



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:05 PM BST

PDB ID : 4AV2
EMDB ID: : EMD-2105
Title : Single particle electron microscopy of PilQ dodecameric complexes from *Neisseria meningitidis*.
Authors : Berry, J.L.; Phelan, M.M.; Collins, R.F.; Adomavicius, T.; Tonjum, T.; Frye, S.A.; Bird, L.; Owens, R.; Ford, R.C.; Lian, L.Y.; Derrick, J.P.
Deposited on : 2012-05-23
Resolution : 26.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

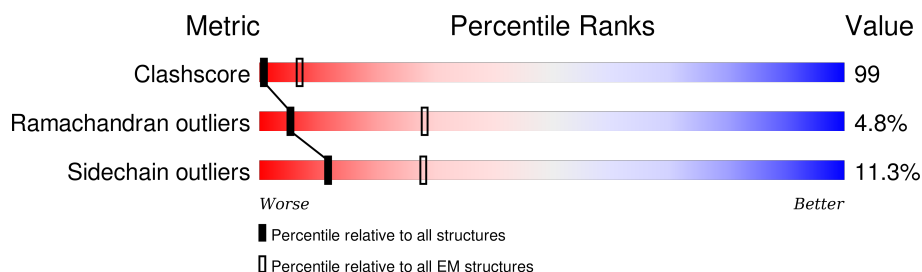
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 26.00 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.

















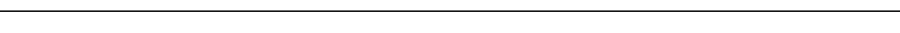
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	745	9% 25% • 63%
1	B	745	9% 25% • 63%
1	C	745	9% 25% • 63%
1	D	745	9% 25% • 63%
1	E	745	9% 25% • 63%
1	F	745	9% 25% • 63%
1	G	745	9% 25% • 63%
1	H	745	9% 25% • 63%
1	I	745	9% 25% • 63%

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Mol	Chain	Length	Quality of chain
1	J	745	
1	K	745	
1	L	745	
2	M	181	
2	N	181	
2	O	181	
2	P	181	
2	Q	181	
2	R	181	
2	S	181	
2	T	181	
2	U	181	
2	V	181	
2	W	181	
2	X	181	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 34704 atoms, of which 1152 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 TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	275	Total	C	N	O	S	0	1
			2152	1354	379	415	4		
1	B	275	Total	C	N	O	S	0	1
			2152	1354	379	415	4		
1	C	275	Total	C	N	O	S	0	1
			2152	1354	379	415	4		
1	D	275	Total	C	N	O	S	0	1
			2152	1354	379	415	4		
1	E	275	Total	C	N	O	S	0	1
			2152	1354	379	415	4		
1	F	275	Total	C	N	O	S	0	1
			2152	1354	379	415	4		
1	G	275	Total	C	N	O	S	0	1
			2152	1354	379	415	4		
1	H	275	Total	C	N	O	S	0	1
			2152	1354	379	415	4		
1	I	275	Total	C	N	O	S	0	1
			2152	1354	379	415	4		
1	J	275	Total	C	N	O	S	0	1
			2152	1354	379	415	4		
1	K	275	Total	C	N	O	S	0	1
			2152	1354	379	415	4		
1	L	275	Total	C	N	O	S	0	1
			2152	1354	379	415	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	428	PHE	LEU	VARIANT	UNP Q70M91
B	428	PHE	LEU	VARIANT	UNP Q70M91
C	428	PHE	LEU	VARIANT	UNP Q70M91
D	428	PHE	LEU	VARIANT	UNP Q70M91
E	428	PHE	LEU	VARIANT	UNP Q70M91

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Chain	Residue	Modelled	Actual	Comment	Reference
F	428	PHE	LEU	VARIANT	UNP Q70M91
G	428	PHE	LEU	VARIANT	UNP Q70M91
H	428	PHE	LEU	VARIANT	UNP Q70M91
I	428	PHE	LEU	VARIANT	UNP Q70M91
J	428	PHE	LEU	VARIANT	UNP Q70M91
K	428	PHE	LEU	VARIANT	UNP Q70M91
L	428	PHE	LEU	VARIANT	UNP Q70M91

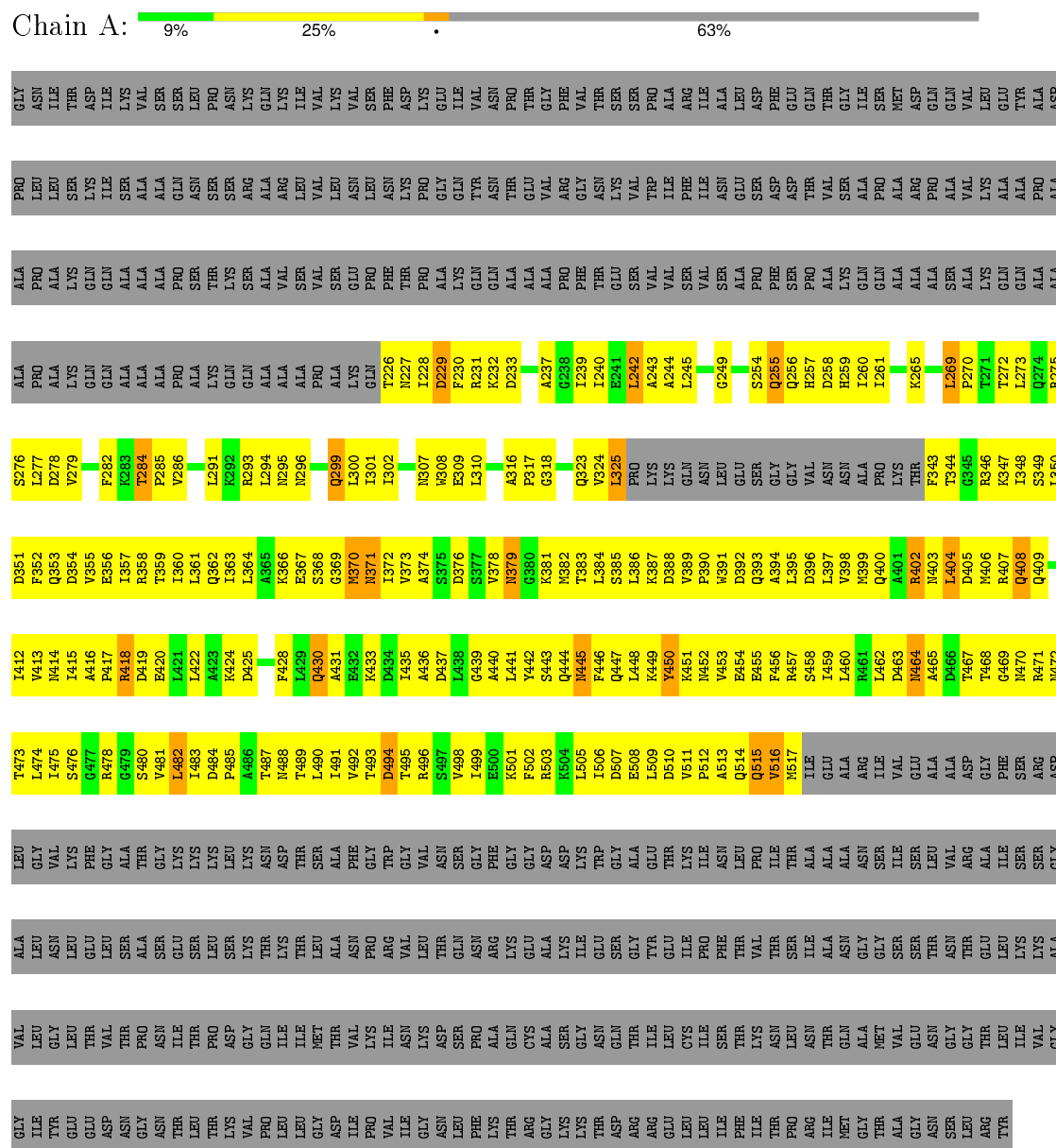
- Molecule 2 is a protein called PILP PROTEIN.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	M	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	N	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	O	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	P	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	Q	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	R	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	S	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	T	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	U	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	V	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	W	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	X	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		

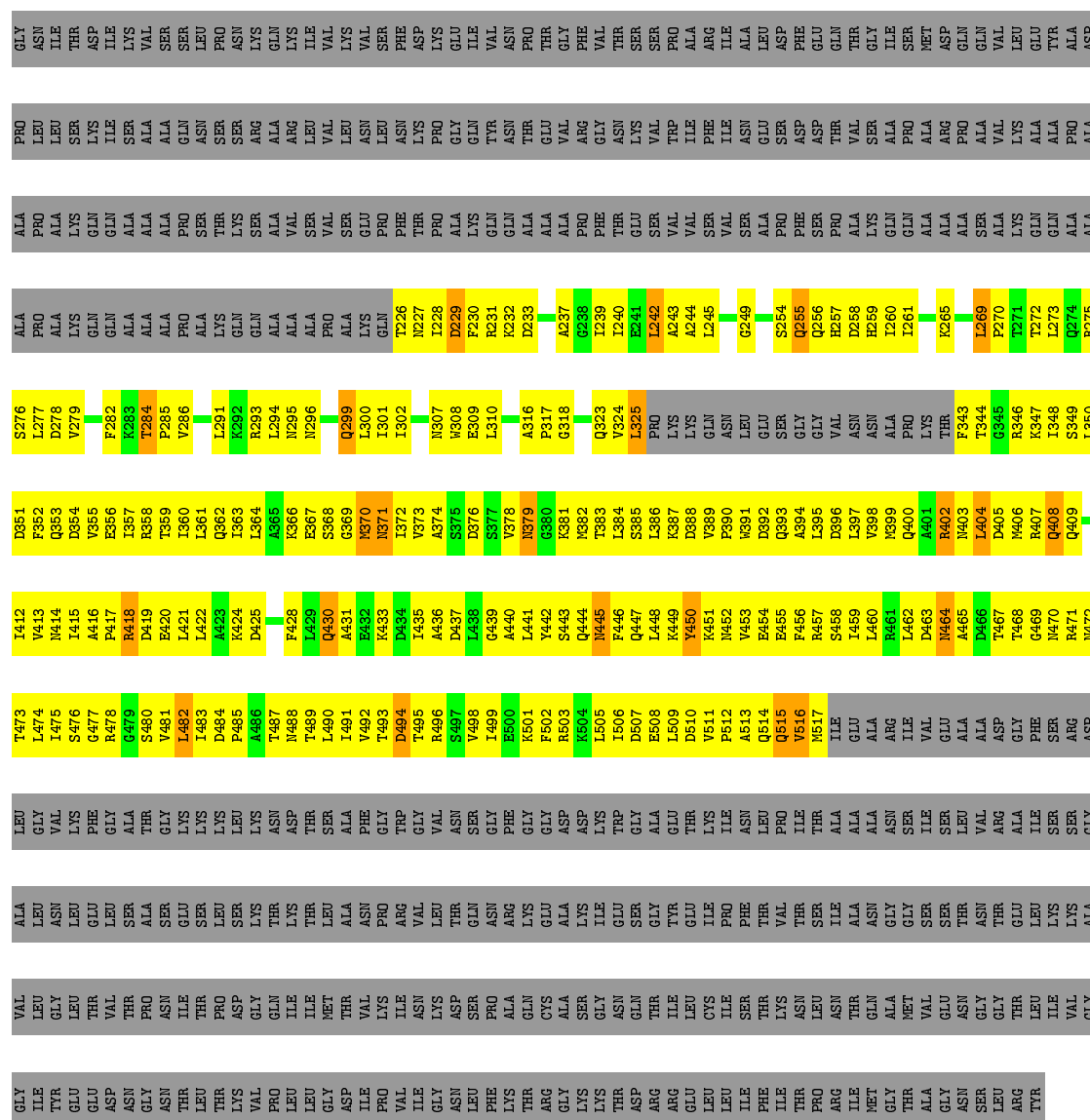
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

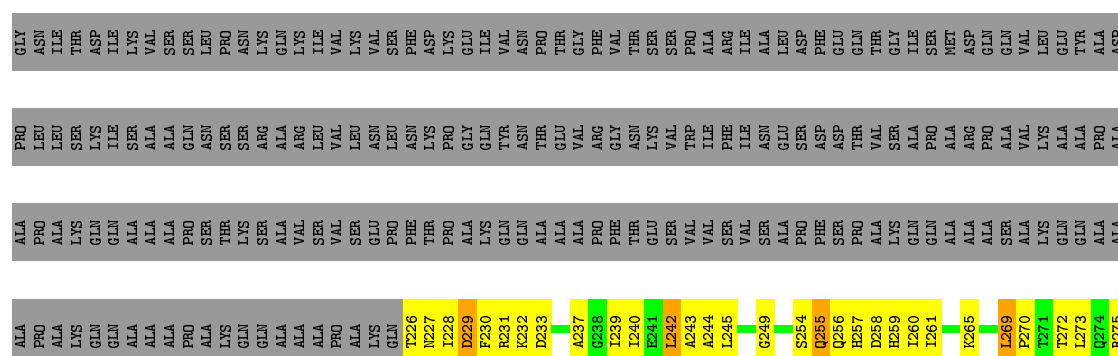
- Molecule 1: TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ

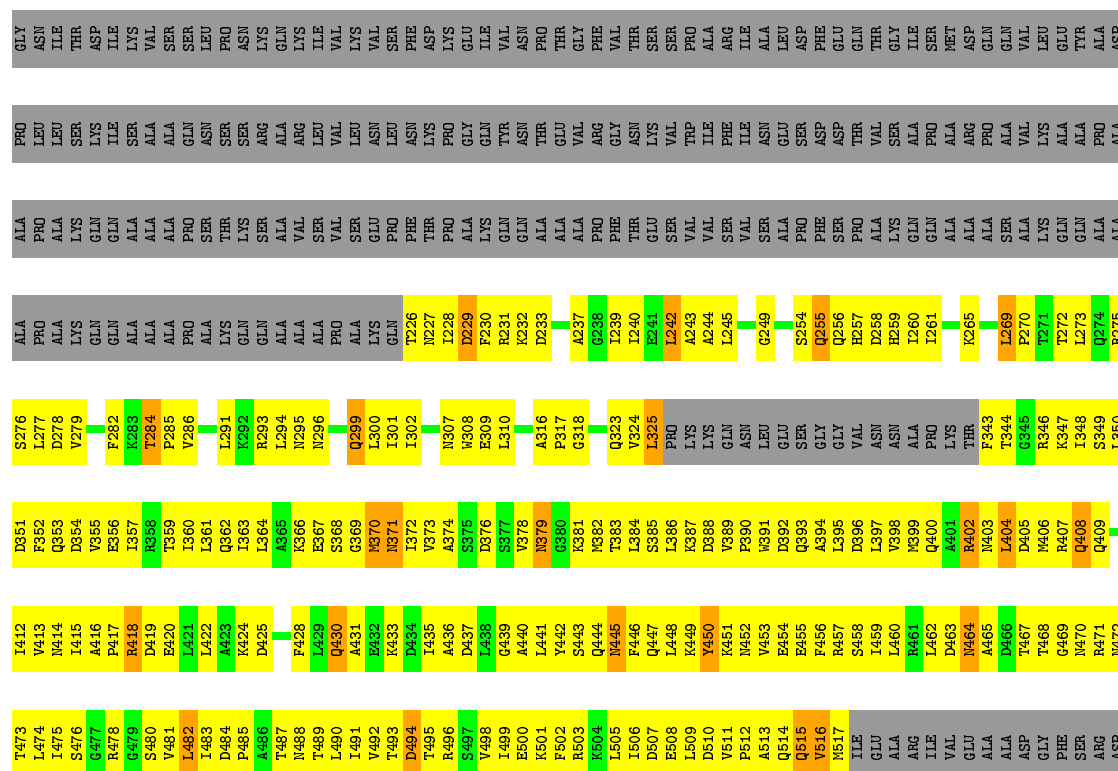


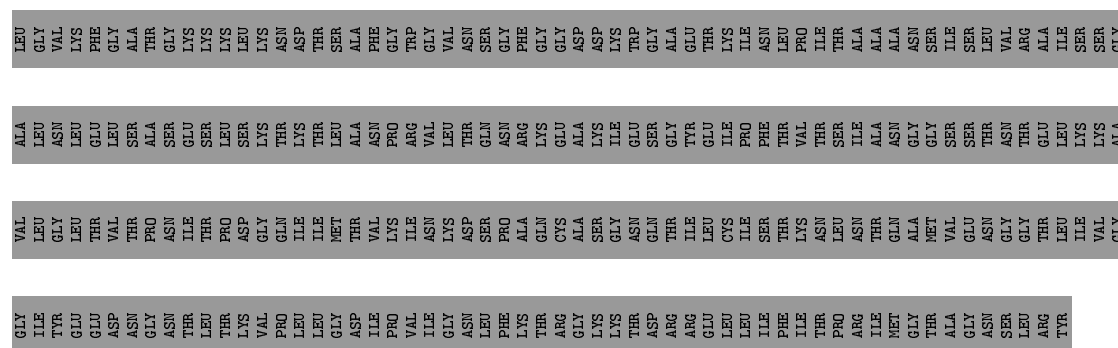
- Molecule 1: TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ



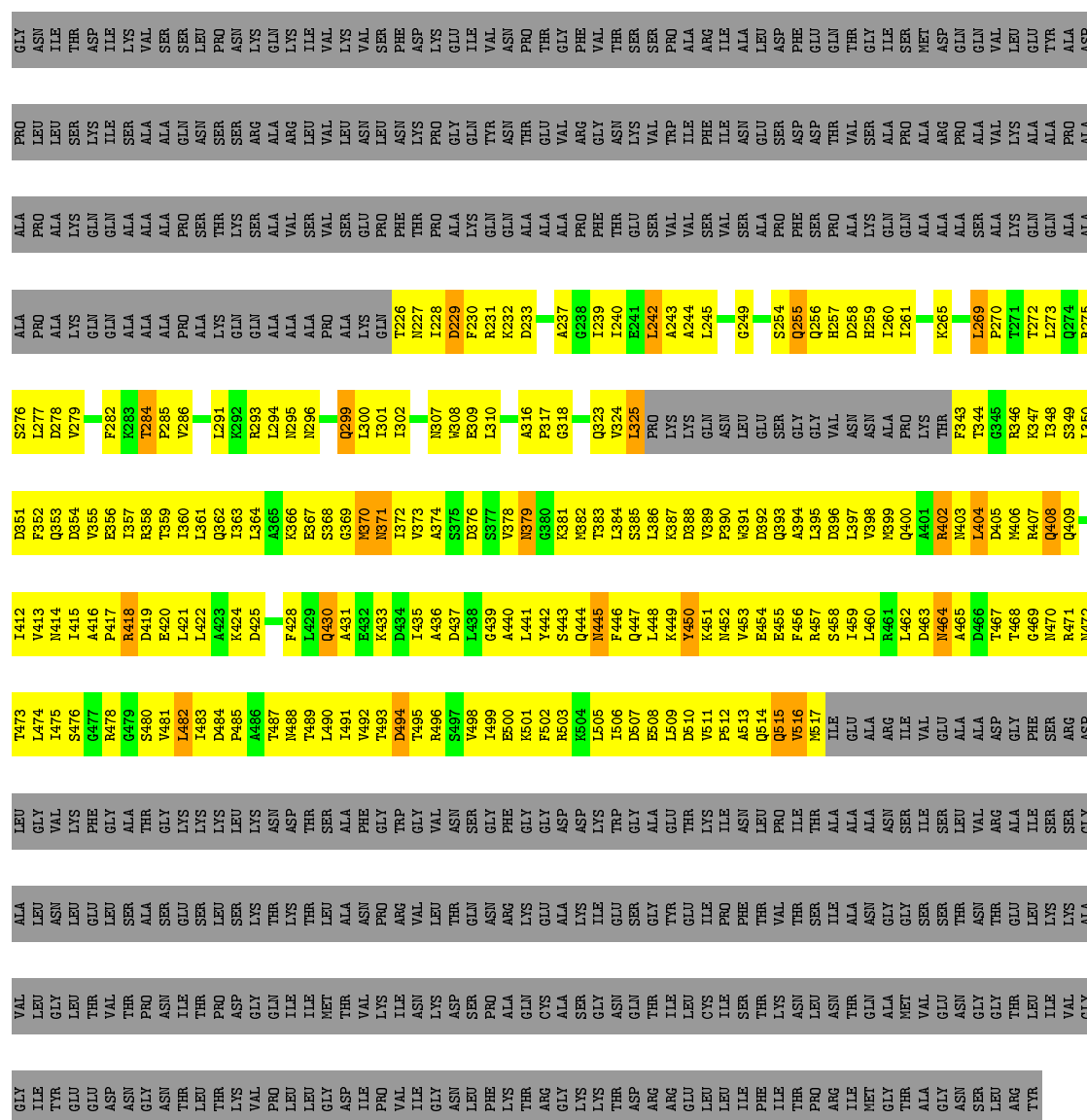
- Molecule 1: TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ



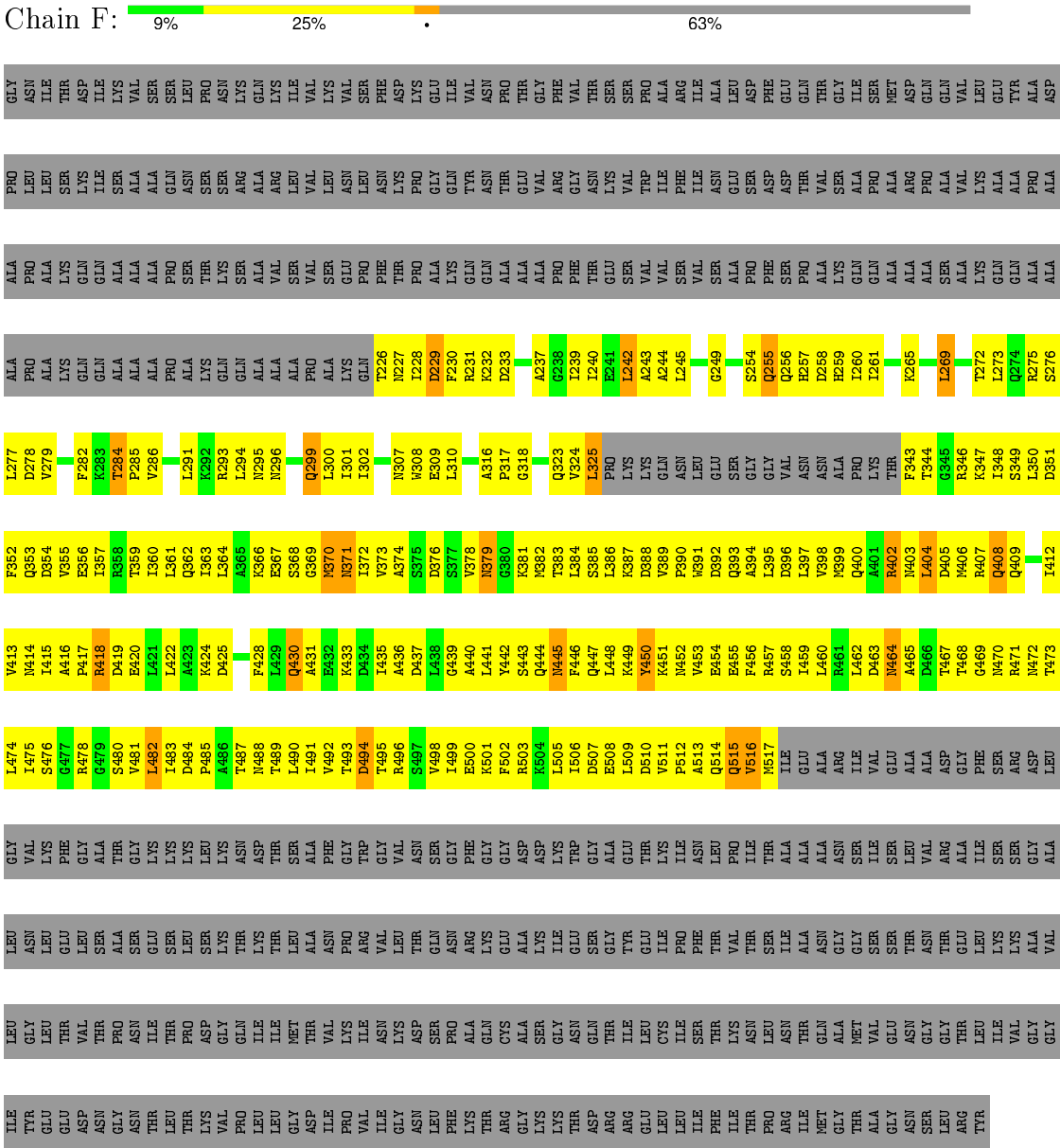




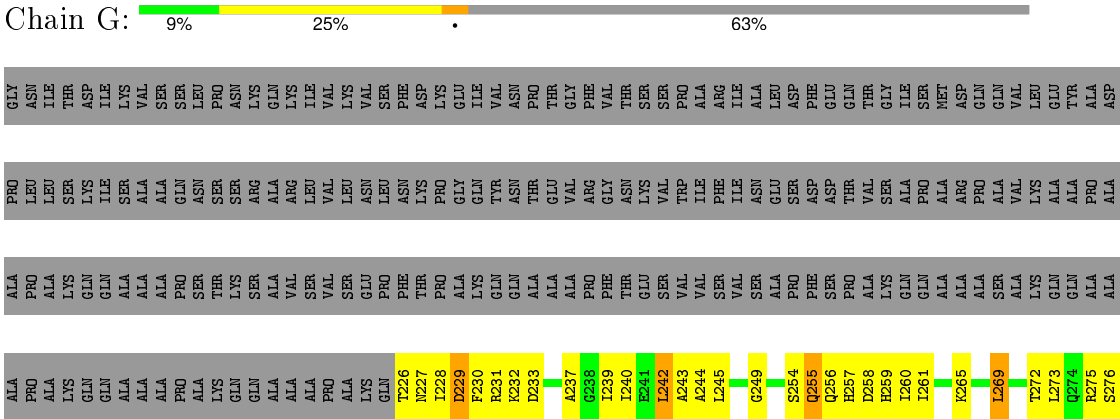
- Molecule 1: TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ

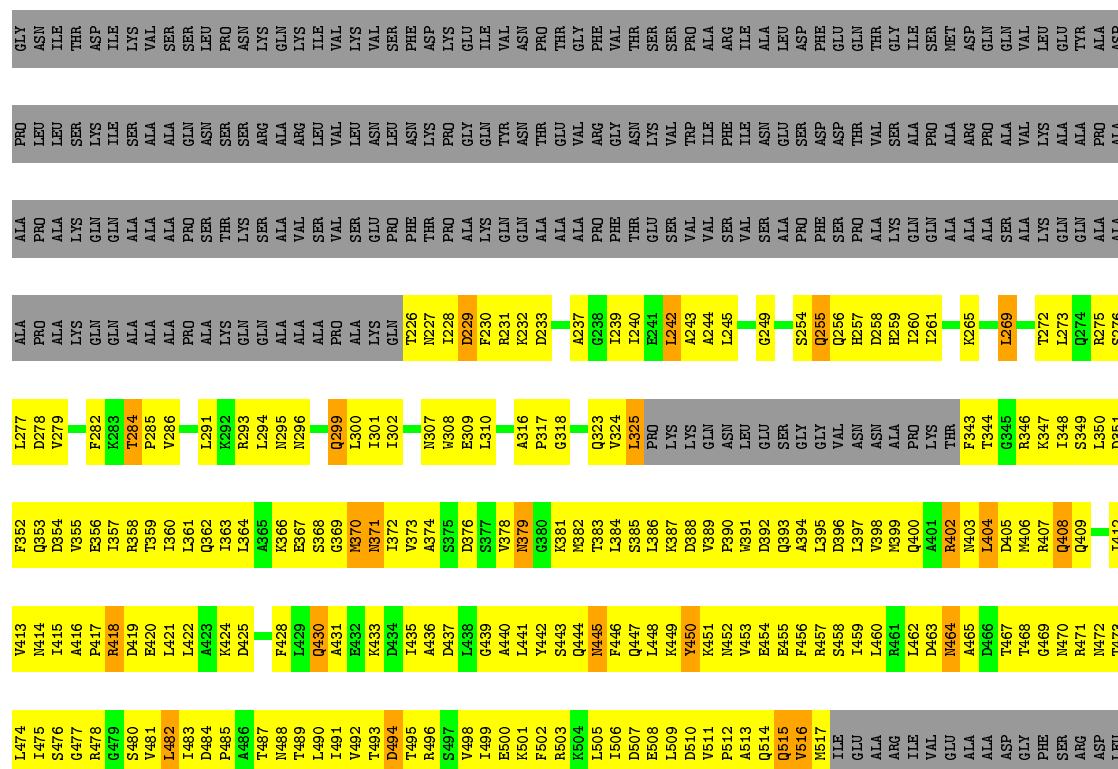


- Molecule 1: TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ



● Molecule 1: TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ





[illegible]

- Molecule 1: TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ

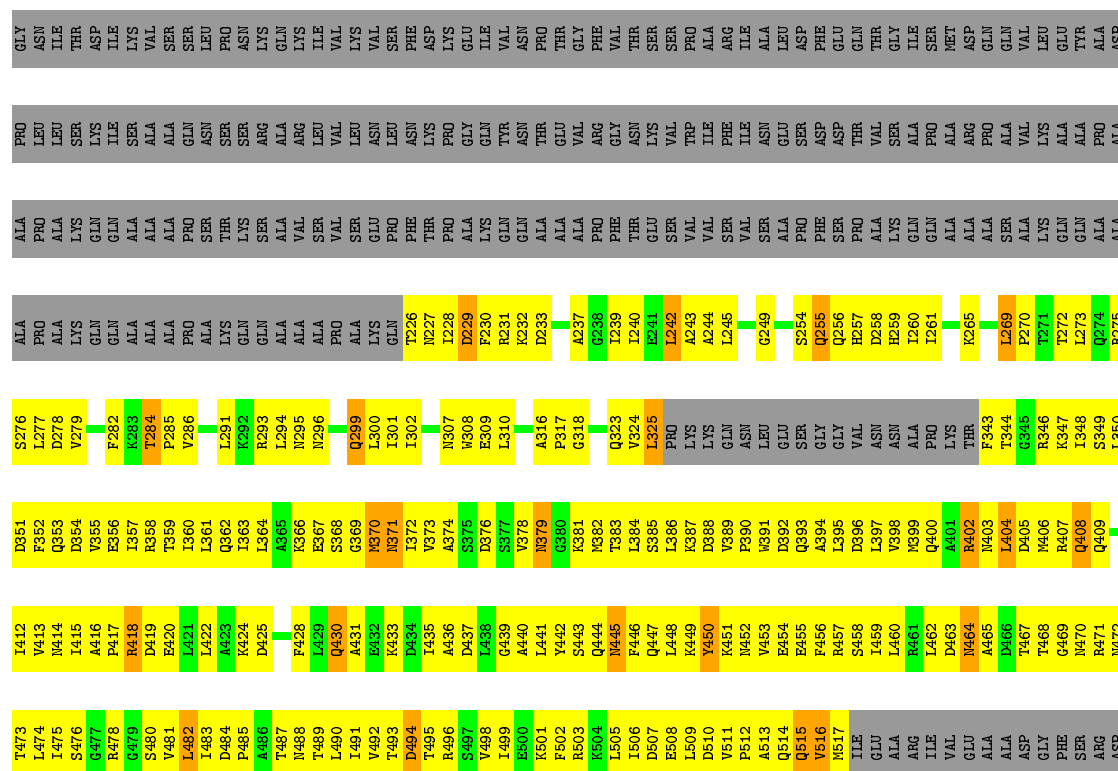
Chain J:  9% 25% . 63%

[illegible]

- Molecule 1: TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ

Chain K:  9% 25% 63%

[illegible]



MET	ASN	Y125
LYS	ALA	L126
HIS	PHE	G127
TYR	ASP	Q128
ALA	PHE	N129
LEU	ARG	Y130
LEU	ARG	G131
ILE	MET	R132
SER	THR	I133
PHE	ASP	E134
LEU	LEU	S135
ALA	LYS	I136
LEU	LYS	T137
SER	GLY	E138
ALA	GLU	D139
CYS	ASN	S140
SER	ALA	I141
GLN	PRO	V142
GLY	ASP	I143
SER	THR	N144
GLU	LYS	E145
ASP	ARG	L146
LEU	ILE	I147
LEU	ILE	E148
ASN	K84	D149
GLU	E85	S150
TRP	T86	L151
MET	L87	G152
ALA	E88	N153
GLN	S91	W154
THR	L92	W155
ARG	L95	S156
ARG	R96	R157
ALA	L97	K158
LYS	Y97	E159
ALA	V98	E160
ALA	G99	L161
GLU	I100	L162
ILE	L101	L163
ILE	K102	N164
PRO	S103	S165
PHE	G104	SER
GLN	Q105	ASP
ALA	K106	LYS
PRO	V107	ASN
THR	S108	THR
LEU	G109	GLU
PRO	F110	VAL
VAL	I111	ALA
ALA	E112	PRO
PRO	A113	VAL
VAL	V117	TYR
TYR	Y118	SER
SER	T119	PRO
PRO	T119	PRO
GLN	V120	GLN
LEU	G121	LEU
THR	V122	THR
GLY	G123	GLY
PRO	N124	ASN

• Molecule 2: PILP PROTEIN

Chain Q: 12% 25% 8% 55%

MET	ASN	Y125
LYS	ALA	L126
HIS	PHE	G127
TYR	ASP	Q128
ALA	PHE	N129
LEU	ARG	Y130
LEU	ARG	G131
ILE	MET	R132
SER	THR	I133
PHE	ASP	E134
LEU	LEU	S135
ALA	LYS	I136
LEU	LYS	T137
SER	GLY	E138
ALA	GLU	D139
CYS	ASN	S140
SER	ALA	I141
GLN	PRO	V142
GLY	ASP	I143
SER	THR	N144
GLU	LYS	E145
ASP	ARG	L146
LEU	ILE	I147
LEU	ILE	E148
ASN	K84	D149
GLU	E85	S150
TRP	T86	L151
MET	L87	G152
ALA	E88	N153
GLN	S91	W154
THR	L92	W155
ARG	L95	S156
ARG	R96	R157
ALA	L97	K158
LYS	Y97	E159
ALA	V98	E160
ALA	G99	L161
GLU	I100	L162
ILE	L101	L163
ILE	K102	N164
PRO	S103	S165
PHE	G104	SER
GLN	Q105	ASP
ALA	K106	LYS
PRO	V107	ASN
THR	S108	THR
LEU	G109	GLU
VAL	F110	VAL
ALA	I111	ALA
ALA	E112	PRO
VAL	A113	VAL
TYR	V117	TYR
SER	Y118	SER
PRO	T119	PRO
PRO	T119	PRO
GLN	V120	GLN
LEU	G121	LEU
THR	V122	THR
GLY	G123	GLY
PRO	N124	ASN

• Molecule 2: PILP PROTEIN

Chain R: 10% 28% 8% 55%

MET	ASN	Y125
LYS	ALA	L126
HIS	PHE	G127
TYR	ASP	Q128
ALA	PHE	N129
LEU	ARG	Y130
LEU	ARG	G131
ILE	MET	R132
SER	THR	I133
PHE	ASP	E134
LEU	LEU	S135
ALA	LYS	I136
LEU	LYS	T137
SER	GLY	E138
ALA	GLU	D139
CYS	ASN	S140
SER	ALA	I141
GLN	PRO	V142
GLY	ASP	I143
SER	THR	N144
GLU	LYS	E145
ASP	ARG	L146
LEU	ILE	I147
LEU	ILE	E148
ASN	K84	D149
GLU	E85	S150
TRP	T86	L151
MET	L87	G152
ALA	E88	N153
GLN	K89	G152
THR	F90	W154
ARG	S91	W155
ARG	L92	S156
GLU	Y155	R157
GLU	S156	K158
ALA	R96	E159
LYS	Y97	E160
ALA	V98	L161
ALA	G99	L162
ILE	I100	L163
ILE	L101	N164
PRO	K102	S165
PHE	S103	SER
GLN	G104	ASP
ALA	Q105	LYS
PRO	K106	ASN
THR	V107	THR
LEU	S108	GLU
LEU	G109	VAL
VAL	F110	ALA
ALA	I111	PRO
ALA	E112	VAL
VAL	A113	TYR
TYR	E114	SER
SER	ALA	PRO
PRO	ALA	PRO
GLN	V117	GLN
LEU	Y118	LEU
THR	T119	THR
GLN	V120	GLN
GLY	G121	GLY
PRO	V122	PRO

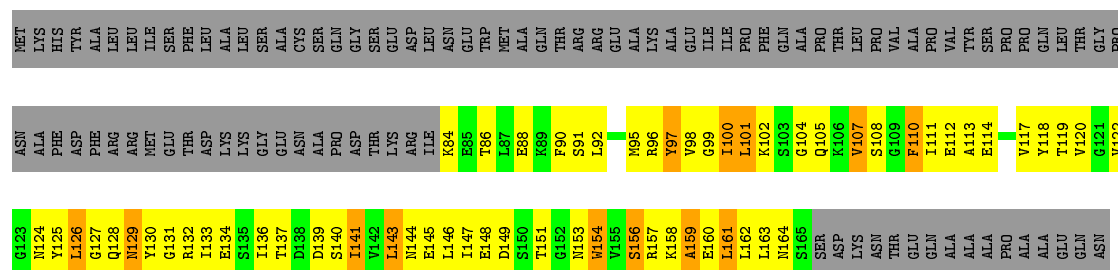
• Molecule 2: PILP PROTEIN

Chain S: 11% 26% 8% 55%

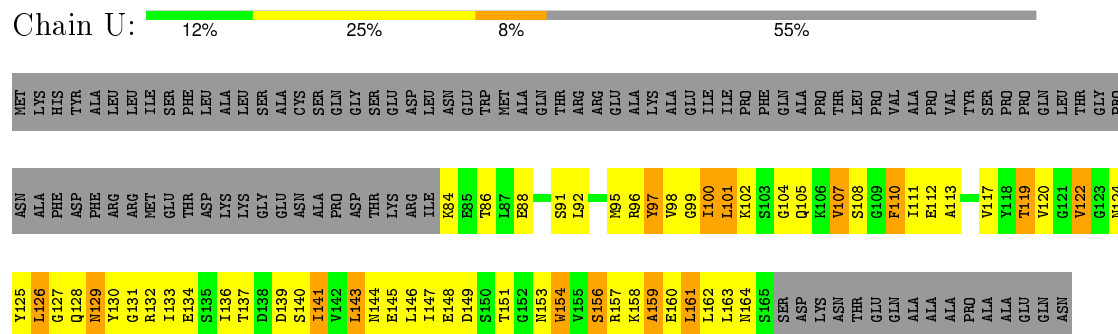
MET	ASN	Y125
LYS	ALA	L126
HIS	PHE	G127
TYR	ASP	Q128
ALA	PHE	N129
LEU	ARG	Y130
LEU	ARG	G131
ILE	MET	R132
SER	THR	I133
PHE	ASP	E134
LEU	LEU	S135
ALA	LYS	I136
LEU	LYS	T137
SER	GLY	E138
ALA	GLU	D139
CYS	ASN	S140
SER	ALA	I141
GLN	PRO	V142
GLY	ASP	I143
SER	THR	N144
GLU	LYS	E145
ASP	ARG	L146
LEU	ILE	I147
LEU	ILE	E148
ASN	K84	D149
GLU	E85	S150
TRP	T86	L151
MET	L87	G152
ALA	E88	N153
GLN	K89	G152
THR	F90	W154
ARG	S91	W155
ARG	L92	S156
GLU	Y155	R157
GLU	S156	K158
ALA	R96	E159
LYS	Y97	E160
ALA	V98	L161
ALA	G99	L162
ILE	I100	L163
ILE	L101	N164
PRO	K102	S165
PHE	S103	SER
GLN	G104	ASP
ALA	Q105	LYS
PRO	K106	ASN
THR	V107	THR
LEU	S108	GLU
LEU	G109	VAL
VAL	F110	ALA
ALA	I111	PRO
ALA	E112	VAL
VAL	A113	TYR
TYR	E114	SER
SER	ALA	PRO
PRO	ALA	PRO
GLN	V117	GLN
LEU	Y118	LEU
THR	T119	THR
GLN	V120	GLN
GLY	G121	GLY
PRO	V122	PRO

• Molecule 2: PILP PROTEIN

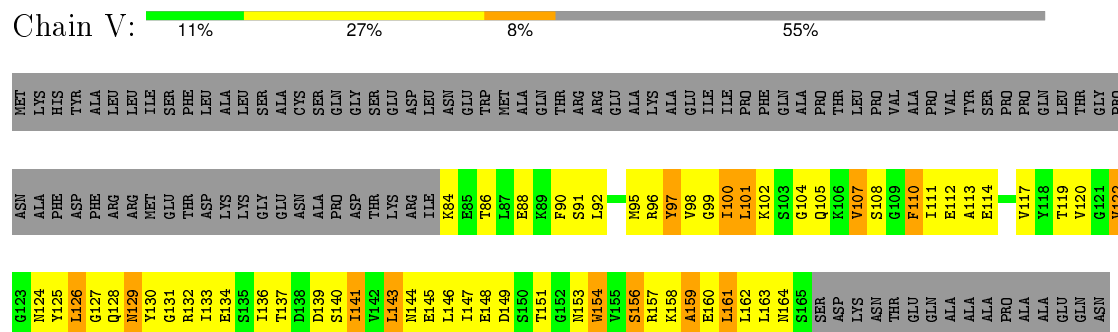
Chain T: 10% 28% 7% 55%



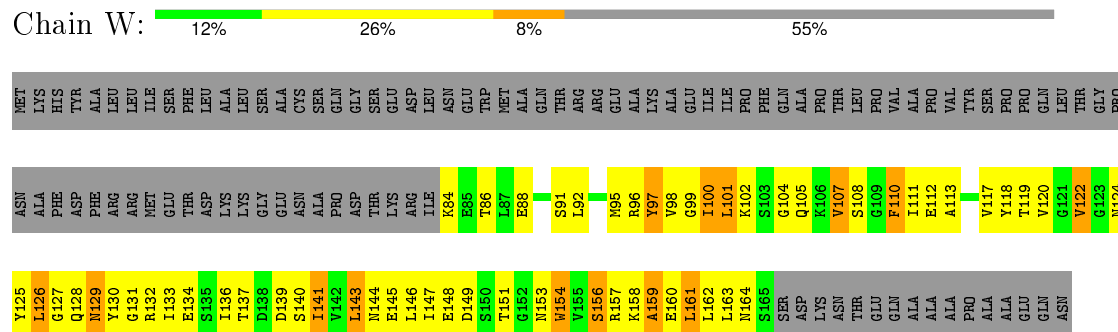
- Molecule 2: PILP PROTEIN



- Molecule 2: PILP PROTEIN



- Molecule 2: PILP PROTEIN



- Molecule 2: PILP PROTEIN

ASN	ASN	MET
ALA	ALA	LYS
PHE	PHE	HIS
ASP	ASP	TYR
PHE	PHE	ALA
Q127	ARG	LEU
Q128	ARG	LEU
M129	ARG	LEU
Y130	MET	ILE
G131	GLU	SER
R132	THR	PHE
I133	ASP	LEU
E134	LYS	ALA
S135	LYS	LEU
I136	GLY	SER
T137	GLU	ALA
D138	ASN	CYS
D139	ALA	SER
S140	PRO	GLN
I141	ASP	GLY
V142	THR	SER
L143	LYS	GLU
N144	ARG	ASP
E145	ILE	LEU
L146	K34	ASN
I147	E85	GLU
E148	T86	TRP
D149	L87	MET
S150	E88	ALA
T151	K89	GLN
G152	F90	THR
N153	S91	ARG
M154	L92	ARG
V155		GLU
S156	N95	ALA
R157	R96	LYS
K158	Y97	ALA
A159	Y98	GLU
E160	G99	ILE
L161	I100	ILE
L162	L101	PRO
L163	K102	PHE
N164	S103	GLN
S165	G104	ALA
SER	Q105	PRO
ASP	K106	THR
LYS	V107	LEU
ASN	S108	PRO
THR	G109	VAL
GLU	F110	ALA
GLN	I111	PRO
ALA	E112	VAL
ALA	A113	TYR
ALA	E114	SER
PRO		PRO
ALA	V117	PRO
ALA	V118	GLN
GLU	T119	LEU
GLN	V120	THR
ASN	G121	GLY
	V122	PRO

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTFFIT EACH MICROGRAPH, Not provided	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	4	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5100	Depositor
Magnification	33000	Depositor
Image detector	GATAN 4K X 4K CCD	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.79	0/2179	1.19	4/2950 (0.1%)
1	B	0.79	0/2179	1.19	4/2950 (0.1%)
1	C	0.79	0/2179	1.19	4/2950 (0.1%)
1	D	0.79	0/2179	1.19	4/2950 (0.1%)
1	E	0.79	0/2179	1.19	4/2950 (0.1%)
1	F	0.79	0/2179	1.19	4/2950 (0.1%)
1	G	0.79	0/2179	1.19	4/2950 (0.1%)
1	H	0.79	0/2179	1.19	4/2950 (0.1%)
1	I	0.79	0/2179	1.19	4/2950 (0.1%)
1	J	0.79	0/2179	1.19	4/2950 (0.1%)
1	K	0.79	0/2179	1.19	4/2950 (0.1%)
1	L	0.79	0/2179	1.19	4/2950 (0.1%)
2	M	0.23	0/652	0.40	0/878
2	N	0.23	0/652	0.40	0/878
2	O	0.23	0/652	0.40	0/878
2	P	0.23	0/652	0.40	0/878
2	Q	0.23	0/652	0.40	0/878
2	R	0.23	0/652	0.40	0/878
2	S	0.23	0/652	0.40	0/878
2	T	0.23	0/652	0.40	0/878
2	U	0.23	0/652	0.40	0/878
2	V	0.23	0/652	0.40	0/878
2	W	0.23	0/652	0.40	0/878
2	X	0.23	0/652	0.40	0/878
All	All	0.70	0/33972	1.06	48/45936 (0.1%)

There are no bond length outliers.

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	408	GLN	CG-CD-OE1	-38.48	44.65	121.60
1	D	408	GLN	CG-CD-OE1	-38.48	44.65	121.60
1	G	408	GLN	CG-CD-OE1	-38.48	44.65	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	408	GLN	CG-CD-OE1	-38.48	44.65	121.60
1	C	408	GLN	CG-CD-OE1	-38.47	44.66	121.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2152	0	2190	607	0
1	B	2152	0	2190	612	0
1	C	2152	0	2190	615	0
1	D	2152	0	2190	610	0
1	E	2152	0	2190	610	0
1	F	2152	0	2190	603	0
1	G	2152	0	2190	601	0
1	H	2152	0	2190	613	0
1	I	2152	0	2190	599	0
1	J	2152	0	2190	605	0
1	K	2152	0	2190	607	0
1	L	2152	0	2190	601	0
2	M	644	96	636	116	0
2	N	644	96	636	115	0
2	O	644	96	636	115	0
2	P	644	96	636	118	0
2	Q	644	96	636	119	0
2	R	644	96	636	119	0
2	S	644	96	636	117	0
2	T	644	96	636	117	0
2	U	644	96	636	113	0
2	V	644	96	636	115	0
2	W	644	96	636	114	0
2	X	644	96	636	117	0
All	All	33552	1152	33912	6674	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 99.

The worst 5 of 6674 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:E:347:LYS:NZ	2:Q:104:GLY:HA2	1.29	1.47
1:C:347:LYS:NZ	2:O:104:GLY:HA2	1.30	1.46
1:G:347:LYS:NZ	2:S:104:GLY:HA2	1.30	1.46
1:A:347:LYS:NZ	2:M:104:GLY:HA2	1.30	1.41
1:I:347:LYS:NZ	2:U:104:GLY:HA2	1.30	1.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	7	45
1	B	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	7	45
1	C	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	7	45
1	D	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	7	45
1	E	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	7	45
1	F	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	7	45
1	G	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	7	45
1	H	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	7	45
1	I	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	7	45
1	J	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	7	45
1	K	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	7	45
1	L	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	7	45
2	M	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	8
2	O	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	8
2	P	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	8
2	Q	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	8
2	R	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	8
2	S	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	8
2	T	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	8
2	U	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	8
2	V	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	8
2	W	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	8
2	X	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	8
All	All	4212/11112 (38%)	3432 (82%)	576 (14%)	204 (5%)	5	32

5 of 204 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	ASN
1	A	402	ARG
1	B	379	ASN
1	B	402	ARG
1	C	379	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	239/615 (39%)	216 (90%)	23 (10%)	10	40
1	B	239/615 (39%)	216 (90%)	23 (10%)	10	40
1	C	239/615 (39%)	216 (90%)	23 (10%)	10	40
1	D	239/615 (39%)	216 (90%)	23 (10%)	10	40
1	E	239/615 (39%)	216 (90%)	23 (10%)	10	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	239/615 (39%)	216 (90%)	23 (10%)	10	40
1	G	239/615 (39%)	216 (90%)	23 (10%)	10	40
1	H	239/615 (39%)	216 (90%)	23 (10%)	10	40
1	I	239/615 (39%)	216 (90%)	23 (10%)	10	40
1	J	239/615 (39%)	216 (90%)	23 (10%)	10	40
1	K	239/615 (39%)	216 (90%)	23 (10%)	10	40
1	L	239/615 (39%)	216 (90%)	23 (10%)	10	40
2	M	71/152 (47%)	59 (83%)	12 (17%)	2	18
2	N	71/152 (47%)	59 (83%)	12 (17%)	2	18
2	O	71/152 (47%)	59 (83%)	12 (17%)	2	18
2	P	71/152 (47%)	59 (83%)	12 (17%)	2	18
2	Q	71/152 (47%)	59 (83%)	12 (17%)	2	18
2	R	71/152 (47%)	59 (83%)	12 (17%)	2	18
2	S	71/152 (47%)	59 (83%)	12 (17%)	2	18
2	T	71/152 (47%)	59 (83%)	12 (17%)	2	18
2	U	71/152 (47%)	59 (83%)	12 (17%)	2	18
2	V	71/152 (47%)	59 (83%)	12 (17%)	2	18
2	W	71/152 (47%)	59 (83%)	12 (17%)	2	18
2	X	71/152 (47%)	59 (83%)	12 (17%)	2	18
All	All	3720/9204 (40%)	3300 (89%)	420 (11%)	12	33

5 of 420 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	269	LEU
1	K	269	LEU
2	V	125	TYR
1	I	300	LEU
1	J	276	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 157 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	408	GLN

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Mol	Chain	Res	Type
1	I	296	ASN
2	S	129	ASN
1	G	445	ASN
1	H	371	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.