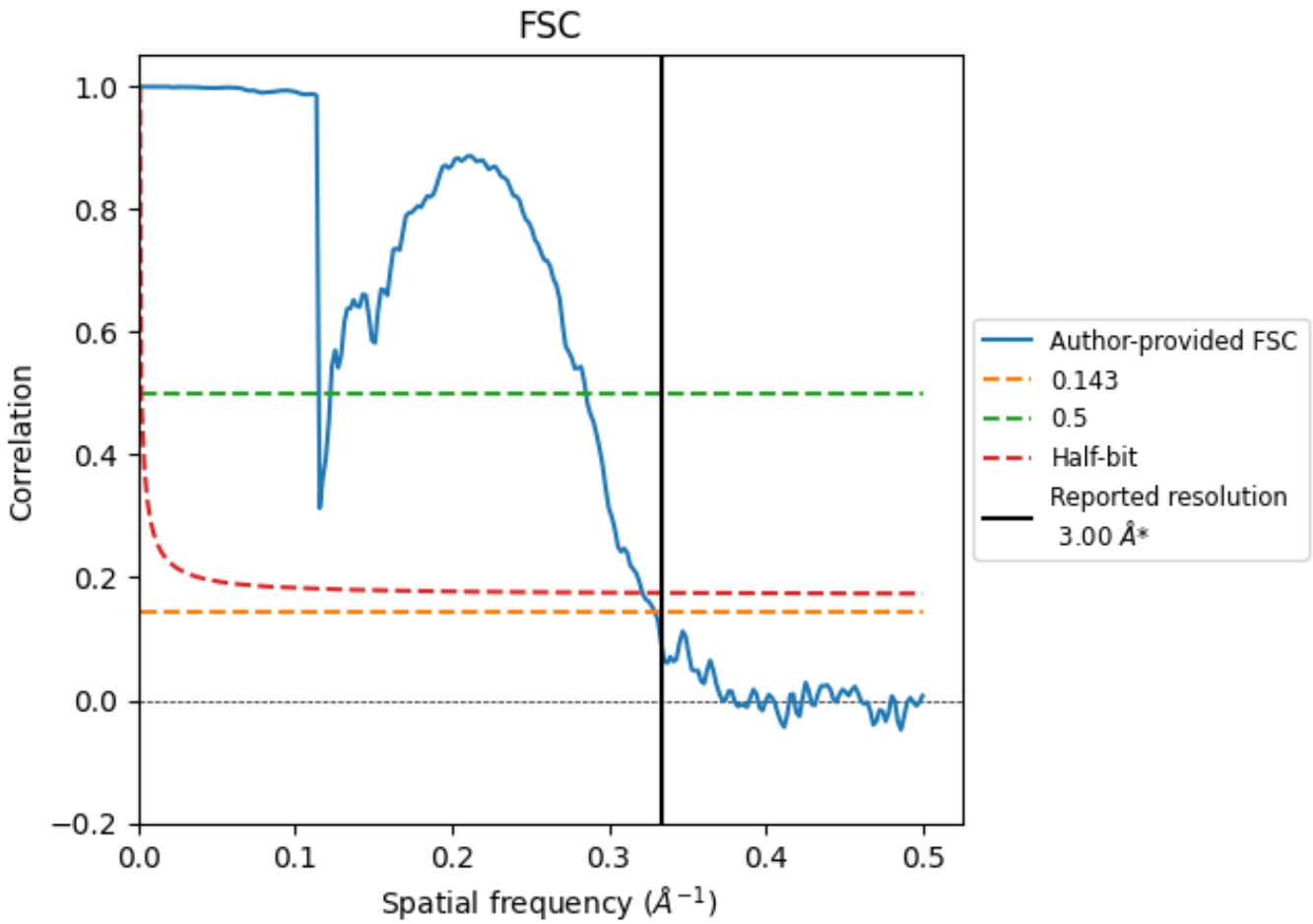


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.03	8.69	3.11
Unmasked-calculated*	-	-	-

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

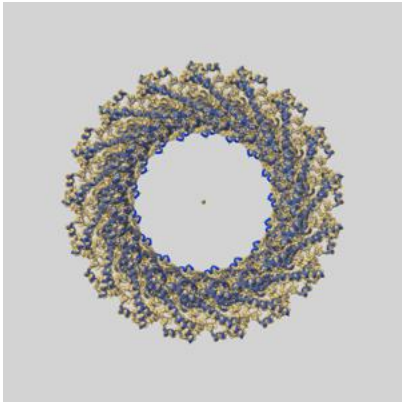
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22077 and PDB model 6X6L. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay (i)

X

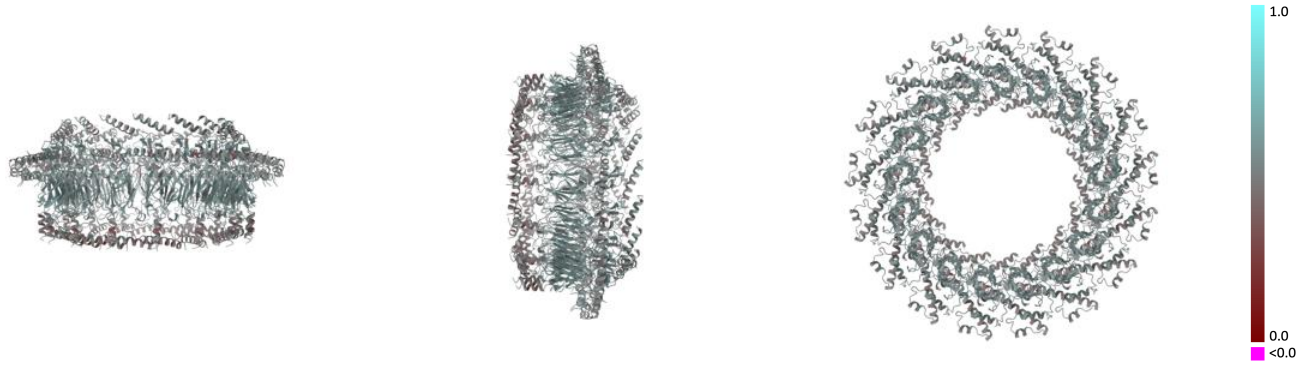
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

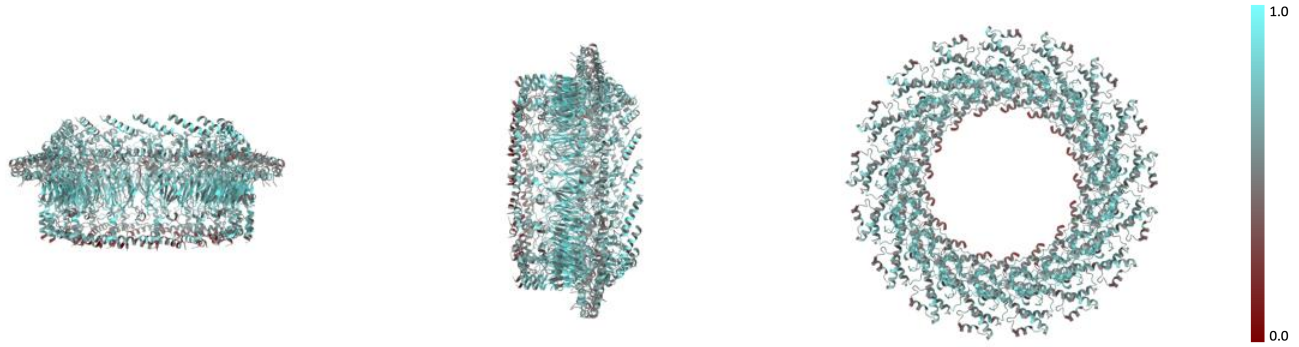
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

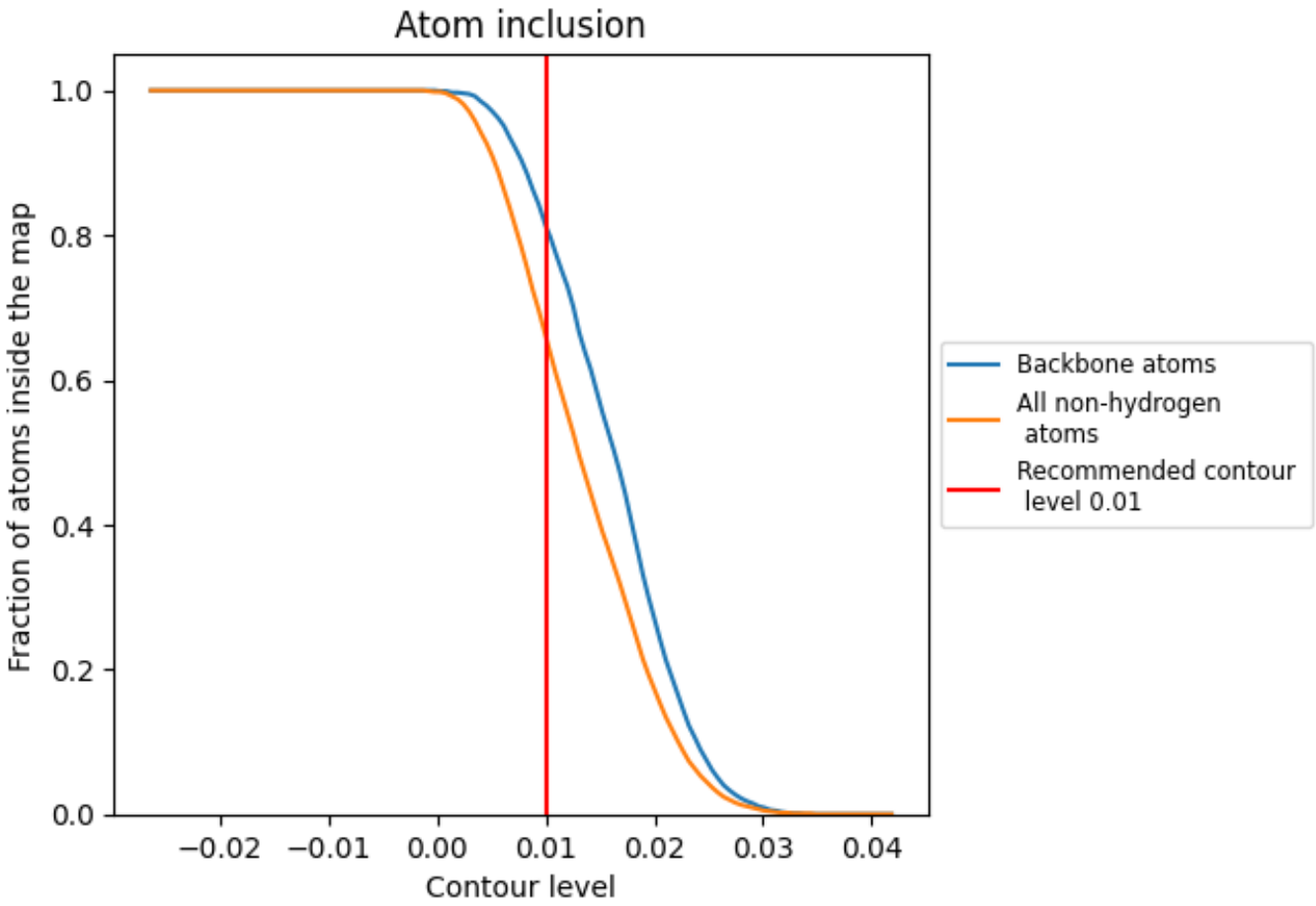
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 66% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6590	0.5180
AX	0.7300	0.5370
AY	0.5760	0.4950
BX	0.7260	0.5360
BY	0.5740	0.4950
CX	0.7260	0.5370
CY	0.5720	0.4940
DX	0.7230	0.5340
DY	0.5760	0.4950
EX	0.7240	0.5360
EY	0.5780	0.4920
FX	0.7300	0.5340
FY	0.5710	0.4930
GX	0.7180	0.5330
GY	0.5720	0.4920
HX	0.7270	0.5340
HY	0.5840	0.4940
IX	0.7250	0.5350
IY	0.5680	0.4940
JX	0.7290	0.5360
JY	0.5700	0.4950
KX	0.7240	0.5370
KY	0.5730	0.4940
LX	0.7290	0.5360
LY	0.5720	0.4930
MX	0.7240	0.5370
MY	0.5740	0.4940
NX	0.7240	0.5390
NY	0.5730	0.4950
OX	0.7300	0.5400
OY	0.5740	0.4960
PX	0.7270	0.5380
PY	0.5800	0.4940
QX	0.7260	0.5380
QY	0.5730	0.4950