



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:55 am GMT

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/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

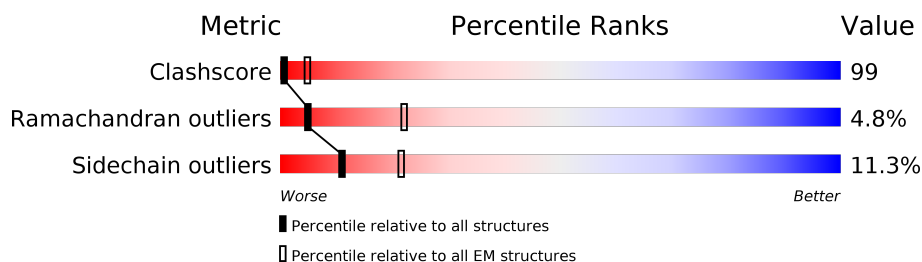
1 Overall quality at a glance

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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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

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

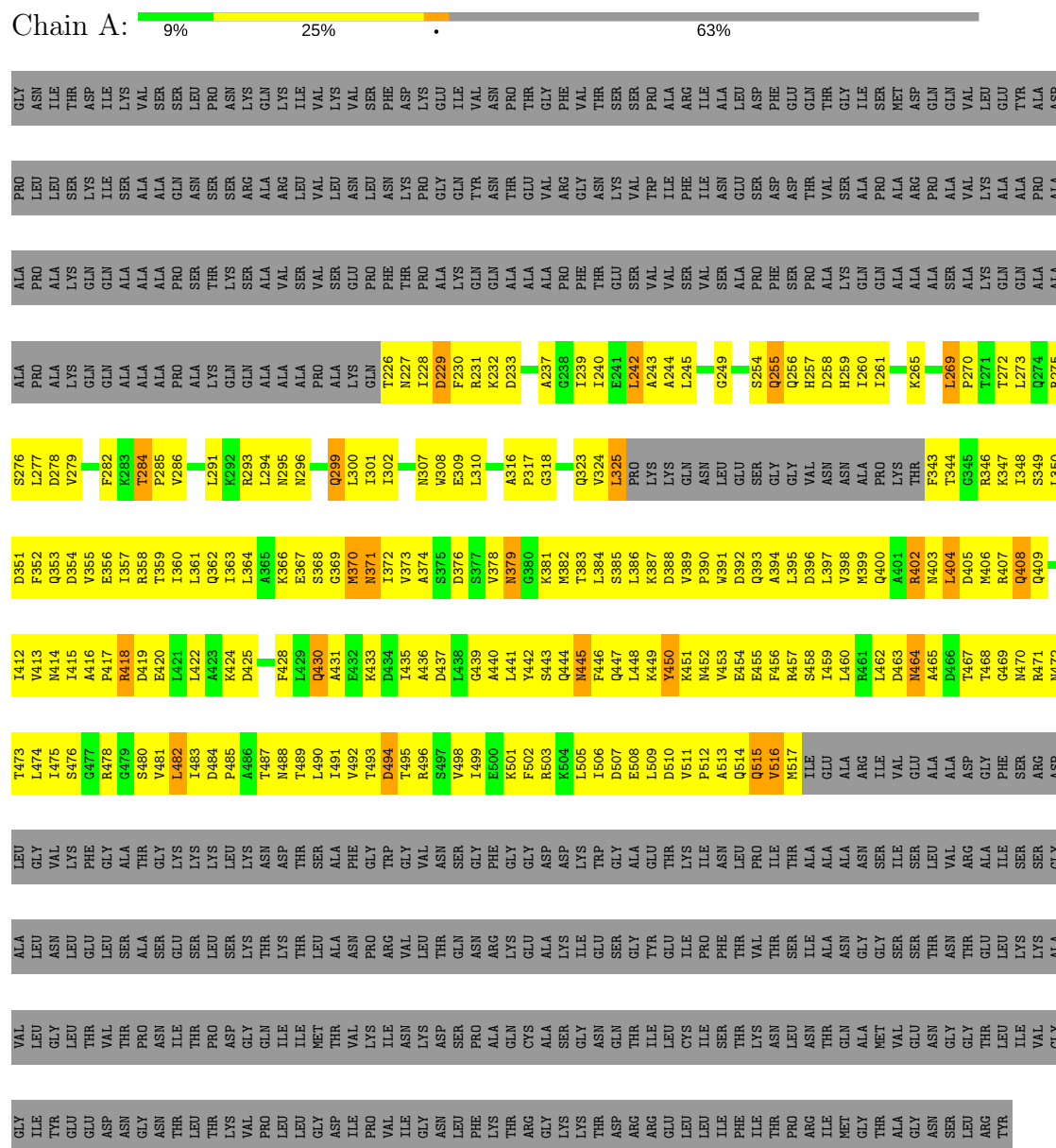
- Molecule 2 is a protein called PILP PROTEIN.

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

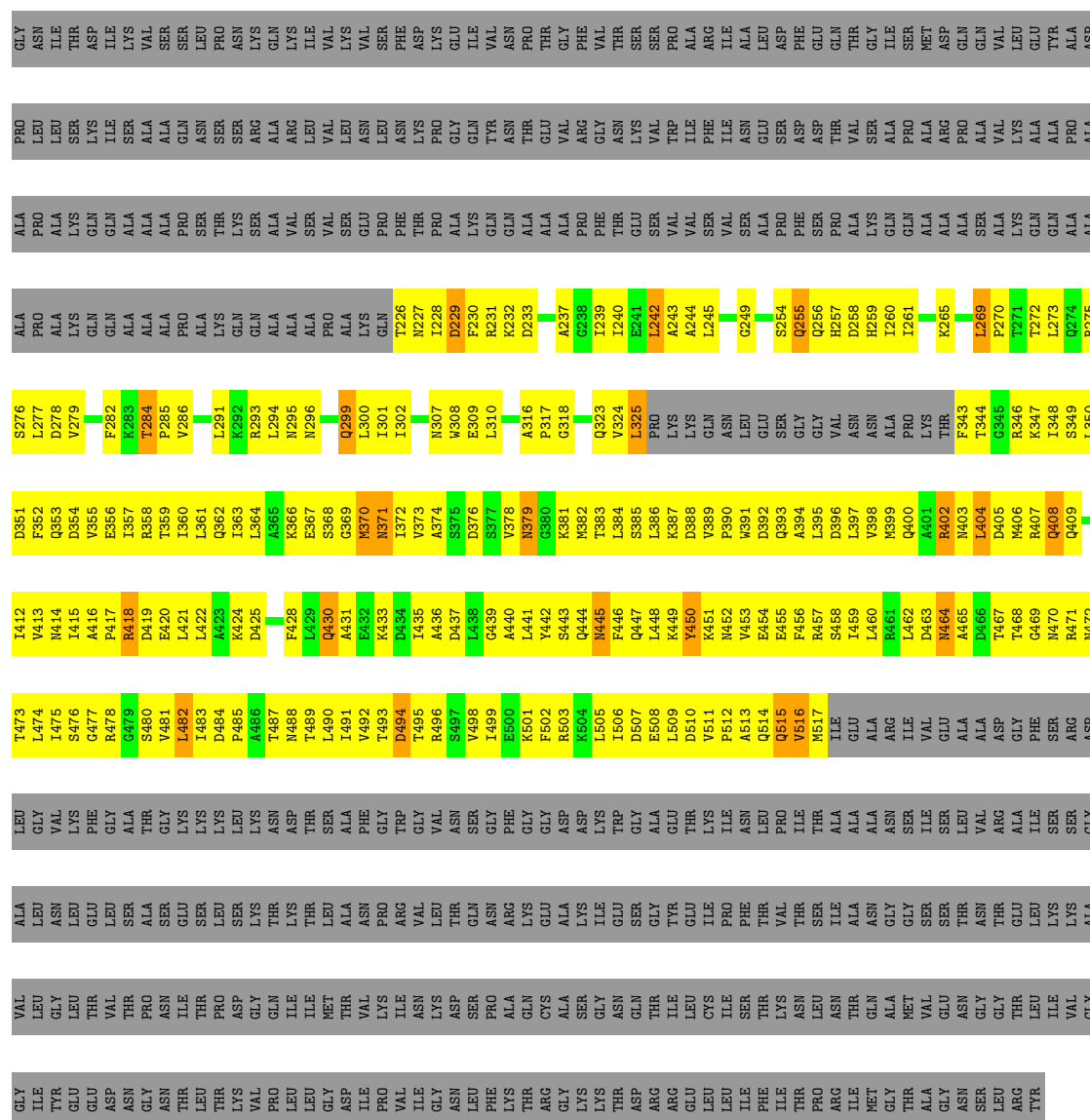
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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



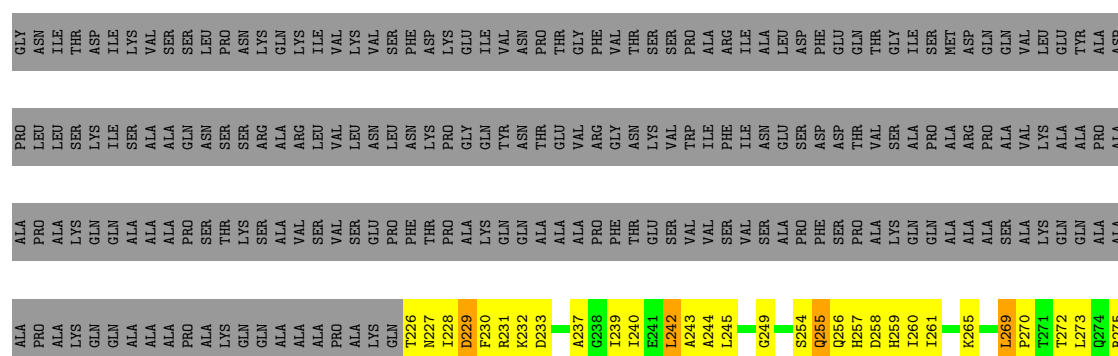
- Molecule 1: TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ

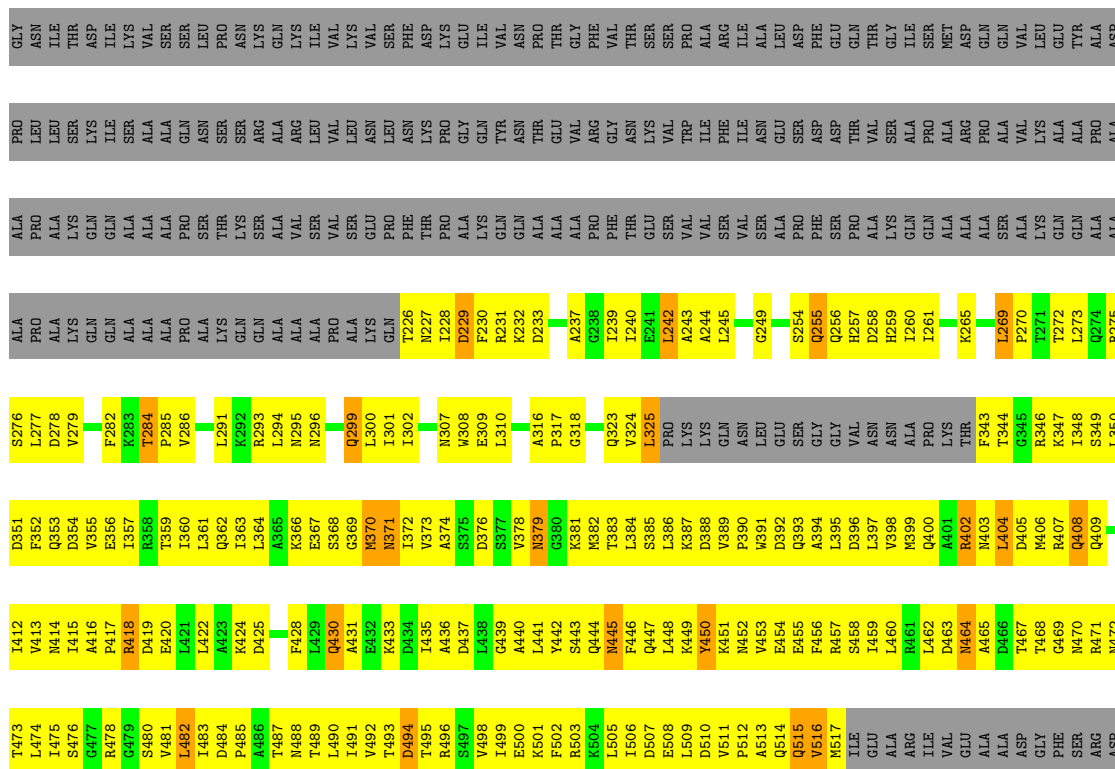
Chain B: 9% 25% . 63%

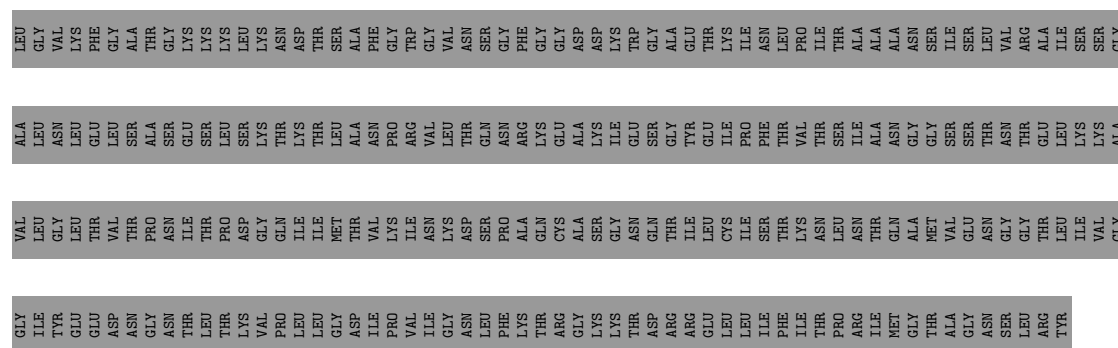


- Molecule 1: TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ

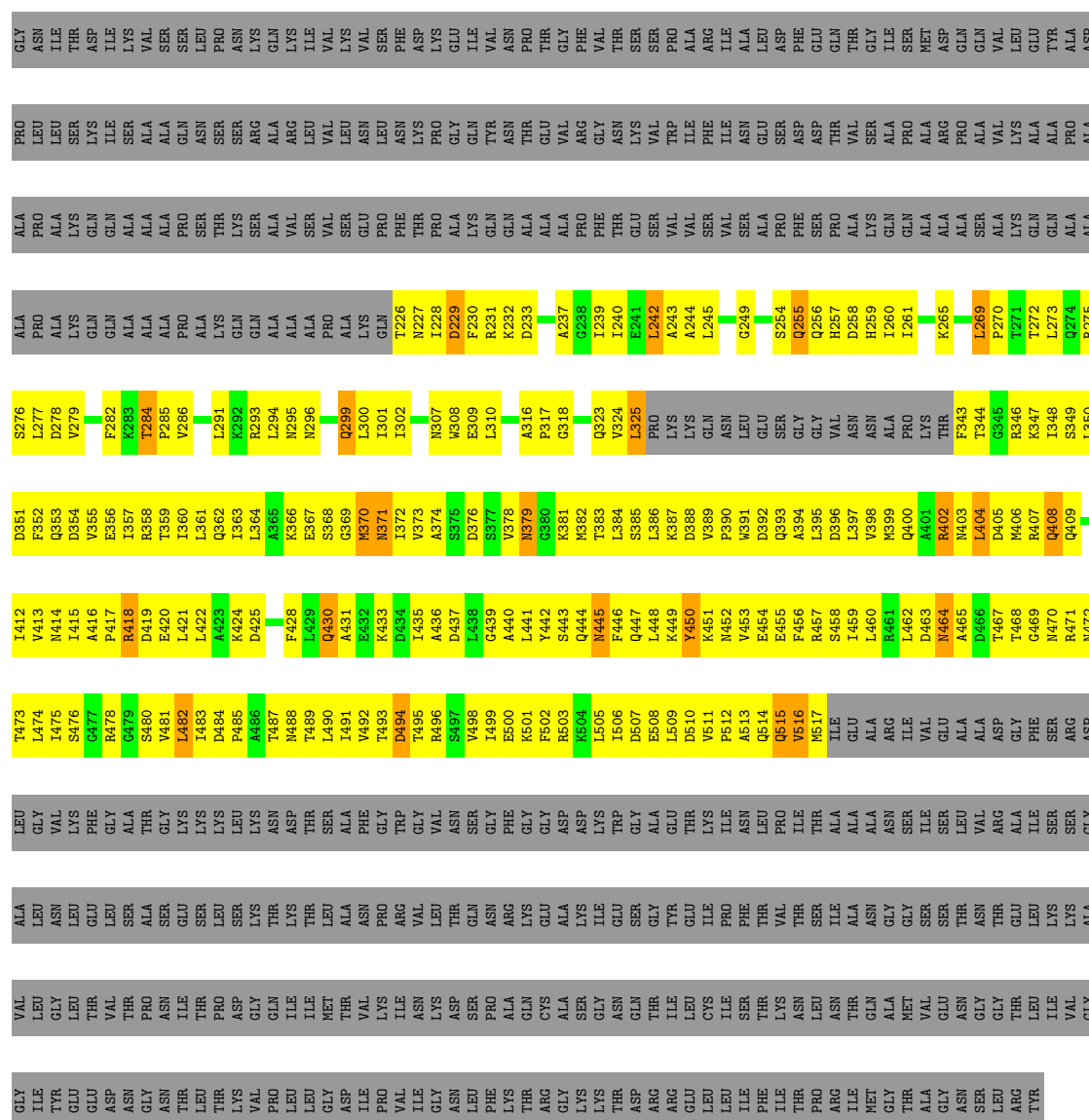
Chain C:  9% 25% 63%







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



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

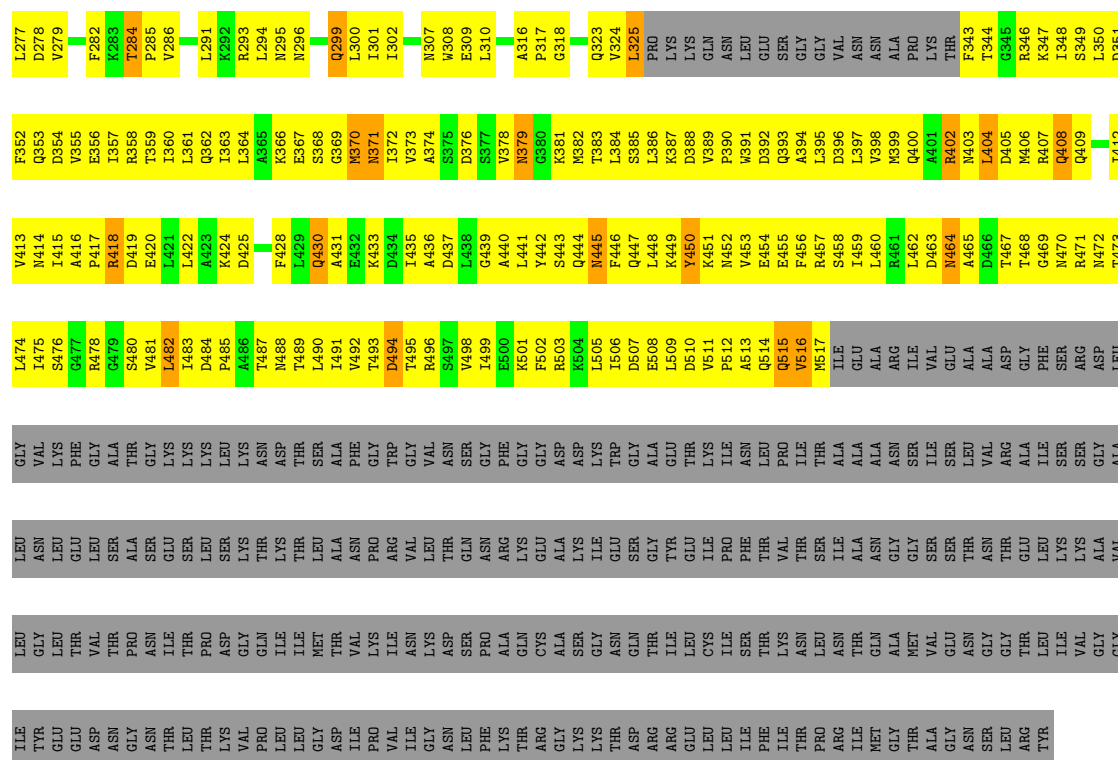
Chain F:  9% 25% . 63%

[illegible]

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

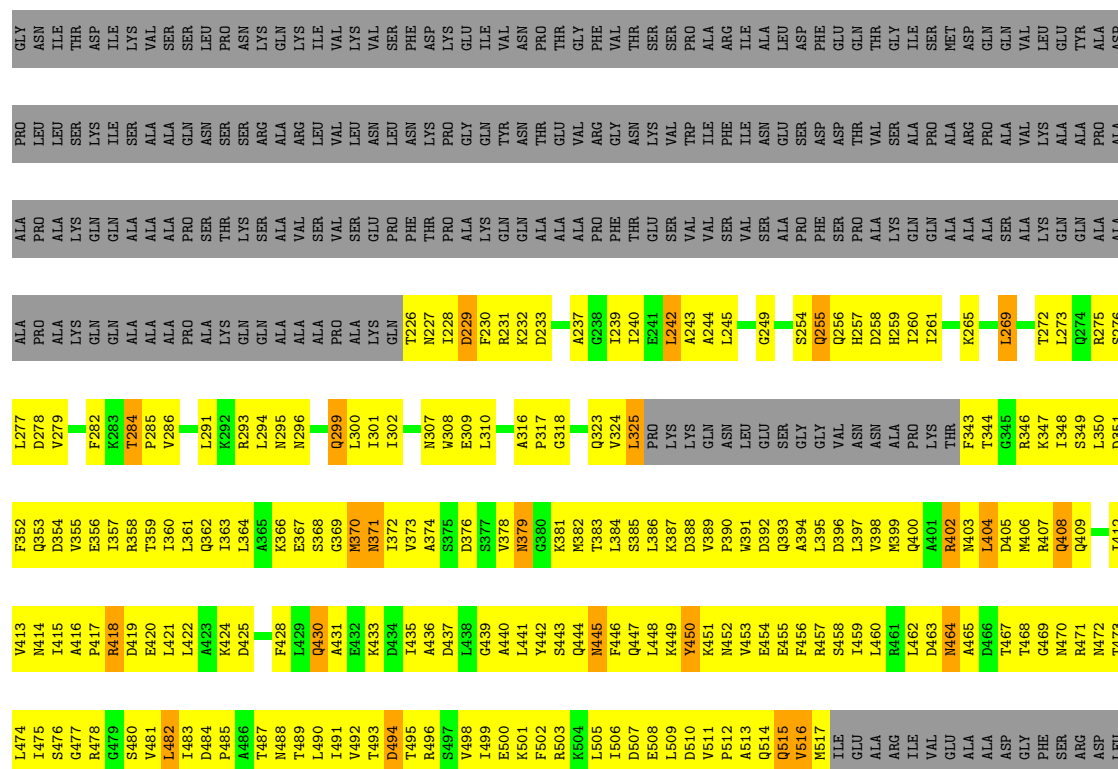
Chain G:  9% 25% 63%

[illegible]



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

Chain H:  9% 25% 0% 63%



[illegible]

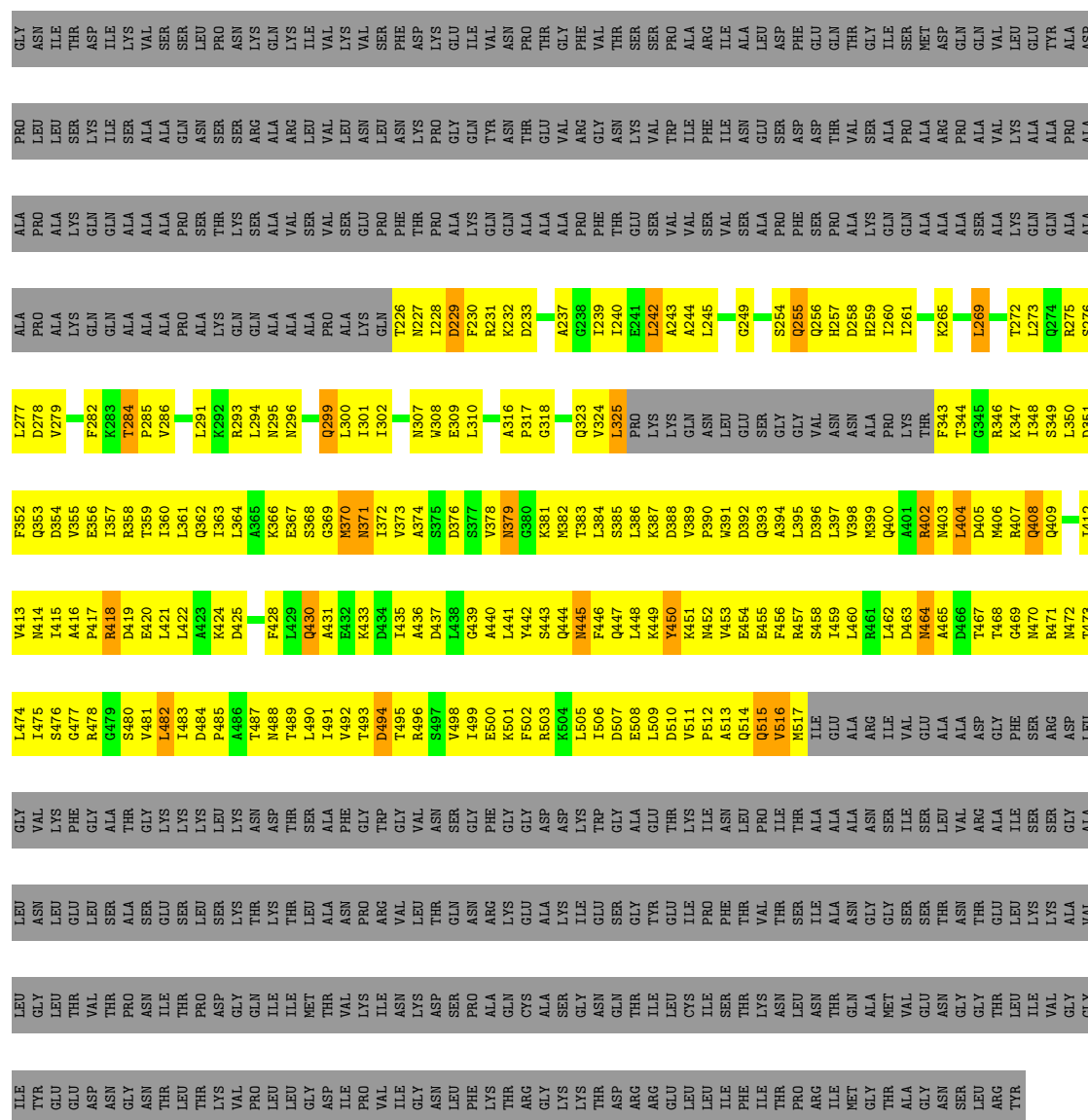
- Molecule 1: TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ

Chain I: 9% 25% . 63%

[illegible]

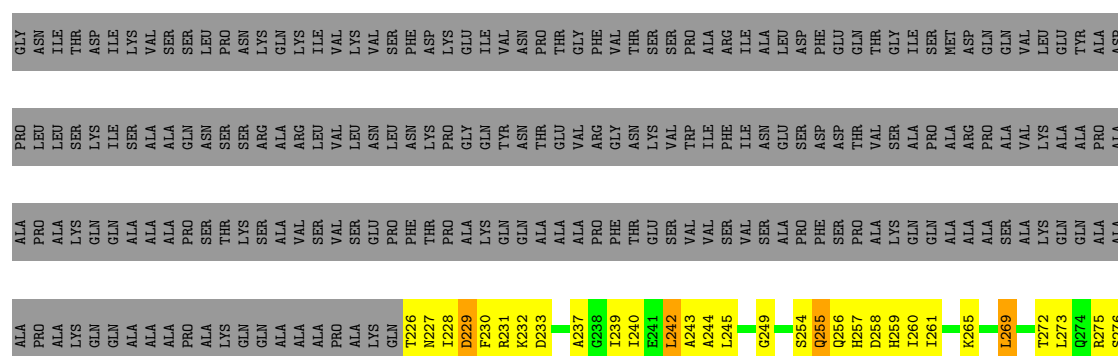
- Molecule 1: TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ

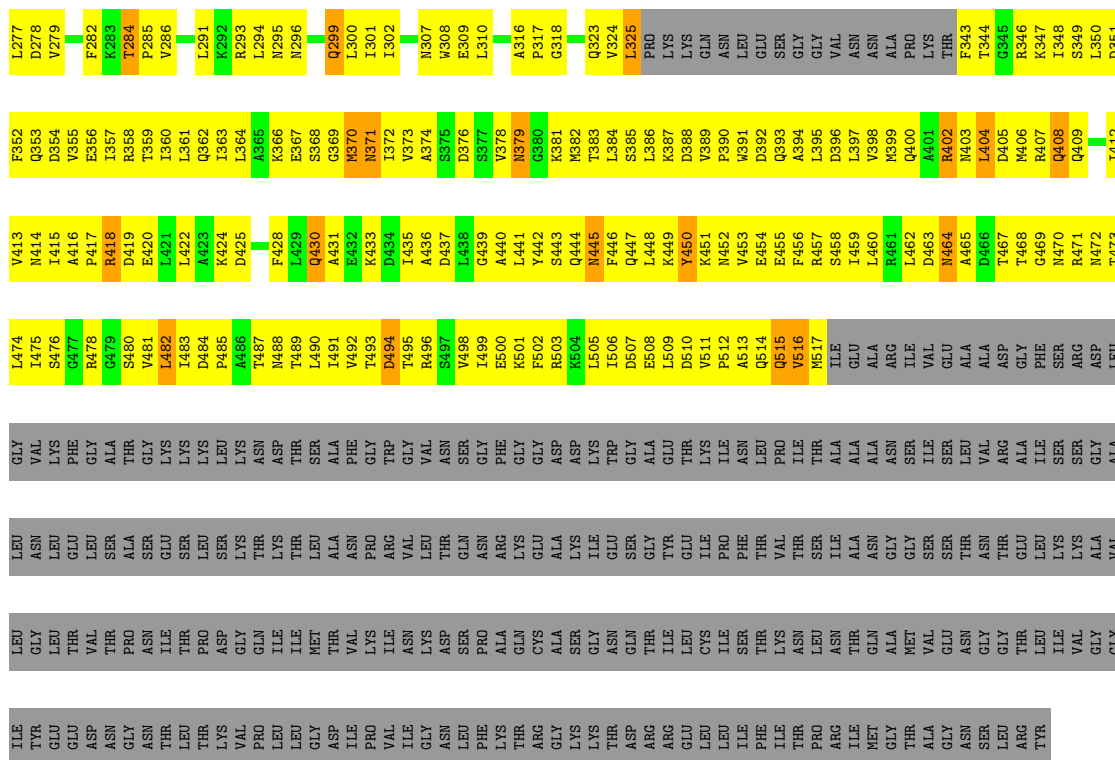
Chain J:  9% 25% . 63%



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

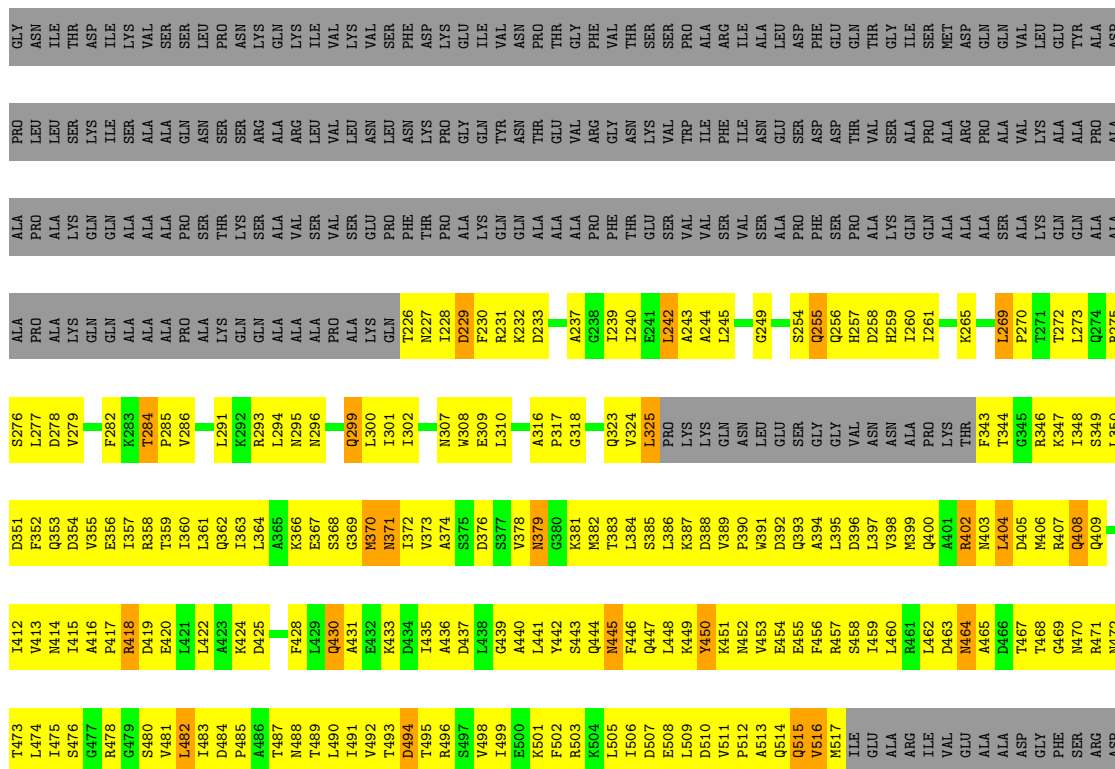
Chain K:  9% 25% . 63%





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

Chain L:  9% 25% . 63%




[illegible]

- Molecule 2: PILP PROTEIN

Chain M: 10% 27% 8% 55%

GL23	GL24	GL25	GL26	GL27	GL28	GL29	GL30	GL31	GL32	GL33	GL34	GL35	GL36	GL37	GL38	GL39	GL40	GL41	GL42	GL43	GL44	GL45	GL46	GL47	GL48	GL49	GL50	GL51	GL52	GL53	GL54	GL55	GL56	GL57	GL58	GL59	GL60	GL61	GL62	GL63	GL64	GL65	GL66	GL67	GL68	GL69	GL70	GL71	GL72	GL73	GL74	GL75	GL76	GL77	GL78	GL79	GL80	GL81	GL82	GL83	GL84	GL85	GL86	GL87	GL88	GL89	GL90	GL91	GL92	GL93	GL94	GL95	GL96	GL97	GL98	GL99	GL100	GL101	GL102	GL103	GL104	GL105	GL106	GL107	GL108	GL109	GL110	GL111	GL112	GL113	GL114	GL115	GL116	GL117	GL118	GL119	GL120	GL121	GL122	GL123	GL124	GL125	GL126	GL127	GL128	GL129	GL130	GL131	GL132	GL133	GL134	GL135	GL136	GL137	GL138	GL139	GL140	GL141	GL142	GL143	GL144	GL145	GL146	GL147	GL148	GL149	GL150	GL151	GL152	GL153	GL154	GL155	GL156	GL157	GL158	GL159	GL160	GL161	GL162	GL163	GL164	GL165	GL166	GL167	GL168	GL169	GL170	GL171	GL172	GL173	GL174	GL175	GL176	GL177	GL178	GL179	GL180	GL181	GL182	GL183	GL184	GL185	GL186	GL187	GL188	GL189	GL190	GL191	GL192	GL193	GL194	GL195	GL196	GL197	GL198	GL199	GL200	GL201	GL202	GL203	GL204	GL205	GL206	GL207	GL208	GL209	GL210	GL211	GL212	GL213	GL214	GL215	GL216	GL217	GL218	GL219	GL220	GL221	GL222	GL223	GL224	GL225	GL226	GL227	GL228	GL229	GL230	GL231	GL232	GL233	GL234	GL235	GL236	GL237	GL238	GL239	GL240	GL241	GL242	GL243	GL244	GL245	GL246	GL247	GL248	GL249	GL250	GL251	GL252	GL253	GL254	GL255	GL256	GL257	GL258	GL259	GL260	GL261	GL262	GL263	GL264	GL265	GL266	GL267	GL268	GL269	GL270	GL271	GL272	GL273	GL274	GL275	GL276	GL277	GL278	GL279	GL280	GL281	GL282	GL283	GL284	GL285	GL286	GL287	GL288	GL289	GL290	GL291	GL292	GL293	GL294	GL295	GL296	GL297	GL298	GL299	GL300	GL301	GL302	GL303	GL304	GL305	GL306	GL307	GL308	GL309	GL310	GL311	GL312	GL313	GL314	GL315	GL316	GL317	GL318	GL319	GL320	GL321	GL322	GL323	GL324	GL325	GL326	GL327	GL328	GL329	GL330	GL331	GL332	GL333	GL334	GL335	GL336	GL337	GL338	GL339	GL340	GL341	GL342	GL343	GL344	GL345	GL346	GL347	GL348	GL349	GL350	GL351	GL352	GL353	GL354	GL355	GL356	GL357	GL358	GL359	GL360	GL361	GL362	GL363	GL364	GL365	GL366	GL367	GL368	GL369	GL370	GL371	GL372	GL373	GL374	GL375	GL376	GL377	GL378	GL379	GL380	GL381	GL382	GL383	GL384	GL385	GL386	GL387	GL388	GL389	GL390	GL391	GL392	GL393	GL394	GL395	GL396	GL397	GL398	GL399	GL400	GL401	GL402	GL403	GL404	GL405	GL406	GL407	GL408	GL409	GL410	GL411	GL412	GL413	GL414	GL415	GL416	GL417	GL418	GL419	GL420	GL421	GL422	GL423	GL424	GL425	GL426	GL427	GL428	GL429	GL430	GL431	GL432	GL433	GL434	GL435	GL436	GL437	GL438	GL439	GL440	GL441	GL442	GL443	GL444	GL445	GL446	GL447	GL448	GL449	GL450	GL451	GL452	GL453	GL454	GL455	GL456	GL457	GL458	GL459	GL460	GL461	GL462	GL463	GL464	GL465	GL466	GL467	GL468	GL469	GL470	GL471	GL472	GL473	GL474	GL475	GL476	GL477	GL478	GL479	GL480	GL481	GL482	GL483	GL484	GL485	
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- Molecule 2: PILP PROTEIN

Chain N: 


GL23	GL123	ASN	MET
M124	ALA	ALA	HIS
Y125	PHE	PHE	TYR
GL126	ASP	ASP	ALA
GL127	PHE	ARG	LEU
GL128	ARG	ARG	LEU
GL129	MET	MET	ILE
Y130	GLU	GLU	SER
GL131	THR	THR	PHE
GL132	THR	ASP	LEU
GL133	ASP	LYS	ALA
GL134	LYS	LYS	LEU
GL135	GLY	GLY	SER
GL136	GLU	GLU	ALA
GL137	GLU	ASN	CYS
GL138	ASN	ALA	SER
GL139	ALA	PRO	GLN
GL140	PRO	ASP	GLY
GL141	ASP	THR	SER
GL142	THR	LYS	GLU
GL143	GLU	ARG	ASP
GL144	ARG	ILE	ASN
GL145	ILE	K84	ASN
GL146	ILE	E85	GLU
GL147	ILE	T86	TRP
GL148	TRP	L87	MET
GL149	TRP	E88	ALA
GL150	ALA	K89	ALA
GL151	ALA	E89	GLN
GL152	GLN	F90	THR
GL153	THR	S91	ARG
GL154	ARG	L92	ARG
GL155	ARG	L93	GLU
GL156	GLU	M95	ALA
GL157	ALA	R96	LYS
GL158	LYS	Y97	ALA
GL159	ALA	V98	GLU
GL160	GLU	G99	ILE
GL161	ILE	I100	ILE
GL162	ILE	L101	ILE
GL163	ILE	K102	PHE
GL164	PHE	L103	PRO
GL165	PRO	G104	GLN
GL166	GLN	Q105	ALA
GL167	ALA	K106	PRO
GL168	PRO	V107	THR
GL169	THR	L108	LEU
GL170	LEU	S108	PRO
GL171	PRO	G109	VAL
GL172	VAL	F110	ALA
GL173	ALA	I111	ALA
GL174	ALA	E112	VAL
GL175	VAL	A113	TYR
GL176	TYR	E114	SER
GL177	SER	PRO	PRO
GL178	PRO	V117	PRO
GL179	PRO	V118	GLN
GL180	GLN	T119	LEU
GL181	LEU	V120	THR
GL182	THR	GLN	GLY
GL183	GLY	G121	GLY
GL184	GLY	V122	GLY

- Molecule 2: PILP PROTEIN

Chain O:


ASN	ALA	PHE	ASP	PHE	ARG	ARG	MET	GLU	THR	ASP	LYS	LYS	LEU	LEU	GLY	ASN	GLU	TRP	MET	ALA	GLN	THR	ARG	ARG	GLU	ALA	LYS	ALA	LYS	MET																											
G123	N124	Y125	L126	G127	Q128	N129	Y130	G131	R132	I133	E134	S135	I136	T137	D138	D139	I140	I141	V142	L143	N144	E145	L146	L147	E148	D149	S150	G151	G152	N153	V154	S155	S156	R157	K158	A159	E160	L161	L162	L163	N164	S165	SER	ASP	LYS	THR	ASN	THR	GLN	ALA	VAL	PRO	GLN	PRO	GLN	THR	GLY

- Molecule 2: PILP PROTEIN

Chain P:  11% 27% 8% 55%


ASN	ALA	PHE	ASP	PHE	ARG	ARG	MET	THR	THR	ASP	LYS	LYS	GLY	GLU	ASN	ALA	PRO	THR	ILE	K84	E85	T86	L87	E88	S91	L92	M95	R96	Y97	V98	G99	I100	L101	K102	S103	G104	Q105	K106	V107	S108	G109	F110	I111	E112	A113	V117	Y118	T119	V120	G121	V122	G123	N124				
MET	LYS	HIS	TYR	ALA	LEU	LEU	ILE	SER	PHE	LEU	LEU	ALA	SER	GLN	GLY	SER	GLU	ASP	LEU	ILE	ASN	TRP	MET	ALA	GLN	THR	ARG	ARG	GLU	LYS	ALA	LYS	ALA	GLU	ILE	PRO	PHE	GLN	ALA	PRO	THR	LEU	VAL	ALA	PRO	VAL	TYR	SER	PRO	GLN	LEU	THR	GLY	PRO			
Y125	L126	G127	Q128	M129	Y130	G131	R132	I133	E134	S135	I136	T137	D138	D139	S140	I141	V142	L143	N144	E145	L146	I147	E148	D149	S150	T151	G152	N153	W154	V155	S156	R157	K158	A159	E160	L161	L162	L163	N164	S165	SER	GLN	ALA	PRO	LYS	ASN	THR	GLU	GLN	ALA	ALA	PRO	TYR	ALA	ALA	GLN	ASN

- Molecule 2: PILP PROTEIN

Chain Q:  12% 25% 8% 55%


MET	LYS	HIS	TYR	ALA	LEU	LEU	ILE	SER	PHE	LEU	LEU	ALA	SER	GLN	GLY	SER	GLU	ASP	LEU	ILE	ASN	TRP	MET	ALA	GLN	THR	ARG	ARG	GLU	LYS	ALA	LYS	ALA	GLU	ILE	PRO	PHE	GLN	ALA	PRO	THR	LEU	VAL	ALA	PRO	VAL	TYR	SER	PRO	GLN	LEU	THR	GLY	PRO			
ASN	ALA	PHE	ASP	PHE	ARG	ARG	MET	THR	THR	ASP	LYS	LYS	GLY	GLU	ASN	ALA	PRO	ASP	THR	ILE	K84	E85	T86	L87	E88	S91	L92	M95	R96	Y97	V98	G99	I100	L101	K102	S103	G104	Q105	K106	V107	S108	G109	F110	I111	E112	A113	V117	Y118	T119	V120	G121	V122	G123	N124			
Y125	L126	G127	Q128	N129	Y130	G131	R132	I133	E134	S135	I136	T137	D138	D139	S140	I141	V142	L143	N144	E145	L146	I147	E148	D149	S150	T151	G152	N153	W154	V155	S156	R157	K158	A159	E160	L161	L162	L163	N164	S165	SER	GLN	ALA	PRO	LYS	ASN	THR	GLU	GLN	ALA	ALA	PRO	TYR	ALA	ALA	GLN	ASN

- Molecule 2: PILP PROTEIN

Chain R:  10% 28% 8% 55%


MET	LYS	HIS	TYR	ALA	LEU	LEU	ILE	SER	PHE	LEU	LEU	ALA	SER	GLY	SER	GLU	ASP	LEU	ILE	ASN	GLU	TRP	MET	ALA	GLN	THR	ARG	ARG	GLU	LYS	ALA	LYS	ALA	GLU	ILE	PRO	PHE	GLN	ALA	PRO	THR	LEU	VAL	ALA	PRO	GLN	LEU	THR	GLY	PRO								
ASN	ALA	PHE	ASP	PHE	ARG	ARG	MET	GLU	THR	ASP	LYS	LYS	GLY	GLU	ASN	ALA	PRO	THR	LYS	ILE	K84	E85	T86	L87	E88	K89	F90	S91	L92		M95	R96	Y97	V98	G99	I100	L101	K102	S103	G104	Q105	K106	V107	S108	G109	F110	I111	E112	A113	E114		V117	Y118	T119	V120	G121	V122	
G123	N124	Y125	L126	Q127	N129	Y130	G131	R132	I133	E134	S135	I136	T137	D138	D139	S140	I141	V142	L143	N144	E145	L146	I147	E148	D149	S150	T151	G152	N153	W154	V155	S156	R157	K158	A159	E160	L161	L162	L163	N164	S165	SER	GLN	ALA	PRO	LYS	ASN	THR	GLU	GLN	ALA	ALA	PRO	TYR	ALA	ALA	GLN	ASN

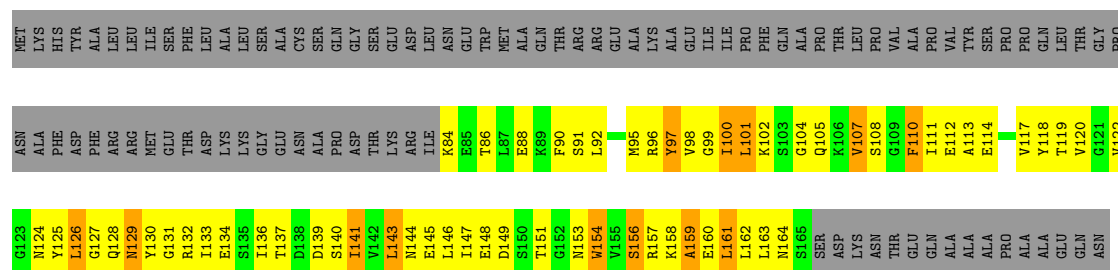
- Molecule 2: PILP PROTEIN

Chain S:  11% 26% 8% 55%

MET	LYS	HIS	TYR	ALA	LEU	LEU	ILE	SER	PHE	LEU	LEU	ALA	SER	GLY	SER	GLU	ASP	LEU	ILE	ASN	TRP	MET	ALA	GLN	THR	ARG	ARG	GLU	LYS	ALA	LYS	ALA	GLU	ILE	PRO	PHE	GLN	ALA	PRO	THR	LEU	VAL	ALA	PRO	VAL	TYR	SER	PRO	GLN	LEU	THR	GLY	PRO					
ASN	ALA	PHE	ASP	PHE	ARG	ARG	MET	GLU	THR	ASP	LYS	LYS	GLY	GLU	ASN	ALA	PRO	THR	ILE	K84	E85	T86	L87	E88	K89	F90	S91	L92	M95	R96	Y97	V98	G99	I100	L101	K102	S103	G104	Q105	K106	V107	S108	G109	F110	I111	E112	A113	E114	V117	Y118	T119	V120	G121	V122				
G123	N124	Y125	L126	Q127	N129	Y130	G131	R132	I133	E134	S135	I136	T137	D138	D139	S140	I141	V142	L143	N144	E145	L146	I147	E148	D149	S150	T151	G152	N153	W154	V155	S156	R157	K158	A159	E160	L161	L162	L163	N164	S165	SER	GLN	ALA	PRO	LYS	ASN	THR	GLU	GLN	ALA	ALA	PRO	TYR	ALA	ALA	GLN	ASN

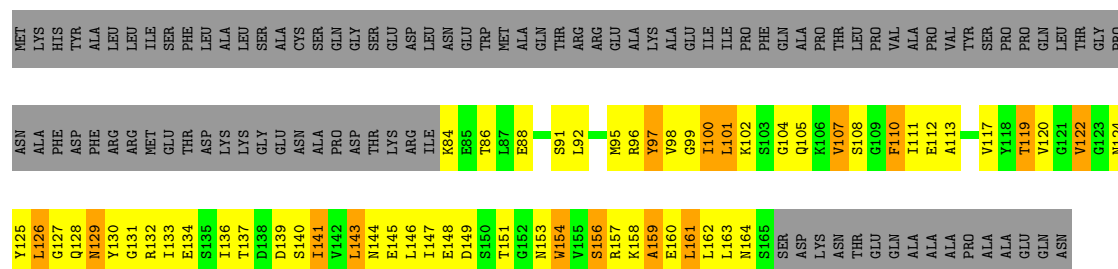
- Molecule 2: PILP PROTEIN

Chain T:  10% 28% 7% 55%



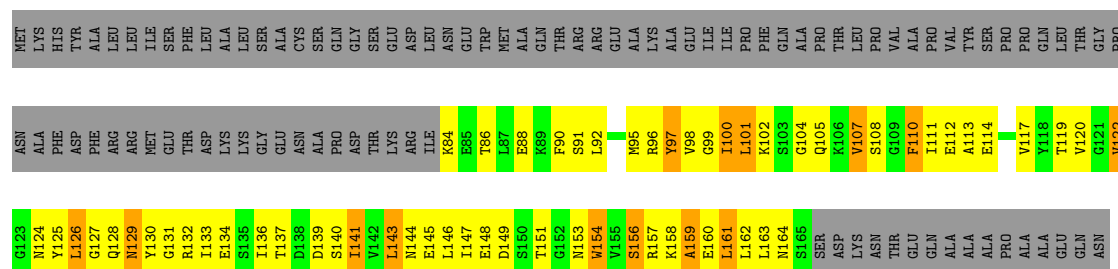
• Molecule 2: PILP PROTEIN

Chain U: 12% 25% 8% 55%



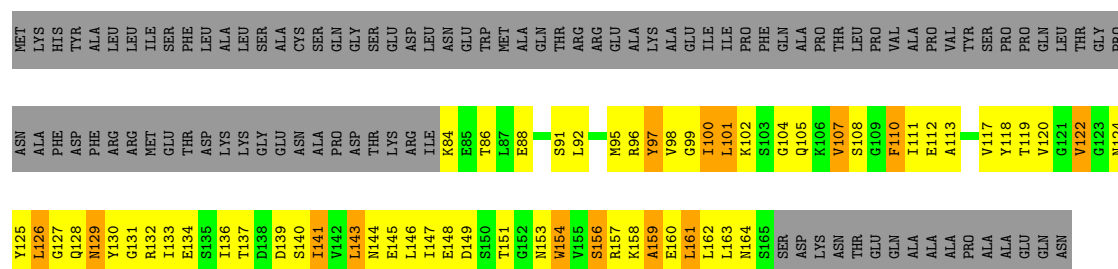
• Molecule 2: PILP PROTEIN

Chain V: 11% 27% 8% 55%



• Molecule 2: PILP PROTEIN

Chain W: 12% 26% 8% 55%



• Molecule 2: PILP PROTEIN

Chain X: 11% 27% 8% 55%

Met	Met	Met
Lys	Lys	Lys
His	His	His
Tyr	Tyr	Tyr
Ala	Ala	Ala
Leu	Leu	Leu
Leu	Leu	Leu
Ile	Ile	Ile
Ser	Ser	Ser
Phe	Phe	Phe
Leu	Leu	Leu
Ala	Ala	Ala
Leu	Leu	Leu
Ser	Ser	Ser
Ala	Ala	Ala
Cys	Cys	Cys
Ser	Ser	Ser
Gln	Gln	Gln
Gly	Gly	Gly
Ser	Ser	Ser
Glu	Glu	Glu
Asp	Asp	Asp
Leu	Leu	Leu
Asn	Asn	Asn
Glu	Glu	Glu
Trp	Trp	Trp
Met	Met	Met
Ala	Ala	Ala
Gln	Gln	Gln
Thr	Thr	Thr
Arg	Arg	Arg
Arg	Arg	Arg
Glu	Glu	Glu
Ala	Ala	Ala
Lys	Lys	Lys
Ala	Ala	Ala
Glu	Glu	Glu
Ile	Ile	Ile
Phe	Phe	Phe
Gln	Gln	Gln
Ala	Ala	Ala
Pro	Pro	Pro
Thr	Thr	Thr
Leu	Leu	Leu
Pro	Pro	Pro
Val	Val	Val
Ala	Ala	Ala
Pro	Pro	Pro
Val	Val	Val
Tyr	Tyr	Tyr
Ser	Ser	Ser
Pro	Pro	Pro
Pro	Pro	Pro
Gln	Gln	Gln
Leu	Leu	Leu
Thr	Thr	Thr
Gly	Gly	Gly
Pro	Pro	Pro

Asn	Asn	Asn
Ala	Ala	Ala
Phe	Phe	Phe
Asp	Asp	Asp
Phe	Phe	Phe
Arg	Arg	Arg
Arg	Arg	Arg
Met	Met	Met
Glu	Glu	Glu
Thr	Thr	Thr
Asp	Asp	Asp
Lys	Lys	Lys
Lys	Lys	Lys
Gly	Gly	Gly
Ala	Ala	Ala
Asn	Asn	Asn
Ala	Ala	Ala
Pro	Pro	Pro
Asp	Asp	Asp
Thr	Thr	Thr
Lys	Lys	Lys
Ile	Ile	Ile
K84	K84	K84
F85	F85	F85
T86	T86	T86
L87	L87	L87
E88	E88	E88
K89	K89	K89
F90	F90	F90
S91	S91	S91
L92	L92	L92
M95	M95	M95
R96	R96	R96
Y97	Y97	Y97
V98	V98	V98
G99	G99	G99
I100	I100	I100
L101	L101	L101
K102	K102	K102
S103	S103	S103
G104	G104	G104
Q105	Q105	Q105
K106	K106	K106
V107	V107	V107
S108	S108	S108
G109	G109	G109
F110	F110	F110
I111	I111	I111
E112	E112	E112
A113	A113	A113
E114	E114	E114
V117	V117	V117
Y118	Y118	Y118
T119	T119	T119
V120	V120	V120
G121	G121	G121
V122	V122	V122

G123	G123	G123
N124	N124	N124
Y125	Y125	Y125
L126	L126	L126
G127	G127	G127
Q128	Q128	Q128
M129	M129	M129
Y130	Y130	Y130
G131	G131	G131
R132	R132	R132
I133	I133	I133
E134	E134	E134
S135	S135	S135
I136	I136	I136
T137	T137	T137
D138	D138	D138
D139	D139	D139
S140	S140	S140
I141	I141	I141
V142	V142	V142
L143	L143	L143
N144	N144	N144
E145	E145	E145
L146	L146	L146
I147	I147	I147
E148	E148	E148
D149	D149	D149
S150	S150	S150
T151	T151	T151
G152	G152	G152
N153	N153	N153
W154	W154	W154
V155	V155	V155
S156	S156	S156
R157	R157	R157
K158	K158	K158
A159	A159	A159
E160	E160	E160
L161	L161	L161
L162	L162	L162
L163	L163	L163
N164	N164	N164
S165	S165	S165
Ser	Ser	Ser
Asp	Asp	Asp
Lys	Lys	Lys
Asn	Asn	Asn
Thr	Thr	Thr
Glu	Glu	Glu
Gln	Gln	Gln
Ala	Ala	Ala
Ala	Ala	Ala
Ala	Ala	Ala
Pro	Pro	Pro
Ala	Ala	Ala
Ala	Ala	Ala
Glu	Glu	Glu
Gln	Gln	Gln
Asn	Asn	Asn

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTFFIT EACH MICROGRAPH	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	33112	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%)	6	40
1	B	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	6	40
1	C	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	6	40
1	D	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	6	40
1	E	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	6	40
1	F	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	6	40
1	G	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	6	40
1	H	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	6	40
1	I	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	6	40
1	J	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	6	40
1	K	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	6	40
1	L	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	6	40
2	M	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	7
2	O	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	7
2	P	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	7
2	Q	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	7
2	R	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	7
2	S	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	7
2	T	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	7
2	U	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	7
2	V	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	7
2	W	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	7
2	X	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	7
All	All	4212/11112 (38%)	3432 (82%)	576 (14%)	204 (5%)	5	28

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	35
1	B	239/615 (39%)	216 (90%)	23 (10%)	10	35
1	C	239/615 (39%)	216 (90%)	23 (10%)	10	35
1	D	239/615 (39%)	216 (90%)	23 (10%)	10	35
1	E	239/615 (39%)	216 (90%)	23 (10%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	239/615 (39%)	216 (90%)	23 (10%)	10	35
1	G	239/615 (39%)	216 (90%)	23 (10%)	10	35
1	H	239/615 (39%)	216 (90%)	23 (10%)	10	35
1	I	239/615 (39%)	216 (90%)	23 (10%)	10	35
1	J	239/615 (39%)	216 (90%)	23 (10%)	10	35
1	K	239/615 (39%)	216 (90%)	23 (10%)	10	35
1	L	239/615 (39%)	216 (90%)	23 (10%)	10	35
2	M	71/152 (47%)	59 (83%)	12 (17%)	2	16
2	N	71/152 (47%)	59 (83%)	12 (17%)	2	16
2	O	71/152 (47%)	59 (83%)	12 (17%)	2	16
2	P	71/152 (47%)	59 (83%)	12 (17%)	2	16
2	Q	71/152 (47%)	59 (83%)	12 (17%)	2	16
2	R	71/152 (47%)	59 (83%)	12 (17%)	2	16
2	S	71/152 (47%)	59 (83%)	12 (17%)	2	16
2	T	71/152 (47%)	59 (83%)	12 (17%)	2	16
2	U	71/152 (47%)	59 (83%)	12 (17%)	2	16
2	V	71/152 (47%)	59 (83%)	12 (17%)	2	16
2	W	71/152 (47%)	59 (83%)	12 (17%)	2	16
2	X	71/152 (47%)	59 (83%)	12 (17%)	2	16
All	All	3720/9204 (40%)	3300 (89%)	420 (11%)	11	29

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 [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 carbohydrates 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.