



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 01:15 PM UTC

PDB ID : 3JC8 / pdb_00003jc8
EMDB ID : EMD-3247
Title : Architectural model of the type IVa pilus machine in a piliated state
Authors : Chang, Y.-W.; Rettberg, L.A.; Jensen, G.J.
Deposited on : 2015-11-24
Resolution : Not provided

This is a wwPDB EM Validation Summary 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

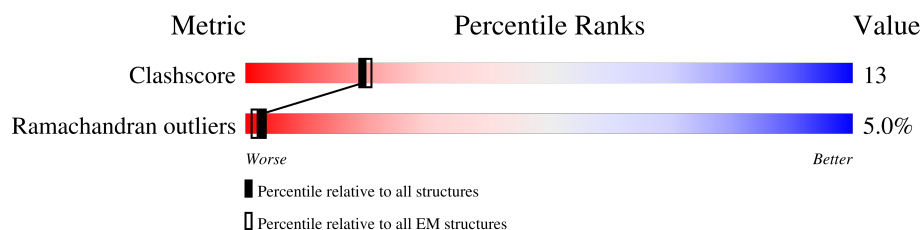
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

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.



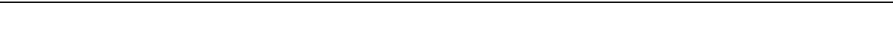
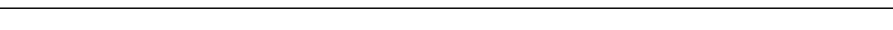
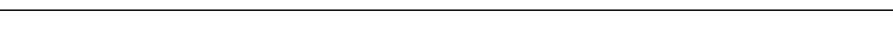
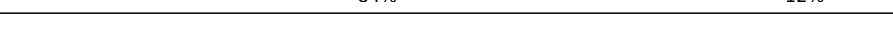
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A1	158	 84% 13% .
1	A2	158	 86% 10% .
1	A3	158	 85% 11% .
1	A4	158	 84% 12% .
1	A5	158	 85% 11% .
1	A6	158	 86% 11% .
1	A7	158	 85% 11% .
1	A8	158	 87% 10% .
1	A9	158	 86% 10% .
1	Aa	158	 82% 14% .

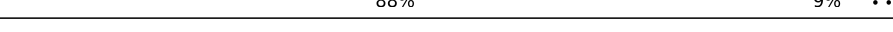
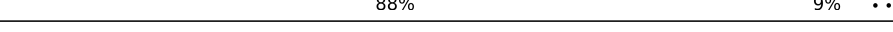
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Mol	Chain	Length	Quality of chain
1	Ab	158	 85% 11% .
1	Ac	158	 85% 11% .
1	Ad	158	 85% 11% .
1	Ae	158	 85% 11% .
1	Af	158	 85% 11% .
1	Ag	158	 85% 11% .
1	Ah	158	 84% 13% .
1	Ai	158	 85% 11% .
1	Aj	158	 85% 11% .
1	Ak	158	 85% 11% .
1	Al	158	 85% 11% .
1	Am	158	 85% 11% .
1	An	158	 83% 12% 5% .
1	Ao	158	 84% 12% .
1	Ap	158	 85% 11% .
1	Aq	158	 86% 10% .
1	Ar	158	 85% 11% .
1	As	158	 86% 11% .
1	At	158	 84% 12% .
1	Au	158	 84% 13% .
1	Av	158	 84% 13% .
1	Aw	158	 85% 11% .
1	Ax	158	 85% 11% .
1	Ay	158	 86% 11% .
1	Az	158	 84% 12% .

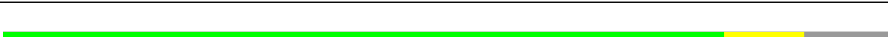
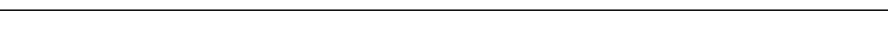
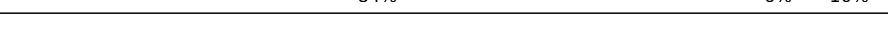
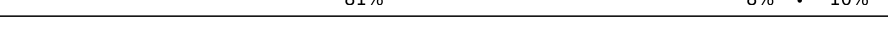
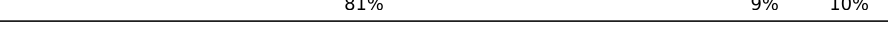
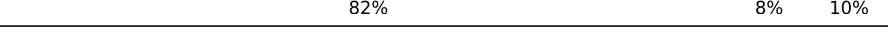
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Mol	Chain	Length	Quality of chain
2	Ba	566	
2	Bb	566	
2	Bc	566	
2	Bd	566	
2	Be	566	
2	Bf	566	
3	Ca	417	
3	Cb	417	
4	Na	225	
4	Nb	225	
4	Nc	225	
4	Nd	225	
4	Ne	225	
4	Nf	225	
4	Ng	225	
4	Nh	225	
4	Ni	225	
4	Nj	225	
4	Nk	225	
4	Nl	225	
5	Oa	205	
5	Ob	205	
5	Oc	205	
5	Od	205	
5	Oe	205	

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Mol	Chain	Length	Quality of chain
5	Of	205	 89% • 8%
5	Og	205	 89% • 8%
5	Oh	205	 89% •• 8%
5	Oi	205	 87% •• 8%
5	Oj	205	 88% • 8%
5	Ok	205	 87% • 8%
5	Ol	205	 88% •• 8%
6	Ma	395	 84% 5% • 10%
6	Mb	395	 81% 9% 10%
6	Mc	395	 84% 5% • 10%
6	Md	395	 81% 9% 10%
6	Me	395	 83% 6% 10%
6	Mf	395	 82% 8% 10%
6	Mg	395	 84% 6% 10%
6	Mh	395	 81% 8% • 10%
6	Mi	395	 83% 6% 10%
6	Mj	395	 81% 9% 10%
6	Mk	395	 84% 6% 10%
6	Ml	395	 82% 8% 10%
7	Qa	901	 40% 5% • 54%
7	Qb	901	 40% 5% • 54%
7	Qc	901	 40% 5% • 54%
7	Qd	901	 40% 5% • 54%
7	Qe	901	 40% 5% • 54%
7	Qf	901	 40% 5% • 54%

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Mol	Chain	Length	Quality of chain
7	Qg	901	
7	Qh	901	
7	Qi	901	
7	Qj	901	
7	Qk	901	
7	Ql	901	
8	Pa	172	
8	Pb	172	
8	Pc	172	
8	Pd	172	
8	Pe	172	
8	Pf	172	
8	Pg	172	
8	Ph	172	
8	Pi	172	
8	Pj	172	
8	Pk	172	
8	Pl	172	
9	Ta	411	
9	Tb	411	
9	Tc	411	
9	Td	411	
9	Te	411	
9	Tf	411	
9	Tg	411	

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Mol	Chain	Length	Quality of chain
9	Th	411	 32% 8% 60%
9	Ti	411	 31% 9% 60%
9	Tj	411	 31% 8% 60%
9	Tk	411	 31% 8% 60%
9	Tl	411	 31% 8% 60%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 107640 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 Pila.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	Aa	158	Total 632	C 316	N 158	O 158	0	0
1	Ab	158	Total 632	C 316	N 158	O 158	0	0
1	Ac	158	Total 632	C 316	N 158	O 158	0	0
1	Ad	158	Total 632	C 316	N 158	O 158	0	0
1	Ae	158	Total 632	C 316	N 158	O 158	0	0
1	Af	158	Total 632	C 316	N 158	O 158	0	0
1	Ag	158	Total 632	C 316	N 158	O 158	0	0
1	Ah	158	Total 632	C 316	N 158	O 158	0	0
1	Ai	158	Total 632	C 316	N 158	O 158	0	0
1	Aj	158	Total 632	C 316	N 158	O 158	0	0
1	Ak	158	Total 632	C 316	N 158	O 158	0	0
1	Al	158	Total 632	C 316	N 158	O 158	0	0
1	Am	158	Total 632	C 316	N 158	O 158	0	0
1	An	158	Total 632	C 316	N 158	O 158	0	0
1	Ao	158	Total 632	C 316	N 158	O 158	0	0
1	Ap	158	Total 632	C 316	N 158	O 158	0	0
1	Aq	158	Total 632	C 316	N 158	O 158	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	Ar	158	Total 632	C 316	N 158	O 158	0	0
1	As	158	Total 632	C 316	N 158	O 158	0	0
1	At	158	Total 632	C 316	N 158	O 158	0	0
1	Au	158	Total 632	C 316	N 158	O 158	0	0
1	Av	158	Total 632	C 316	N 158	O 158	0	0
1	Aw	158	Total 632	C 316	N 158	O 158	0	0
1	Ax	158	Total 632	C 316	N 158	O 158	0	0
1	Ay	158	Total 632	C 316	N 158	O 158	0	0
1	Az	158	Total 632	C 316	N 158	O 158	0	0
1	A1	158	Total 632	C 316	N 158	O 158	0	0
1	A2	158	Total 632	C 316	N 158	O 158	0	0
1	A3	158	Total 632	C 316	N 158	O 158	0	0
1	A4	158	Total 632	C 316	N 158	O 158	0	0
1	A5	158	Total 632	C 316	N 158	O 158	0	0
1	A6	158	Total 632	C 316	N 158	O 158	0	0
1	A7	158	Total 632	C 316	N 158	O 158	0	0
1	A8	158	Total 632	C 316	N 158	O 158	0	0
1	A9	158	Total 632	C 316	N 158	O 158	0	0

- Molecule 2 is a protein called Type IV-A pilus assembly ATPase PilB.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	Ba	452	Total 1808	C 904	N 452	O 452	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	Bb	452	Total	C	N	O	0	0
			1808	904	452	452		
2	Bc	452	Total	C	N	O	0	0
			1808	904	452	452		
2	Bd	452	Total	C	N	O	0	0
			1808	904	452	452		
2	Be	452	Total	C	N	O	0	0
			1808	904	452	452		
2	Bf	452	Total	C	N	O	0	0
			1808	904	452	452		

- Molecule 3 is a protein called Type 4 fimbrial assembly protein PilC.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	Ca	316	Total	C	N	O	0	0
			1264	632	316	316		
3	Cb	316	Total	C	N	O	0	0
			1264	632	316	316		

- Molecule 4 is a protein called PilN.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	Na	223	Total	C	N	O	0	0
			892	446	223	223		
4	Nb	223	Total	C	N	O	0	0
			892	446	223	223		
4	Nc	223	Total	C	N	O	0	0
			892	446	223	223		
4	Nd	223	Total	C	N	O	0	0
			892	446	223	223		
4	Ne	223	Total	C	N	O	0	0
			892	446	223	223		
4	Nf	223	Total	C	N	O	0	0
			892	446	223	223		
4	Ng	223	Total	C	N	O	0	0
			892	446	223	223		
4	Nh	223	Total	C	N	O	0	0
			892	446	223	223		
4	Ni	223	Total	C	N	O	0	0
			892	446	223	223		
4	Nj	223	Total	C	N	O	0	0
			892	446	223	223		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	Nk	223	Total	C	N	O	0	0
			892	446	223	223		
4	Nl	223	Total	C	N	O	0	0
			892	446	223	223		

- Molecule 5 is a protein called PilO.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	Oa	189	Total	C	N	O	0	0
			756	378	189	189		
5	Ob	189	Total	C	N	O	0	0
			756	378	189	189		
5	Oc	189	Total	C	N	O	0	0
			756	378	189	189		
5	Od	189	Total	C	N	O	0	0
			756	378	189	189		
5	Oe	189	Total	C	N	O	0	0
			756	378	189	189		
5	Of	189	Total	C	N	O	0	0
			756	378	189	189		
5	Og	189	Total	C	N	O	0	0
			756	378	189	189		
5	Oh	189	Total	C	N	O	0	0
			756	378	189	189		
5	Oi	189	Total	C	N	O	0	0
			756	378	189	189		
5	Oj	189	Total	C	N	O	0	0
			756	378	189	189		
5	Ok	189	Total	C	N	O	0	0
			756	378	189	189		
5	Ol	189	Total	C	N	O	0	0
			756	378	189	189		

- Molecule 6 is a protein called Type IV pilus biogenesis protein PilM.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	Ma	355	Total	C	N	O	0	0
			1420	710	355	355		
6	Mb	355	Total	C	N	O	0	0
			1420	710	355	355		
6	Mc	355	Total	C	N	O	0	0
			1420	710	355	355		

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	Md	355	Total	C	N	O	0	0
			1420	710	355	355		
6	Me	355	Total	C	N	O	0	0
			1420	710	355	355		
6	Mf	355	Total	C	N	O	0	0
			1420	710	355	355		
6	Mg	355	Total	C	N	O	0	0
			1420	710	355	355		
6	Mh	355	Total	C	N	O	0	0
			1420	710	355	355		
6	Mi	355	Total	C	N	O	0	0
			1420	710	355	355		
6	Mj	355	Total	C	N	O	0	0
			1420	710	355	355		
6	Mk	355	Total	C	N	O	0	0
			1420	710	355	355		
6	ML	355	Total	C	N	O	0	0
			1420	710	355	355		

- Molecule 7 is a protein called PilQ.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	Qa	418	Total	C	N	O	0	0
			1672	836	418	418		
7	Qb	418	Total	C	N	O	0	0
			1672	836	418	418		
7	Qc	418	Total	C	N	O	0	0
			1672	836	418	418		
7	Qd	418	Total	C	N	O	0	0
			1672	836	418	418		
7	Qe	418	Total	C	N	O	0	0
			1672	836	418	418		
7	Qf	418	Total	C	N	O	0	0
			1672	836	418	418		
7	Qg	418	Total	C	N	O	0	0
			1672	836	418	418		
7	Qh	418	Total	C	N	O	0	0
			1672	836	418	418		
7	Qi	418	Total	C	N	O	0	0
			1672	836	418	418		
7	Qj	418	Total	C	N	O	0	0
			1672	836	418	418		

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Mol	Chain	Residues	Atoms				AltConf	Trace
7	Qk	418	Total	C	N	O	0	0
			1672	836	418	418		
7	Ql	418	Total	C	N	O	0	0
			1672	836	418	418		

- Molecule 8 is a protein called PilP.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	Pa	155	Total	C	N	O	0	0
			620	310	155	155		
8	Pb	155	Total	C	N	O	0	0
			620	310	155	155		
8	Pc	155	Total	C	N	O	0	0
			620	310	155	155		
8	Pd	155	Total	C	N	O	0	0
			620	310	155	155		
8	Pe	155	Total	C	N	O	0	0
			620	310	155	155		
8	Pf	155	Total	C	N	O	0	0
			620	310	155	155		
8	Pg	155	Total	C	N	O	0	0
			620	310	155	155		
8	Ph	155	Total	C	N	O	0	0
			620	310	155	155		
8	Pi	155	Total	C	N	O	0	0
			620	310	155	155		
8	Pj	155	Total	C	N	O	0	0
			620	310	155	155		
8	Pk	155	Total	C	N	O	0	0
			620	310	155	155		
8	Pl	155	Total	C	N	O	0	0
			620	310	155	155		

- Molecule 9 is a protein called LysM domain protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	Ta	163	Total	C	N	O	0	0
			652	326	163	163		
9	Tb	163	Total	C	N	O	0	0
			652	326	163	163		
9	Tc	163	Total	C	N	O	0	0
			652	326	163	163		

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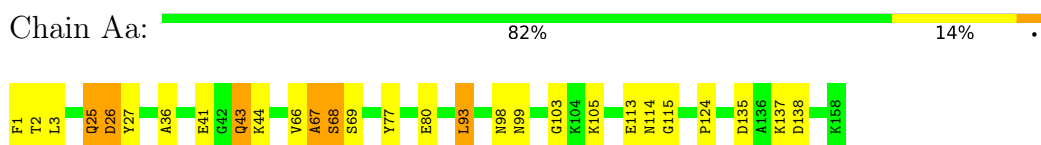
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Mol	Chain	Residues	Atoms				AltConf	Trace
9	Td	163	Total 652	C 326	N 163	O 163	0	0
9	Te	163	Total 652	C 326	N 163	O 163	0	0
9	Tf	163	Total 652	C 326	N 163	O 163	0	0
9	Tg	163	Total 652	C 326	N 163	O 163	0	0
9	Th	163	Total 652	C 326	N 163	O 163	0	0
9	Ti	163	Total 652	C 326	N 163	O 163	0	0
9	Tj	163	Total 652	C 326	N 163	O 163	0	0
9	Tk	163	Total 652	C 326	N 163	O 163	0	0
9	Tl	163	Total 652	C 326	N 163	O 163	0	0

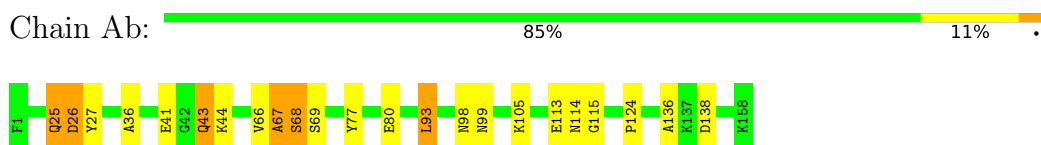
3 Residue-property plots [i](#)

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. 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.

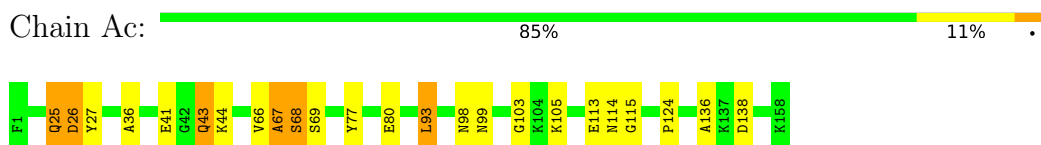
- Molecule 1: PilA



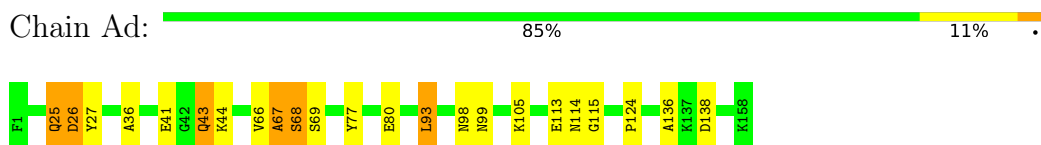
- Molecule 1: PilA



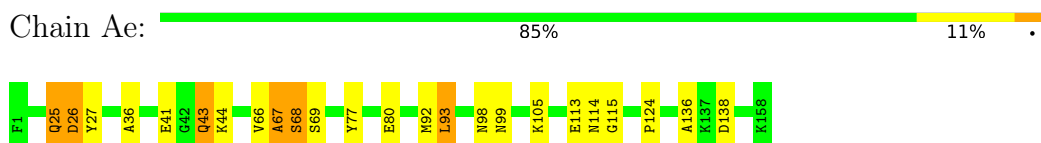
- Molecule 1: PilA



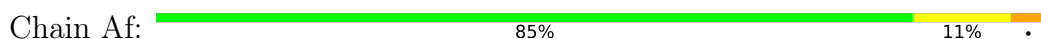
- Molecule 1: PilA



- Molecule 1: PilA

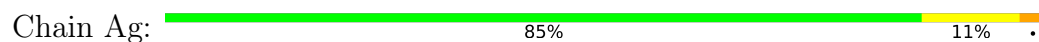


- Molecule 1: PilA

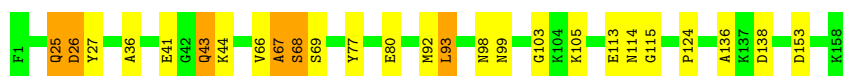
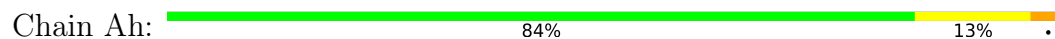




- Molecule 1: PilA



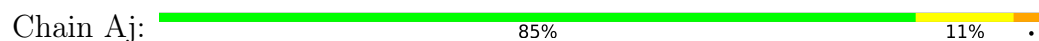
- Molecule 1: PilA



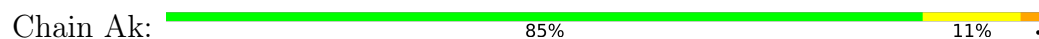
- Molecule 1: PilA



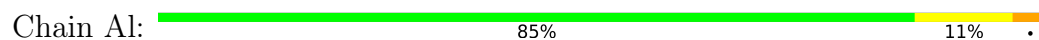
- Molecule 1: PilA



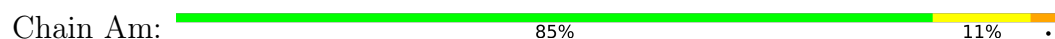
- Molecule 1: PilA



- Molecule 1: PilA



- Molecule 1: PilA





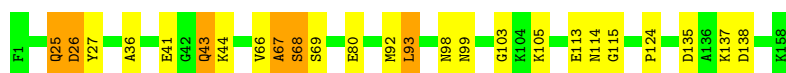
- Molecule 1: PilA

Chain An: 83% 12% 5%



- Molecule 1: PilA

Chain Ao: 84% 12% .



- Molecule 1: PilA

Chain Ap: 85% 11% .



- Molecule 1: PilA

Chain Aq: 86% 10% .



- Molecule 1: PilA

Chain Ar: 85% 11% .



- Molecule 1: PilA

Chain As: 86% 11% .



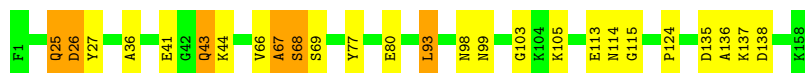
- Molecule 1: PilA

Chain At: 84% 12% .



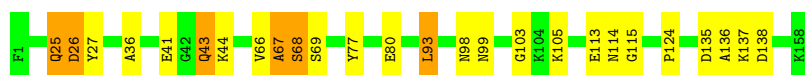
- Molecule 1: PilA

Chain Au: 84% 13% .



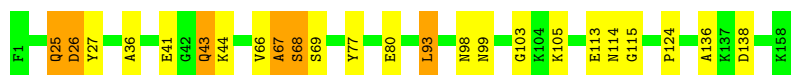
- Molecule 1: PilA

Chain Av: 84% 13% .



- Molecule 1: PilA

Chain Aw: 85% 11% .



- Molecule 1: PilA

Chain Ax: 85% 11% .



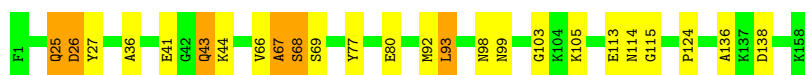
- Molecule 1: PilA

Chain Ay: 86% 11% .



- Molecule 1: PilA

Chain Az: 84% 12% .



- Molecule 1: PilA

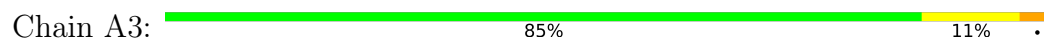
Chain A1: 84% 13% .



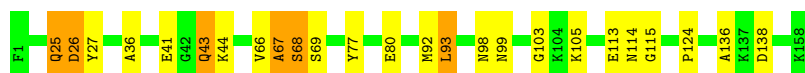
- Molecule 1: PilA



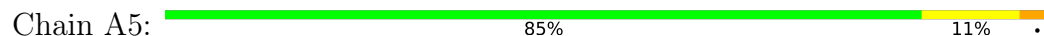
- Molecule 1: PilA



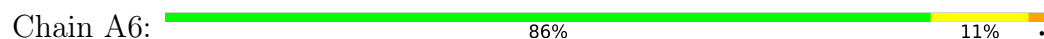
- Molecule 1: PilA



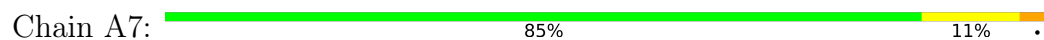
- Molecule 1: PilA



- Molecule 1: PilA



- Molecule 1: PilA



- Molecule 1: PilA

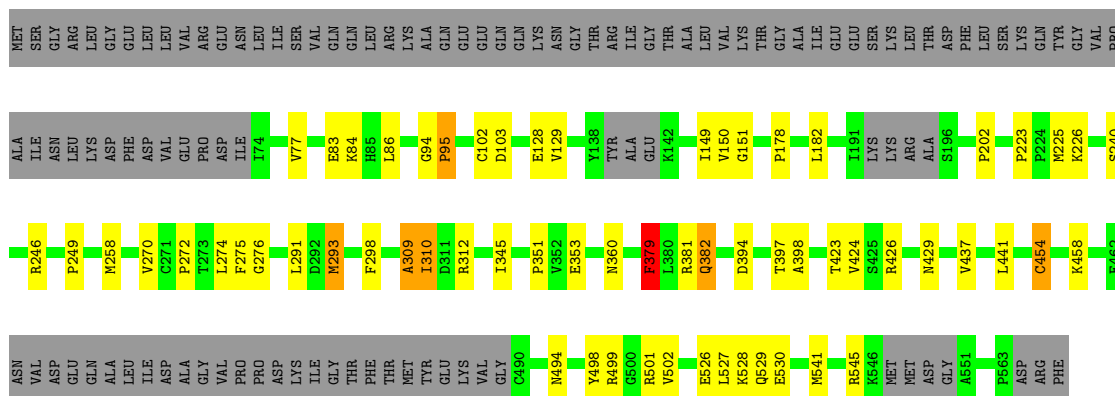




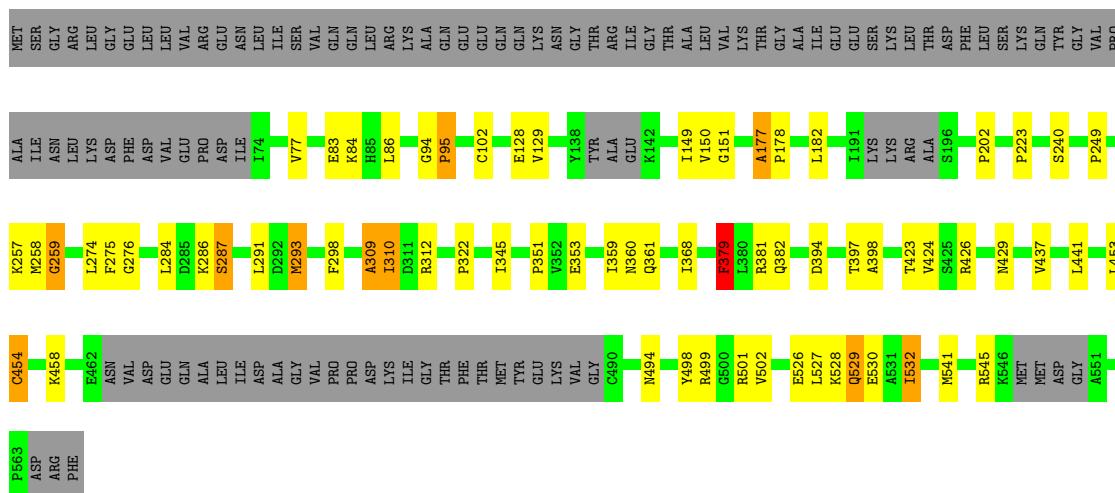
- Molecule 1: PilA



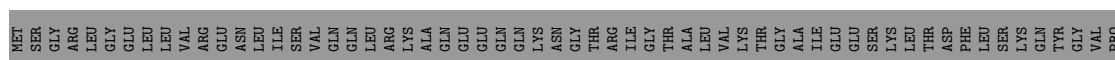
- Molecule 2: Type IV-A pilus assembly ATPase PilB

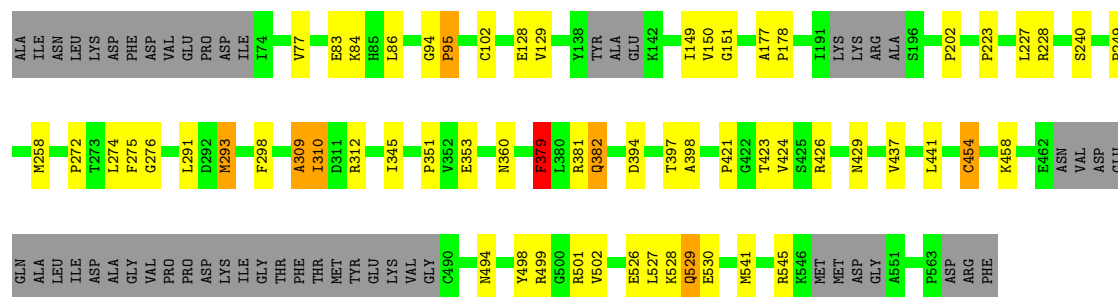


- Molecule 2: Type IV-A pilus assembly ATPase PilB



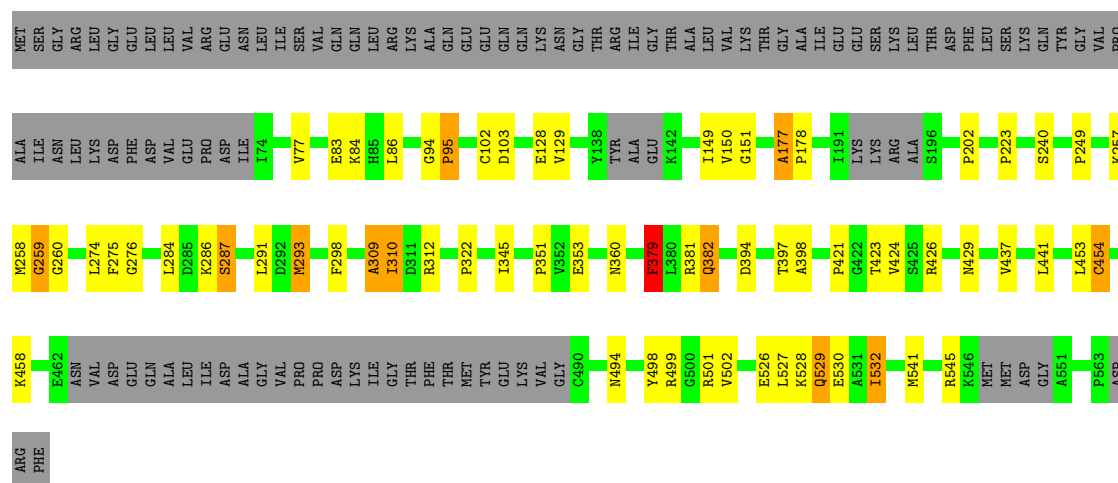
- Molecule 2: Type IV-A pilus assembly ATPase PilB





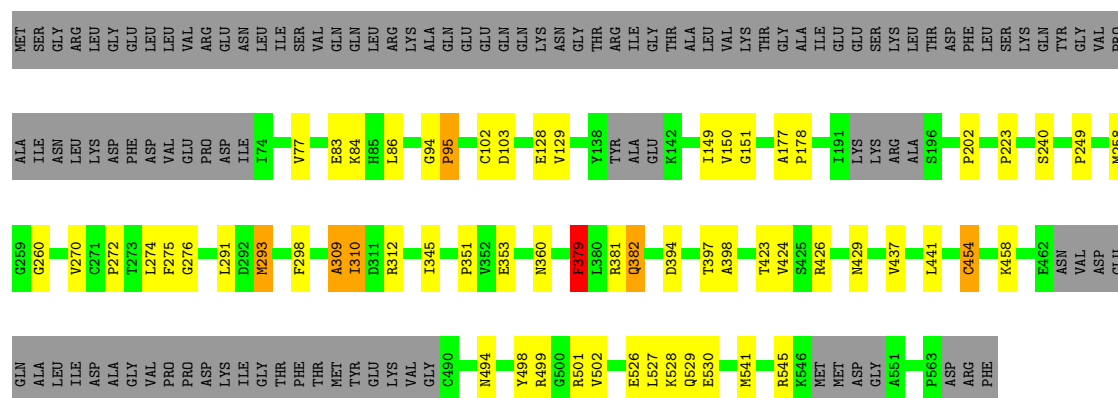
• Molecule 2: Type IV-A pilus assembly ATPase PilB

Chain Bd: 68% 10% 20%



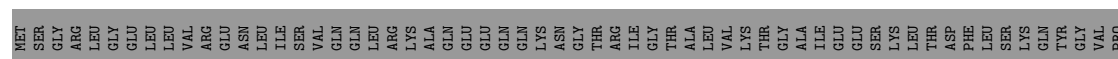
• Molecule 2: Type IV-A pilus assembly ATPase PilB

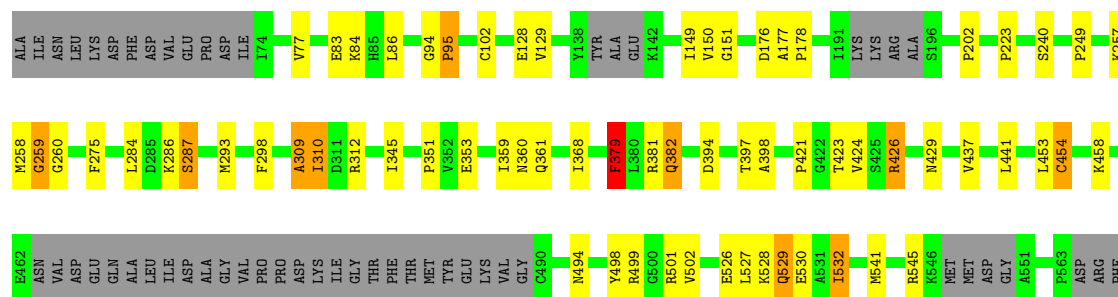
Chain Be: 69% 10% 20%



• Molecule 2: Type IV-A pilus assembly ATPase PilB

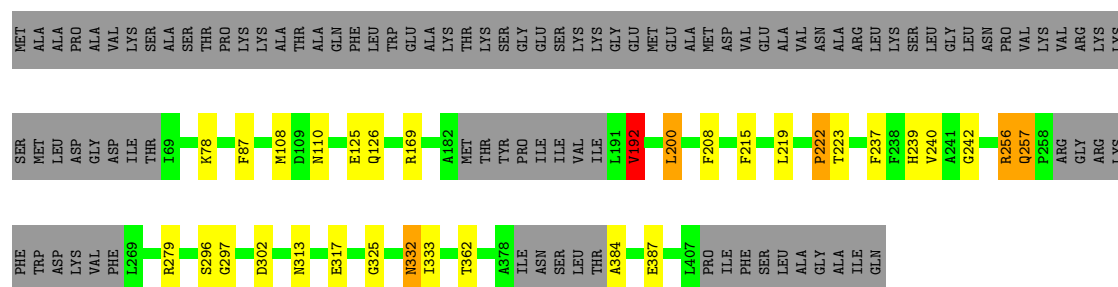
Chain Bf: 68% 10% 20%





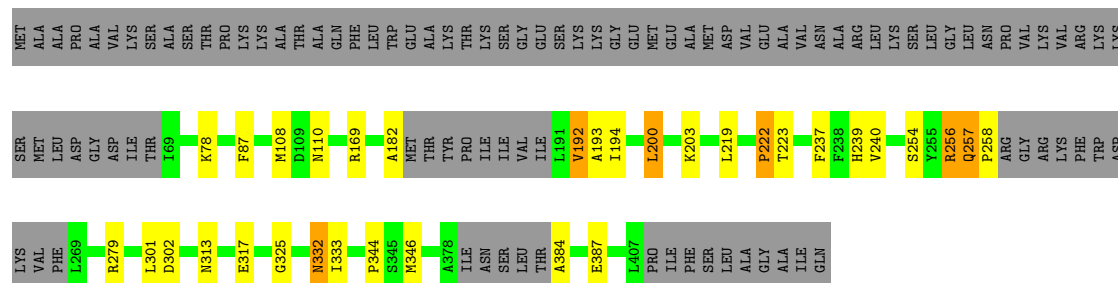
- Molecule 3: Type 4 fimbrial assembly protein PilC

Chain Ca: 68% 6% 24%



- Molecule 3: Type 4 fimbrial assembly protein PilC

Chain Cb: 68% 6% 24%



- Molecule 4: PilN

Chain Na: 85% 11% ..



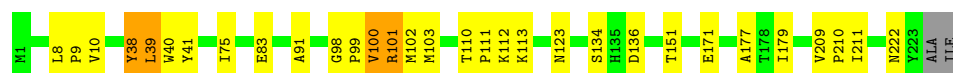
- Molecule 4: PilN

Chain Nb: 86% 11% ..



- Molecule 4: PilN

Chain Nc:  85% 12% ..



• Molecule 4: PiIN

Chain Nd:  87% 10% ..



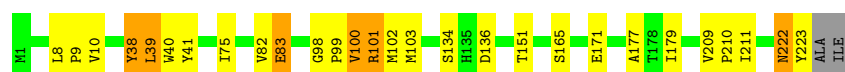
• Molecule 4: PiIN

Chain Ne:  87% 10% ..



• Molecule 4: PiIN

Chain Nf:  87% 10% ..



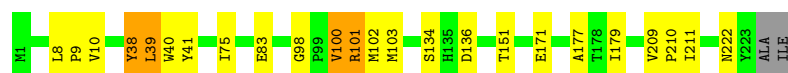
• Molecule 4: PiIN

Chain Ng:  88% 9% ..



• Molecule 4: PiIN

Chain Nh:  88% 9% ..



• Molecule 4: PiIN

Chain Ni:  88% 9% ..



• Molecule 4: PiIN

Chain Nj:  87% 10% ..



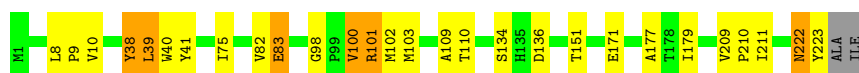
- Molecule 4: PilN

Chain Nk: 88% 9% ..



- Molecule 4: PilN

Chain Nl: 87% 10% ..



- Molecule 5: PilO

Chain Oa: 86% 5% 8%



- Molecule 5: PilO

Chain Ob: 87% 5% 8%



- Molecule 5: PilO

Chain Oc: 89% .. 8%



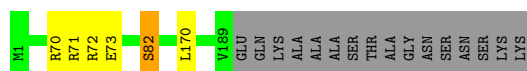
- Molecule 5: PilO

Chain Od: 88% • 8%



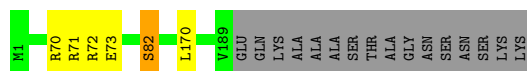
- Molecule 5: PilO

Chain Oe: 89% • 8%



- Molecule 5: Pi1O

Chain Of: 89% 8%



- Molecule 5: Pi1O

Chain Og: 89% 8%



- Molecule 5: Pi1O

Chain Oh: 89% 8%



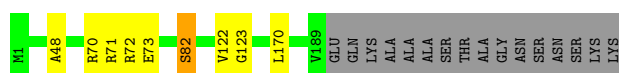
- Molecule 5: Pi1O

Chain Oi: 87% 8%



- Molecule 5: Pi1O

Chain Oj: 88% 8%



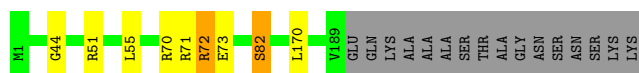
- Molecule 5: Pi1O

Chain Ok: 87% 8%



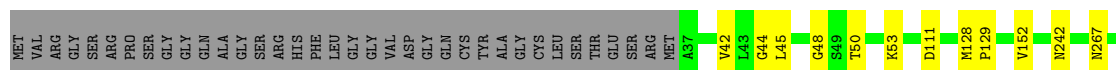
- Molecule 5: Pi1O

Chain Ol: 88% 8%



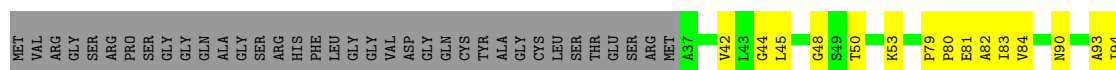
• Molecule 6: Type IV pilus biogenesis protein PilM

Chain Ma: 84% 5% 10%



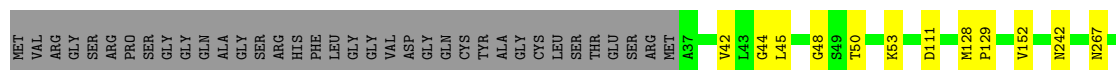
• Molecule 6: Type IV pilus biogenesis protein PilM

Chain Mb: 81% 9% 10%



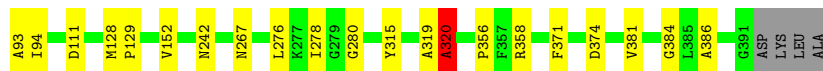
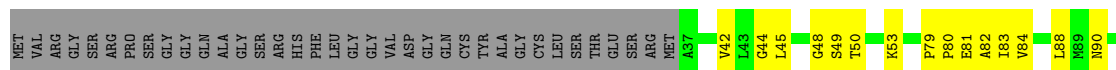
• Molecule 6: Type IV pilus biogenesis protein PilM

Chain Mc: 84% 5% 10%



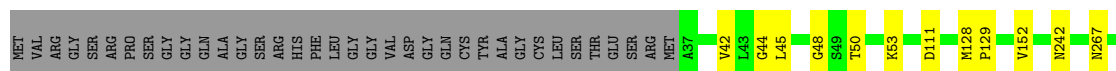
• Molecule 6: Type IV pilus biogenesis protein PilM

Chain Md: 81% 9% 10%



• Molecule 6: Type IV pilus biogenesis protein PilM

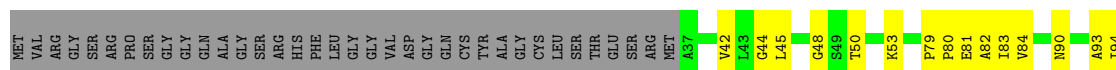
Chain Me: 83% 6% 10%





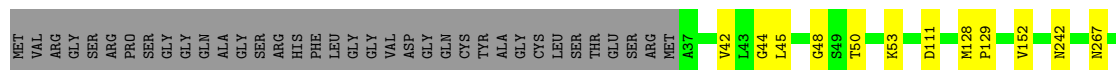
- Molecule 6: Type IV pilus biogenesis protein PilM

Chain Mf: 82% 8% 10%



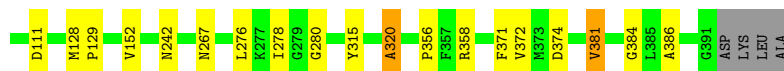
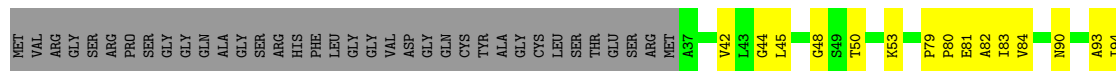
- Molecule 6: Type IV pilus biogenesis protein PilM

Chain Mg: 84% 6% 10%



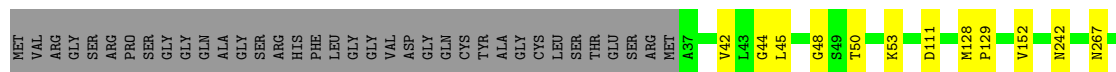
- Molecule 6: Type IV pilus biogenesis protein PilM

Chain Mh: 81% 8% 10%



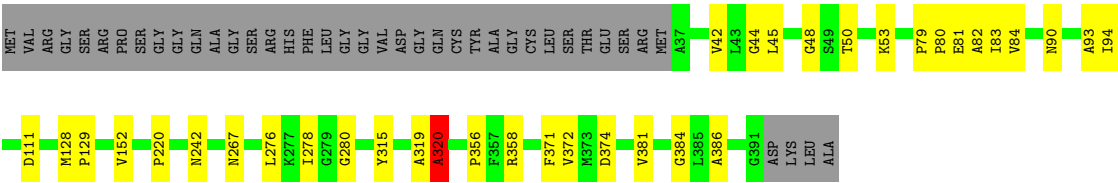
- Molecule 6: Type IV pilus biogenesis protein PilM

Chain Mi: 83% 6% 10%

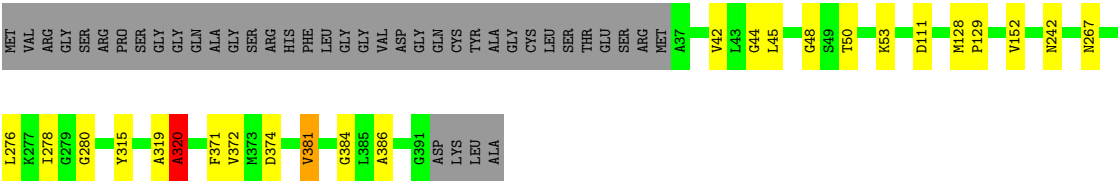
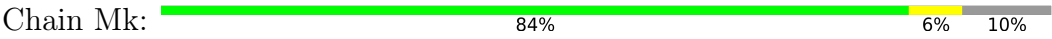


- Molecule 6: Type IV pilus biogenesis protein PilM

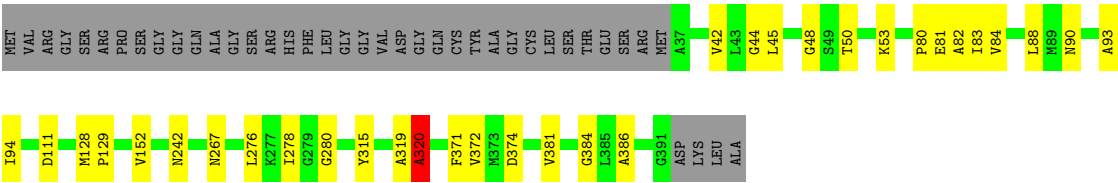
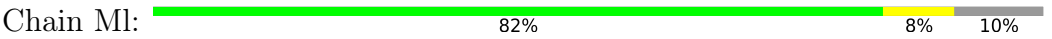
Chain Mj: 81% 9% 10%



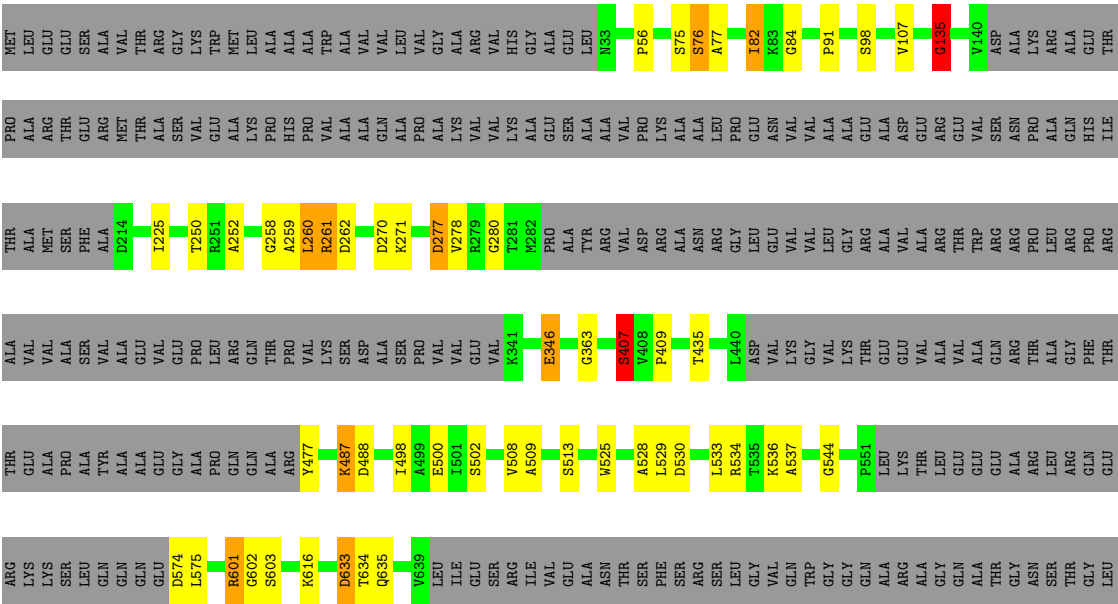
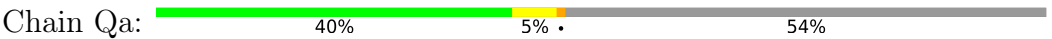
• Molecule 6: Type IV pilus biogenesis protein PilM



• Molecule 6: Type IV pilus biogenesis protein PilM



• Molecule 7: PilQ



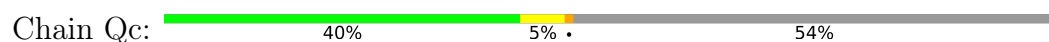
[illegible]

- Molecule 7: PilQ

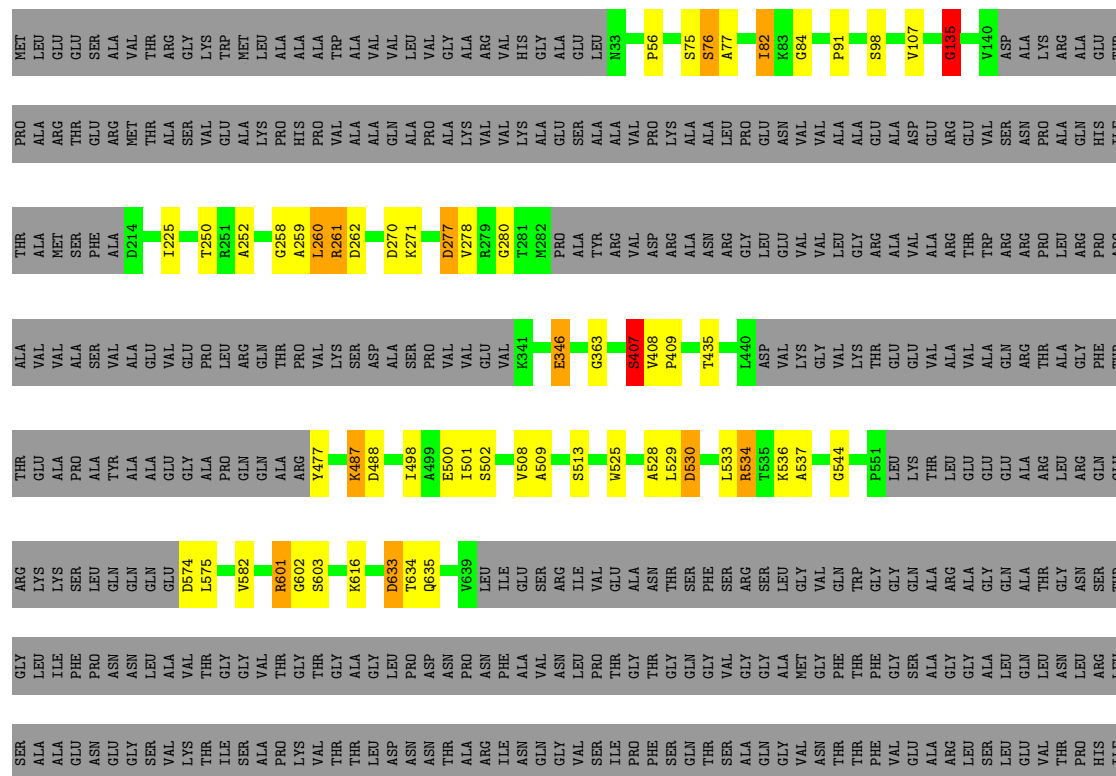


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VAL	VAL	GLY	GLU	GLY	PRO	ASN	LYS	ALA	VAL	VAL	VAL	VAL	THR	ALA	GLN	GLU	THR	GLU
PHE	VAL	VAL	GLU	GLY	ASN	GLY	LEU	THR	VAL	VAL	VAL	VAL	THR	VAL	THR	VAL	ARG	ALA
LEU	LEU	LEU	LEU	SER	SER	LEU	GLN	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	THR
ARG	SER	VAL	VAL	VAL	VAL	VAL	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	ARG
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PRO	PRO	ASN	THR	THR	THR	THR	D574	ALA	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	VAL	THR
VAL	VAL	ALA	ALA	ILE	GLY	GLY	L576	GLY	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	GLY	TRP
SER	SER	ALA	SER	SER	GLY	GLY	E600	GLN	ARG	GLN	GLN	GLN	GLN	GLN	GLN	GLN	VAL	TRP
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VAL	LEU	ALA	ALA	ILE	GLY	GLY	D633	LEU	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ALA
LEU	LEU	VAL	SER	SER	GLY	GLY	T634	GLY	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	ALA
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THR	THR	GLN	GLN	ALA	ASN	ASN	V639	ASN	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	ALA
ARG	ARG	GLY	GLY	ILE	ASN	ASN	LEU	ASN	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	ALA
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PHE	ARG	SER	ILE	ILE	PRO	PRO	W525	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA
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PRO	ALA	ASN	ASN	PHE	THR	THR	A528	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	LYS
ARG	ARG	ASN	ASN	THR	GLY	GLY	L529	SER	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	ALA
ILE	ILE	GLN	GLN	GLN	GLN	GLN	D530	PHE	THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA
LEU	LEU	LEU	THR	THR	THR	THR	S533	GLY	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	ALA
ARG	ARG	LEU	ALA	ALA	GLY	GLY	R534	ARG	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	PRO
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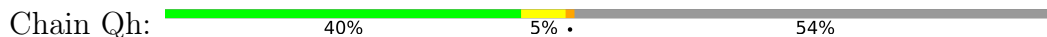
- Molecule 7: PilQ



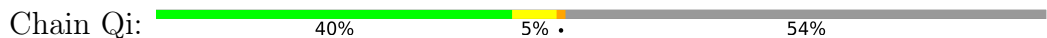
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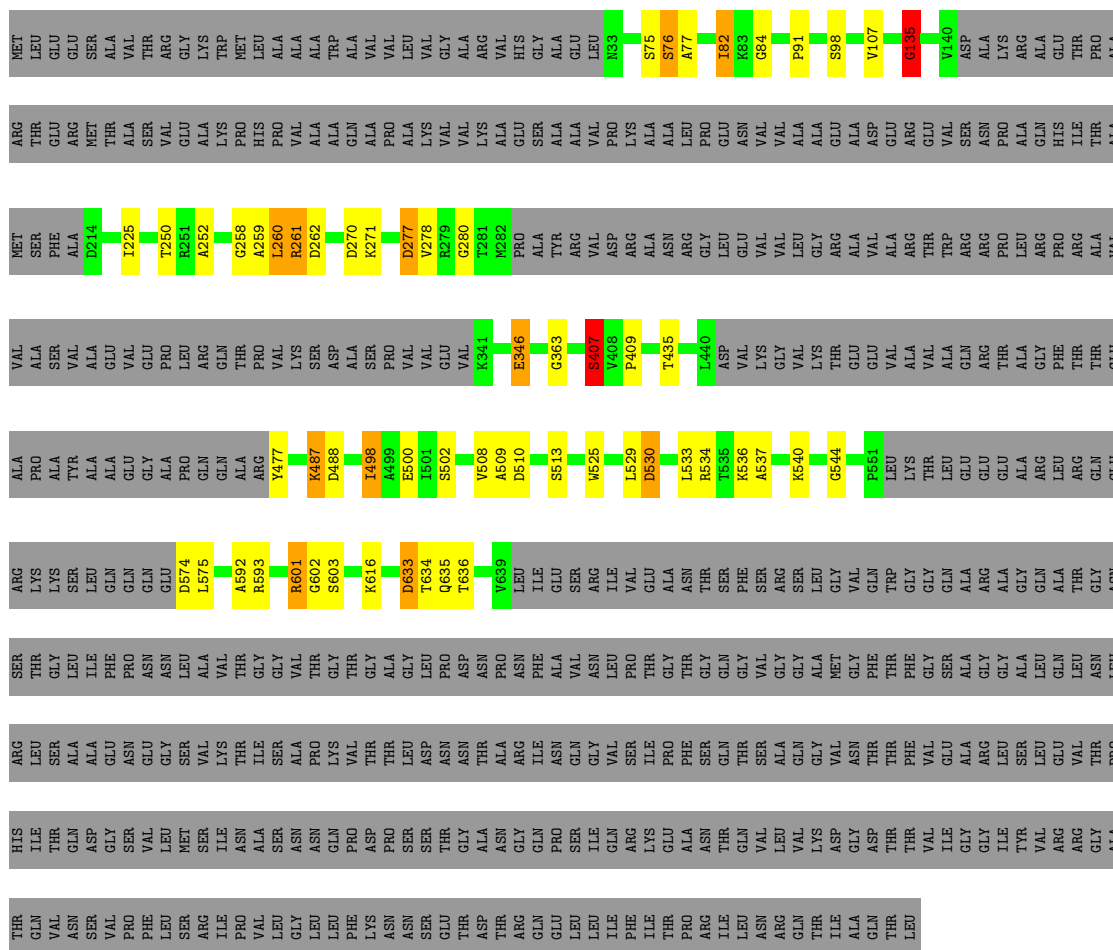


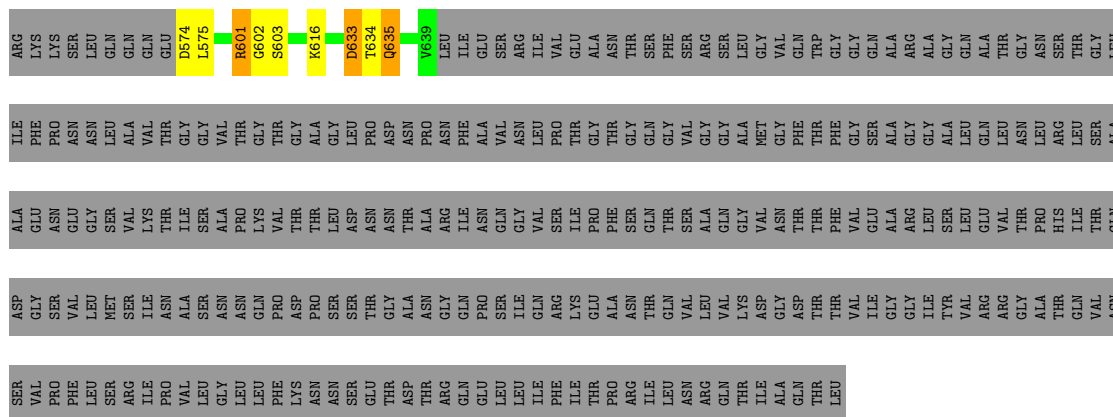
- Molecule 7: PilQ

[illegible]

- Molecule 7: PilQ

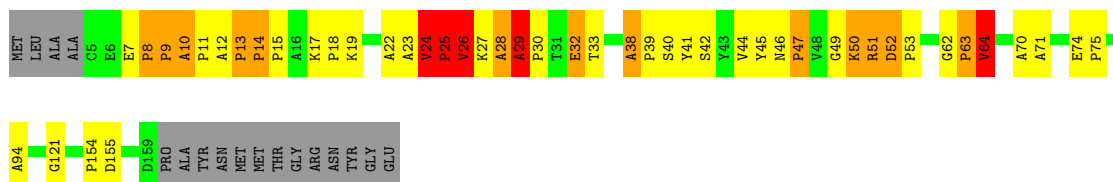
[illegible]





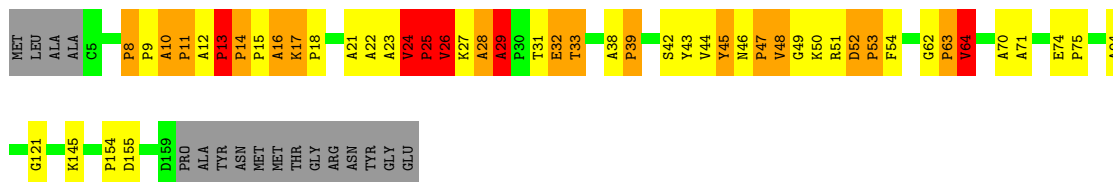
• Molecule 8: PilP

Chain Pa: 62% 17% 8% • 10%



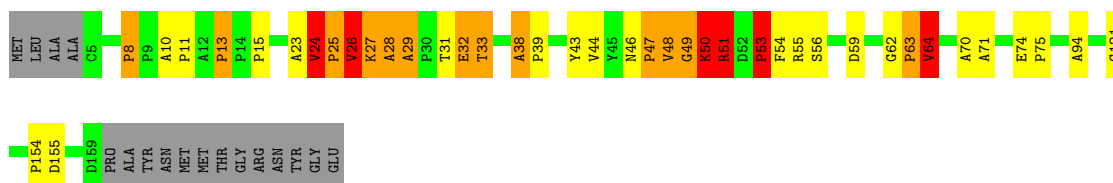
• Molecule 8: PilP

Chain Pb: 61% 16% 9% • 10%



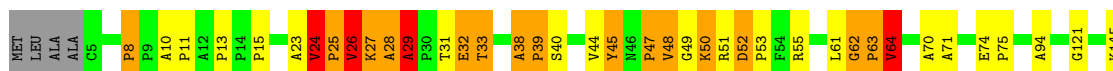
• Molecule 8: PilP

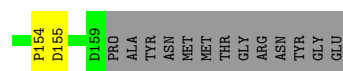
Chain Pc: 66% 13% 8% • 10%



• Molecule 8: PilP

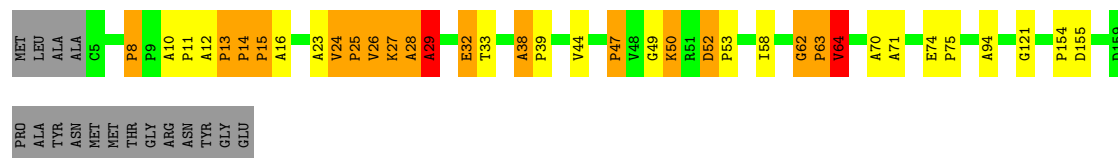
Chain Pd: 66% 13% 9% • 10%





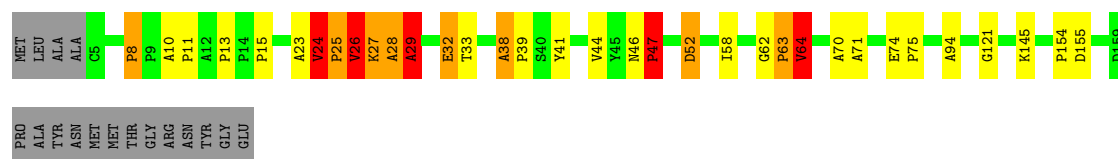
• Molecule 8: PilP

Chain Pe: 69% 11% 9% • 10%



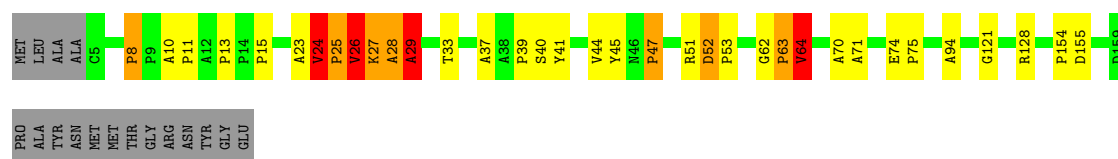
• Molecule 8: PilP

Chain Pf: 70% 12% 5% • 10%



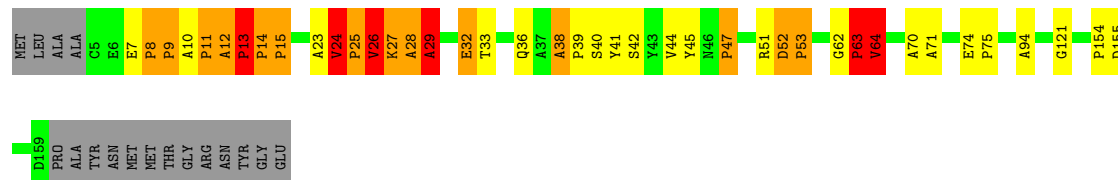
• Molecule 8: PilP

Chain Pg: 70% 14% • • 10%



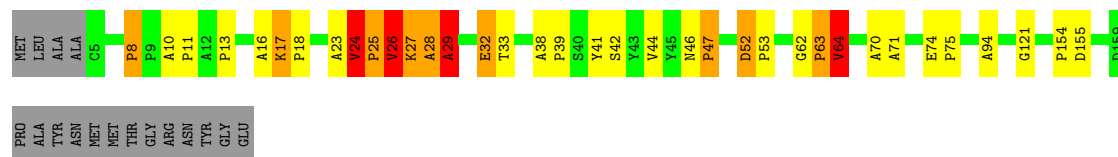
• Molecule 8: PilP

Chain Ph: 66% 12% 8% • 10%



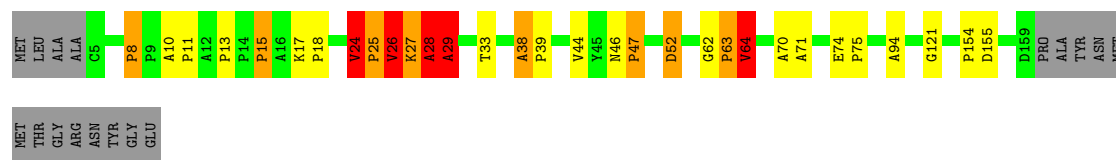
• Molecule 8: PilP

Chain Pi: 69% 13% 5% • 10%



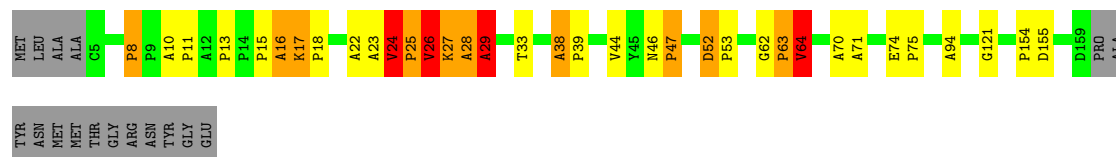
- Molecule 8: PilP

Chain Pj: 



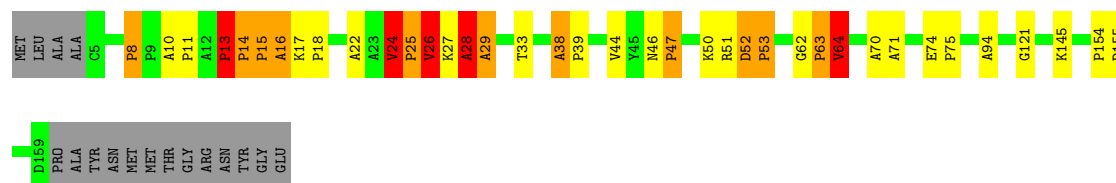
- Molecule 8: PilP

Chain Pk: 



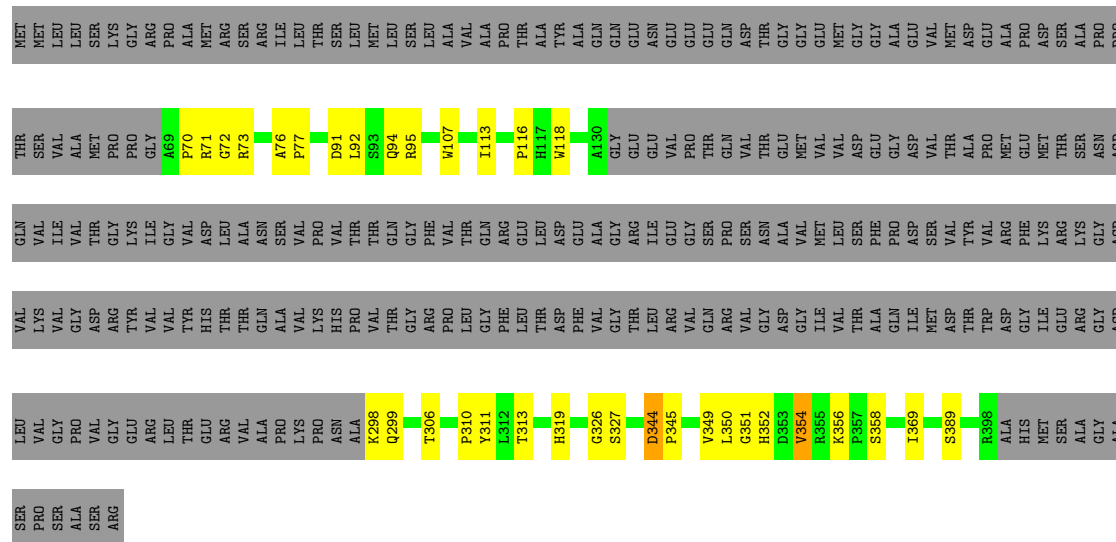
- Molecule 8: PilP

Chain Pl: 



- Molecule 9: LysM domain protein

Chain Ta: 



- Molecule 9: LysM domain protein

SER	LEU	VAL	GLN	THR	MET
PRO	VAL	LYS	VAL	SER	LEU
SER	GLY	VAL	ILE	VAL	LEU
ALA	PRO	GLY	THR	ALA	SER
SER	VAL	ASP	THR	MET	LEU
ARG	GLY	ARG	GLY	PRO	SER
	GLU	TYR	LYS	PRO	LYS
	ARG	VAL	ILE	GLY	GLY
	LEU	VAL	VAL	A69	PRO
	THR	TYR	VAL	P70	ALA
	GLU	HIS	ASP	R71	MET
	ARG	THR	LEU	G72	ARG
	VAL	THR	ALA	R73	SER
	PRO	GLN	ASN		SER
	LYS	VAL	VAL	A76	ILE
	ASN	HIS	PRO	P77	THR
	ALA	VAL	VAL		SER
	PRO	VAL	THR	D91	LEU
	ASN	PRO	THR	L92	LEU
	ALA	VAL	THR	S93	MET
	PRO	VAL	GLN	Q94	LEU
	Q299	THR	GLY	R95	SER
		GLY	PHE		LEU
	T306	ARG	VAL	W07	ALA
		PRO	THR		VAL
	P310	LEU	THR		ALA
	G311	GLY	GLN	I113	PRO
	L312	PHE	ARG		THR
	T313	LEU	LEU	P116	ALA
		THR	LEU	W117	ALA
	H319	ASP	ASP	W118	TYR
		PHE	GLU		ALA
	G326	VAL	ALA	A130	GLN
	S327	GLY	GLY	GLY	GLN
		THR	ARG	GLU	GLU
	D344	LEU	ILE	GLU	ASN
	P345	ARG	GLU	VAL	GLU
		VAL	GLY	PRO	GLU
	V349	GLN	SER	THR	GLU
	L350	ARG	PRO	GLN	GLN
	G351	VAL	SER	VAL	ASP
	H352	GLY	ASN	THR	THR
	B353	ASP	ALA	GLU	GLY
	V354	ILE	VAL	MET	GLY
	R355	VAL	LEU	VAL	MET
	K356	THR	SER	ASP	GLY
	P357	ALA	PHE	GLU	GLY
	S358	GLN	PRO	GLY	ALA
		ILE	ASP	ASP	GLU
	T369	MET	SER	THR	VAL
		ASP	VAL	VAL	VAL
	S389	THR	TYR	ALA	ASP
		TRP	ARG	PRO	GLY
	R398	ASP	VAL	MET	ALA
	ALA	GLY	PHE	GLU	PRO
	HIS	ILE	LYS	THR	ASP
	MET	GLU	ARG	THR	SER
	SER	GLU	LYS	SER	ALA
	ALA	ARG	GLY	ASN	PRO
	GLY	GLY	ASP	ASP	PRO
	ALA	ASP	ASP	ASP	PRO

GLY	LEU	VAL	GLN	THR	MET
ALA	GLY	LYS	VAL	SER	MET
SER	VAL	VAL	ILE	VAL	LEU
PRO	PRO	GLY	THR	ALA	SER
SER	VAL	ASP	THR	MET	LEU
ALA	GLY	ARG	GLY	PRO	SER
ARG	GLU	TYR	LYS	PRO	LYS
	LEU	VAL	ILE	GLY	GLY
	THR	TYR	VAL	A69	PRO
	GLU	HIS	ASP	P70	ALA
	ARG	THR	LEU	R71	MET
	VAL	THR	ALA	G72	ARG
	PRO	ALA	ASN	R73	SER
	LYS	VAL	SER	A76	ARG
	ASN	HIS	VAL	P77	LEU
	ALA	PRO	VAL	D91	THR
	K298	PRO	THR	L92	SER
	Q299	VAL	THR	S93	LEU
	V300	THR	GLN	Q94	LEU
	D301	GLY	GLY	R95	SER
	T306	ARG	PHE	W107	LEU
	P310	PRO	VAL	I113	ALA
	V311	GLY	GLN	P116	VAL
	L312	LEU	LEU	H117	ALA
	T313	THR	GLY	W118	THR
		ASP	ASP	A130	TYR
		PHE	GLU	SER	ALA
	H319	VAL	ALA	GLN	GLN
	G326	GLY	GLY	GLY	GLY
	S327	THR	ARG	GLU	ASN
	D344	LEU	ILE	VAL	GLU
	P345	ARG	GLY	PRO	GLU
	V349	GLN	PRO	GLN	GLU
	L350	VAL	SER	VAL	THR
	G351	GLY	ASN	THR	ASP
	H352	ASP	ALA	GLU	GLY
	D353	ILE	VAL	MET	GLY
	V354	VAL	LEU	VAL	MET
	R355	THR	SER	ASP	GLY
	K356	GLN	PHE	GLY	GLY
	P357	ALA	PRO	GLY	ALA
	S358	ILE	ASP	ASP	GLU
		MET	SER	VAL	VAL
	I369	THR	TYR	THR	ASP
	S389	TRP	ARG	PRO	GLY
	K396	ASP	THR	MET	ALA
	ALA	GLY	PHE	THR	PRO
	HIS	ILE	LYS	MET	ASP
	THR	GLU	ARG	THR	SER
	MET	ARG	LYS	SER	ALA
	SER	GLY	GLY	ASN	PRO
	ALA	ASP	ASP	THR	PRO

[illegible]

PRO	VAL	LYS	VAL	THR	THR	MET
SER	GLY	VAL	ILE	SER	SER	MET
ALA	PRO	GLY	VAL	VAL	LEU	LEU
SER	VAL	ASP	THR	GLY	ALA	SER
ARG	GLY	ARG	THR	THR	MET	SER
	GLU	TYR	LYS	PRO	LYS	LYS
	ARG	VAL	ILE	GLY	GLY	GLY
	LEU	VAL	VAL	VAL	ASP	ARG
	THR	TYR	VAL	ASP	A69	PRO
	GLU	HIS	THR	LEU	P70	ALA
	ARG	THR	THR	ALA	R71	MET
	VAL	THR	GLN	ASN	G72	ARG
	ALA	ALA	SER	SER	R73	SER
	PRO	VAL	VAL	VAL	A76	ARG
	LYS	VAL	PRO	PRO	P77	ILE
	PRO	HIS	VAL	THR	D91	THR
	ASN	PRO	THR	THR		SER
	ALA	VAL	THR	THR		LEU
	K298	VAL	THR	GLN	Q94	MET
	Q299	GLY	GLY	GLY	R95	LEU
		ARG	PHE	PHE		SER
	T306	PRO	VAL	VAL	W107	LEU
	P310	LEU	THR	THR		ALA
	Y311	GLY	GLN	GLN	I113	VAL
	I312	PHE	ARG	ARG		ALA
	T313	LEU	GLU	GLU	P116	PRO
		THR	LEU	ASP	H117	THR
	H319	ASP	ASP	GLY	W118	ALA
		PHE	GLU			TYR
	G326	VAL	ALA	ALA	A130	GLN
	S327	GLY	GLY	GLY		LEU
		THR	ARG	ARG		GLU
	D344	LEU	ILE	ILE		GLU
	P345	ARG	GLU	GLU	VAL	ASN
		VAL	GLY	PRO	VAL	GLU
	V349	GLN	SER	THR	THR	GLU
	I350	ARG	PRO	GLN	GLN	GLU
	G351	VAL	SER	VAL	VAL	GLN
	H352	GLY	ASN	THR	ASP	ASP
	D353	ASP	ALA	GLU	GLU	THR
	V354	GLY	VAL	THR	THR	GLY
	R355	ILE	LEU	VAL	VAL	GLY
	K356	THR	SER	ASP	VAL	GLY
	P357	THR	SER	GLY	GLY	MET
	S358	ALA	PHE	PRO	ASP	GLY
		GLN	THR	ASP	VAL	ALA
	I369	ILE	SER	SER	THR	GLU
		MET	THR	THR	VAL	VAL
	S389	ASP	VAL	ALA	ALA	MET
		TRP	VAL	VAL	PRO	ASP
	R398	ASP	ARG	THR	GLU	GLU
	ALA	GLY	PHE	THR	MET	ALA
	HIS	ILE	LYS	LYS	THR	PRO
	MET	GLU	ARG	THR	SER	ASP
	SER	ALA	ARG	LYS	ASN	SER
	ALA	GLY	GLY	GLY	ASP	ALA
	ALA	ASP	ASP	ASP	ASP	PRO

PRO	VAL	LYS	VAL	THR	MET
SER	GLY	VAL	ILE	SER	LEU
ALA	PRO	GLY	VAL	VAL	LEU
SER	VAL	ASP	THR	ALA	SER
ARG	GLY	ARG	GLY	MET	LEU
	GLU	TYR	LYS	PRO	SER
	ARG	VAL	ILE	PRO	GLY
	LEU	VAL	GLY	GLY	ARG
	THR	HIS	ASP	A69	PRO
	GLU	THR	ASP	P70	ALA
	ARG	THR	LEU	R71	MET
	VAL	THR	ALA	G72	ARG
	ALA	GLN	ASN	R73	SER
	PRO	ALA	SER		ARG
	LYS	VAL	VAL	A76	ILE
	PRO	PRO	PRO	P77	LEU
	ASN	HIS	VAL		THR
	ALA	PRO	THR	D91	SER
	K298	VAL	THR	L92	LEU
	K299	THR	GLN	S93	MET
		GLY	GLY	Q94	LEU
	T306	ARG	PHE		SER
		PRO	VAL	W107	LEU
	P810	LEU	THR		ALA
	Y311	GLY	GLN	I113	VAL
	L312	PHE	ARG		ALA
	T313	LEU	GLU	P116	PRO
		THR	LEU	H117	THR
	H319	ASP	ASP	W118	ALA
		PHE	GLU		TYR
	G326	VAL	ALA	A130	GLY
	S327	GLY	GLY		GLN
		THR	ARG	GLU	GLN
	D344	LEU	ILE	GLU	GLU
	P345	ARG	GLU	VAL	ASN
		VAL	GLY	PRO	GLU
	V349	GLN	SER	THR	GLU
	L350	ARG	PRO	GLN	GLU
	G351	VAL	SER	VAL	GLN
	H352	GLY	ASN	THR	ASP
	D353	ASP	ALA	GLU	THR
	V354	GLY	VAL	GLU	GLY
	R355	ILE	MET	MET	GLY
	K356	VAL	LEU	VAL	GLU
	P357	THR	SER	ASP	MET
	S358	ALA	PHE	GLU	GLY
		GLN	PRO	GLY	GLY
		ILE	ASP	ASP	ALA
		MET	SER	VAL	GLU
		THR	TYR	THR	VAL
	S389	ASP	VAL	ALA	MET
		TRP	VAL	PRO	ASP
	R398	ASP	ARG	MET	GLU
	ALA	GLY	PHE	GLU	ALA
	HIS	ILE	LYS	MET	PRO
	MET	GLU	ARG	THR	ASP
	SER	ARG	LYS	SER	SER
	ALA	GLY	GLY	ASN	ALA
	ALA	ASP	ASP	ASP	PRO

[illegible]

Device Type	Percentage
Smartphones	31%
Tablets	8%
Feature Phones	60%



4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of tilted images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	150	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	27500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MEA

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	A1	1.13	1/627 (0.2%)	1.44	11/782 (1.4%)
1	A2	1.14	1/627 (0.2%)	1.43	9/782 (1.2%)
1	A3	1.14	1/627 (0.2%)	1.44	11/782 (1.4%)
1	A4	1.14	1/627 (0.2%)	1.44	11/782 (1.4%)
1	A5	1.14	1/627 (0.2%)	1.44	10/782 (1.3%)
1	A6	1.11	1/627 (0.2%)	1.45	11/782 (1.4%)
1	A7	1.13	1/627 (0.2%)	1.44	11/782 (1.4%)
1	A8	1.14	1/627 (0.2%)	1.44	10/782 (1.3%)
1	A9	1.14	1/627 (0.2%)	1.44	10/782 (1.3%)
1	Aa	1.14	1/627 (0.2%)	1.43	10/782 (1.3%)
1	Ab	1.14	1/627 (0.2%)	1.44	10/782 (1.3%)
1	Ac	1.13	1/627 (0.2%)	1.43	11/782 (1.4%)
1	Ad	1.14	1/627 (0.2%)	1.44	10/782 (1.3%)
1	Ae	1.14	1/627 (0.2%)	1.43	10/782 (1.3%)
1	Af	1.13	1/627 (0.2%)	1.42	9/782 (1.2%)
1	Ag	1.14	1/627 (0.2%)	1.43	11/782 (1.4%)
1	Ah	1.13	1/627 (0.2%)	1.43	12/782 (1.5%)
1	Ai	1.12	1/627 (0.2%)	1.44	11/782 (1.4%)
1	Aj	1.14	1/627 (0.2%)	1.43	11/782 (1.4%)
1	Ak	1.14	1/627 (0.2%)	1.44	10/782 (1.3%)
1	Al	1.13	1/627 (0.2%)	1.43	10/782 (1.3%)
1	Am	1.13	1/627 (0.2%)	1.44	11/782 (1.4%)
1	An	1.11	1/627 (0.2%)	1.42	9/782 (1.2%)
1	Ao	1.13	1/627 (0.2%)	1.43	10/782 (1.3%)
1	Ap	1.13	1/627 (0.2%)	1.44	10/782 (1.3%)
1	Aq	1.14	1/627 (0.2%)	1.42	9/782 (1.2%)
1	Ar	1.13	1/627 (0.2%)	1.44	11/782 (1.4%)
1	As	1.14	1/627 (0.2%)	1.43	10/782 (1.3%)
1	At	1.14	1/627 (0.2%)	1.43	10/782 (1.3%)
1	Au	1.14	1/627 (0.2%)	1.43	11/782 (1.4%)
1	Av	1.14	1/627 (0.2%)	1.44	11/782 (1.4%)
1	Aw	1.14	1/627 (0.2%)	1.43	11/782 (1.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Ax	1.14	1/627 (0.2%)	1.44	10/782 (1.3%)
1	Ay	1.14	1/627 (0.2%)	1.43	10/782 (1.3%)
1	Az	1.13	1/627 (0.2%)	1.44	11/782 (1.4%)
2	Ba	0.61	0/1803	1.13	17/2245 (0.8%)
2	Bb	0.79	2/1803 (0.1%)	1.16	19/2245 (0.8%)
2	Bc	0.61	0/1803	1.14	17/2245 (0.8%)
2	Bd	0.66	1/1803 (0.1%)	1.18	22/2245 (1.0%)
2	Be	0.61	0/1803	1.13	17/2245 (0.8%)
2	Bf	0.65	2/1803 (0.1%)	1.19	22/2245 (1.0%)
3	Ca	1.09	1/1260 (0.1%)	1.71	10/1568 (0.6%)
3	Cb	1.10	1/1260 (0.1%)	1.71	10/1568 (0.6%)
4	Na	0.37	0/891	0.89	1/1112 (0.1%)
4	Nb	0.38	0/891	0.90	1/1112 (0.1%)
4	Nc	0.38	0/891	0.90	1/1112 (0.1%)
4	Nd	0.38	0/891	0.90	1/1112 (0.1%)
4	Ne	0.39	0/891	0.90	1/1112 (0.1%)
4	Nf	0.38	0/891	0.90	1/1112 (0.1%)
4	Ng	0.38	0/891	0.90	1/1112 (0.1%)
4	Nh	0.39	0/891	0.90	1/1112 (0.1%)
4	Ni	0.38	0/891	0.90	1/1112 (0.1%)
4	Nj	0.39	0/891	0.90	1/1112 (0.1%)
4	Nk	0.37	0/891	0.90	1/1112 (0.1%)
4	Nl	0.37	0/891	0.90	1/1112 (0.1%)
5	Oa	0.32	0/755	0.69	0/942
5	Ob	0.33	0/755	0.68	0/942
5	Oc	0.32	0/755	0.69	2/942 (0.2%)
5	Od	0.33	0/755	0.68	0/942
5	Oe	0.33	0/755	0.68	0/942
5	Of	0.32	0/755	0.69	0/942
5	Og	0.32	0/755	0.69	0/942
5	Oh	0.32	0/755	0.69	2/942 (0.2%)
5	Oi	0.34	0/755	0.69	2/942 (0.2%)
5	Oj	0.32	0/755	0.69	0/942
5	Ok	0.32	0/755	0.68	0/942
5	Ol	0.33	0/755	0.69	2/942 (0.2%)
6	Ma	0.39	0/1419	0.81	4/1772 (0.2%)
6	Mb	0.40	0/1419	0.81	2/1772 (0.1%)
6	Mc	0.39	0/1419	0.81	4/1772 (0.2%)
6	Md	0.39	0/1419	0.82	2/1772 (0.1%)
6	Me	0.38	0/1419	0.81	2/1772 (0.1%)
6	Mf	0.38	0/1419	0.83	4/1772 (0.2%)
6	Mg	0.38	0/1419	0.80	4/1772 (0.2%)
6	Mh	0.39	0/1419	0.82	4/1772 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	Mi	0.38	0/1419	0.82	2/1772 (0.1%)
6	Mj	0.39	0/1419	0.82	2/1772 (0.1%)
6	Mk	0.38	0/1419	0.80	4/1772 (0.2%)
6	Ml	0.39	0/1419	0.82	2/1772 (0.1%)
7	Qa	1.05	6/1667 (0.4%)	2.32	28/2075 (1.3%)
7	Qb	1.06	7/1667 (0.4%)	2.31	29/2075 (1.4%)
7	Qc	1.06	7/1667 (0.4%)	2.32	28/2075 (1.3%)
7	Qd	1.06	8/1667 (0.5%)	2.32	29/2075 (1.4%)
7	Qe	1.06	6/1667 (0.4%)	2.32	32/2075 (1.5%)
7	Qf	1.06	7/1667 (0.4%)	2.32	32/2075 (1.5%)
7	Qg	1.06	7/1667 (0.4%)	2.32	29/2075 (1.4%)
7	Qh	1.06	6/1667 (0.4%)	2.32	29/2075 (1.4%)
7	Qi	1.05	6/1667 (0.4%)	2.31	30/2075 (1.4%)
7	Qj	1.05	5/1667 (0.3%)	2.32	28/2075 (1.3%)
7	Qk	1.06	7/1667 (0.4%)	2.32	28/2075 (1.3%)
7	Ql	1.06	5/1667 (0.3%)	2.32	29/2075 (1.4%)
8	Pa	1.35	1/619 (0.2%)	1.81	12/772 (1.6%)
8	Pb	1.34	1/619 (0.2%)	1.76	9/772 (1.2%)
8	Pc	1.38	2/619 (0.3%)	1.79	11/772 (1.4%)
8	Pd	1.39	1/619 (0.2%)	1.80	10/772 (1.3%)
8	Pe	1.38	1/619 (0.2%)	1.85	12/772 (1.6%)
8	Pf	1.42	2/619 (0.3%)	1.91	12/772 (1.6%)
8	Pg	1.38	2/619 (0.3%)	1.81	12/772 (1.6%)
8	Ph	1.30	1/619 (0.2%)	1.76	10/772 (1.3%)
8	Pi	1.42	2/619 (0.3%)	1.92	13/772 (1.7%)
8	Pj	1.39	1/619 (0.2%)	1.91	13/772 (1.7%)
8	Pk	1.44	2/619 (0.3%)	1.90	14/772 (1.8%)
8	Pl	1.39	1/619 (0.2%)	1.86	13/772 (1.7%)
9	Ta	1.13	1/650 (0.2%)	1.45	4/809 (0.5%)
9	Tb	1.14	0/650	1.46	4/809 (0.5%)
9	Tc	1.14	1/650 (0.2%)	1.46	4/809 (0.5%)
9	Td	1.14	2/650 (0.3%)	1.46	4/809 (0.5%)
9	Te	1.15	1/650 (0.2%)	1.46	4/809 (0.5%)
9	Tf	1.15	0/650	1.47	4/809 (0.5%)
9	Tg	1.13	0/650	1.46	4/809 (0.5%)
9	Th	1.14	0/650	1.47	4/809 (0.5%)
9	Ti	1.15	2/650 (0.3%)	1.47	6/809 (0.7%)
9	Tj	1.14	0/650	1.46	4/809 (0.5%)
9	Tk	1.13	0/650	1.45	4/809 (0.5%)
9	Tl	1.15	0/650	1.47	6/809 (0.7%)
All	All	0.90	143/107295 (0.1%)	1.50	1097/133760 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	Ba	0	3
2	Bb	0	7
2	Bc	0	4
2	Bd	0	7
2	Be	0	4
2	Bf	0	7
3	Ca	0	18
3	Cb	0	18
4	Na	0	6
4	Nb	0	6
4	Nc	0	5
4	Nd	0	5
4	Ne	0	5
4	Nf	0	5
4	Ng	0	5
4	Nh	0	5
4	Ni	0	5
4	Nj	0	5
4	Nk	0	5
4	Nl	0	5
5	Oa	0	1
5	Ob	0	1
5	Oc	0	1
5	Od	0	1
5	Oe	0	1
5	Of	0	1
5	Og	0	1
5	Oh	0	1
5	Oi	0	1
5	Oj	0	1
5	Ok	0	1
5	Ol	0	1
6	Ma	0	2
6	Mb	0	2
6	Mc	0	2
6	Md	0	2
6	Me	0	2
6	Mf	0	2
6	Mg	0	2
6	Mh	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	Mi	0	2
6	Mj	0	2
6	Mk	0	2
6	Ml	0	2
7	Qa	0	20
7	Qb	0	23
7	Qc	0	21
7	Qd	0	21
7	Qe	0	21
7	Qf	0	20
7	Qg	0	21
7	Qh	0	20
7	Qi	0	22
7	Qj	0	23
7	Qk	0	21
7	Ql	0	21
8	Pa	0	25
8	Pb	0	28
8	Pc	0	20
8	Pd	0	24
8	Pe	0	22
8	Pf	0	21
8	Pg	0	21
8	Ph	0	26
8	Pi	0	21
8	Pj	0	19
8	Pk	0	19
8	Pl	0	21
9	Ta	0	6
9	Tb	0	6
9	Tc	0	7
9	Td	0	6
9	Te	0	6
9	Tf	0	6
9	Tg	0	6
9	Th	0	6
9	Ti	0	7
9	Tj	0	7
9	Tk	0	6
9	Tl	0	6
All	All	0	762

The worst 5 of 143 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Pc	63	PRO	C-N	24.45	1.66	1.33
8	Pk	63	PRO	C-N	24.28	1.66	1.33
8	Pi	63	PRO	C-N	24.26	1.66	1.33
1	Ay	26	ASP	N-CA	24.21	1.76	1.46
1	Ae	26	ASP	N-CA	24.12	1.76	1.46

The worst 5 of 1097 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Qi	407	SER	O-C-N	-64.94	36.22	122.59
7	Qj	407	SER	O-C-N	-64.94	36.22	122.59
7	Qb	407	SER	O-C-N	-64.93	36.23	122.59
7	Qk	407	SER	O-C-N	-64.93	36.23	122.59
7	Qe	407	SER	O-C-N	-64.93	36.23	122.59

There are no chirality outliers.

5 of 762 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Ba	293	MET	Peptide
2	Ba	345	ILE	Peptide
2	Ba	379	PHE	Peptide
2	Bb	177	ALA	Peptide
2	Bb	284	LEU	Peptide

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	A1	632	0	174	17	0
1	A2	632	0	174	13	0
1	A3	632	0	174	14	0
1	A4	632	0	174	17	0
1	A5	632	0	174	15	0
1	A6	632	0	174	11	0
1	A7	632	0	174	13	0
1	A8	632	0	174	13	0
1	A9	632	0	174	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Aa	632	0	174	26	0
1	Ab	632	0	174	13	0
1	Ac	632	0	174	12	0
1	Ad	632	0	174	12	0
1	Ae	632	0	174	17	0
1	Af	632	0	174	15	0
1	Ag	632	0	174	14	0
1	Ah	632	0	174	16	0
1	Ai	632	0	174	14	0
1	Aj	632	0	174	15	0
1	Ak	632	0	174	16	0
1	Al	632	0	174	18	0
1	Am	632	0	174	14	0
1	An	632	0	174	28	0
1	Ao	632	0	174	16	0
1	Ap	632	0	174	15	0
1	Aq	632	0	174	15	0
1	Ar	632	0	174	14	0
1	As	632	0	174	14	0
1	At	632	0	174	16	0
1	Au	632	0	174	17	0
1	Av	632	0	174	15	0
1	Aw	632	0	174	14	0
1	Ax	632	0	174	16	0
1	Ay	632	0	174	14	0
1	Az	632	0	174	14	0
2	Ba	1808	0	487	43	0
2	Bb	1808	0	487	37	0
2	Bc	1808	0	487	31	0
2	Bd	1808	0	487	39	0
2	Be	1808	0	487	34	0
2	Bf	1808	0	487	33	0
3	Ca	1264	0	354	9	0
3	Cb	1264	0	354	21	0
4	Na	892	0	248	23	0
4	Nb	892	0	248	16	0
4	Nc	892	0	248	31	0
4	Nd	892	0	248	13	0
4	Ne	892	0	248	9	0
4	Nf	892	0	248	11	0
4	Ng	892	0	248	8	0
4	Nh	892	0	248	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Ni	892	0	248	6	0
4	Nj	892	0	248	8	0
4	Nk	892	0	248	8	0
4	Nl	892	0	248	14	0
5	Oa	756	0	207	14	0
5	Ob	756	0	207	14	0
5	Oc	756	0	207	3	0
5	Od	756	0	207	6	0
5	Oe	756	0	207	2	0
5	Of	756	0	207	2	0
5	Og	756	0	207	3	0
5	Oh	756	0	207	4	0
5	Oi	756	0	207	9	0
5	Oj	756	0	207	5	0
5	Ok	756	0	207	15	0
5	Ol	756	0	207	6	0
6	Ma	1420	0	396	11	0
6	Mb	1420	0	396	32	0
6	Mc	1420	0	396	10	0
6	Md	1420	0	396	29	0
6	Me	1420	0	396	13	0
6	Mf	1420	0	396	34	0
6	Mg	1420	0	396	12	0
6	Mh	1420	0	396	33	0
6	Mi	1420	0	396	13	0
6	Mj	1420	0	396	31	0
6	Mk	1420	0	396	12	0
6	Ml	1420	0	396	38	0
7	Qa	1672	0	462	33	0
7	Qb	1672	0	462	36	0
7	Qc	1672	0	462	35	0
7	Qd	1672	0	462	36	0
7	Qe	1672	0	462	37	0
7	Qf	1672	0	462	34	0
7	Qg	1672	0	462	35	0
7	Qh	1672	0	462	34	0
7	Qi	1672	0	462	36	0
7	Qj	1672	0	462	44	0
7	Qk	1672	0	462	35	0
7	Ql	1672	0	462	35	0
8	Pa	620	0	155	37	0
8	Pb	620	0	155	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	Pc	620	0	155	38	0
8	Pd	620	0	155	18	0
8	Pe	620	0	155	12	0
8	Pf	620	0	155	11	0
8	Pg	620	0	155	8	0
8	Ph	620	0	155	15	0
8	Pi	620	0	155	9	0
8	Pj	620	0	155	10	0
8	Pk	620	0	155	24	0
8	Pl	620	0	155	18	0
9	Ta	652	0	177	51	0
9	Tb	652	0	177	51	0
9	Tc	652	0	177	51	0
9	Td	652	0	177	51	0
9	Te	652	0	177	51	0
9	Tf	652	0	177	51	0
9	Tg	652	0	177	51	0
9	Th	652	0	177	51	0
9	Ti	652	0	177	51	0
9	Tj	652	0	177	51	0
9	Tk	652	0	177	51	0
9	Tl	652	0	177	51	0
All	All	107640	0	29460	1744	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 13.

The worst 5 of 1744 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:Ac:26:ASP:N	1:Ac:26:ASP:CA	1.76	1.49
1:A2:26:ASP:N	1:A2:26:ASP:CA	1.76	1.49
1:Af:26:ASP:N	1:Af:26:ASP:CA	1.76	1.49
1:An:26:ASP:N	1:An:26:ASP:CA	1.76	1.49
1:Aw:26:ASP:N	1:Aw:26:ASP:CA	1.76	1.49

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	A1	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	A2	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	A3	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	A4	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	A5	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	A6	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	A7	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	A8	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	A9	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Aa	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ab	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ac	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ad	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ae	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Af	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ag	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ah	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ai	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Aj	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ak	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Al	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Am	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	An	156/158 (99%)	135 (86%)	11 (7%)	10 (6%)	1	1
1	Ao	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ap	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Aq	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ar	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	As	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	At	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Au	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Av	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Aw	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ax	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ay	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Az	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
2	Ba	442/566 (78%)	362 (82%)	55 (12%)	25 (6%)	1	1
2	Bb	442/566 (78%)	365 (83%)	49 (11%)	28 (6%)	1	1
2	Bc	442/566 (78%)	363 (82%)	54 (12%)	25 (6%)	1	1
2	Bd	442/566 (78%)	363 (82%)	51 (12%)	28 (6%)	1	1
2	Be	442/566 (78%)	362 (82%)	55 (12%)	25 (6%)	1	1
2	Bf	442/566 (78%)	362 (82%)	52 (12%)	28 (6%)	1	1
3	Ca	308/417 (74%)	292 (95%)	9 (3%)	7 (2%)	5	5
3	Cb	308/417 (74%)	292 (95%)	10 (3%)	6 (2%)	6	6
4	Na	221/225 (98%)	180 (81%)	27 (12%)	14 (6%)	1	1
4	Nb	221/225 (98%)	181 (82%)	25 (11%)	15 (7%)	1	1
4	Nc	221/225 (98%)	182 (82%)	25 (11%)	14 (6%)	1	1
4	Nd	221/225 (98%)	182 (82%)	25 (11%)	14 (6%)	1	1
4	Ne	221/225 (98%)	181 (82%)	25 (11%)	15 (7%)	1	1
4	Nf	221/225 (98%)	181 (82%)	25 (11%)	15 (7%)	1	1
4	Ng	221/225 (98%)	181 (82%)	26 (12%)	14 (6%)	1	1
4	Nh	221/225 (98%)	182 (82%)	25 (11%)	14 (6%)	1	1
4	Ni	221/225 (98%)	182 (82%)	24 (11%)	15 (7%)	1	1
4	Nj	221/225 (98%)	183 (83%)	24 (11%)	14 (6%)	1	1
4	Nk	221/225 (98%)	181 (82%)	26 (12%)	14 (6%)	1	1
4	Nl	221/225 (98%)	181 (82%)	26 (12%)	14 (6%)	1	1
5	Oa	187/205 (91%)	169 (90%)	15 (8%)	3 (2%)	7	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Ob	187/205 (91%)	169 (90%)	15 (8%)	3 (2%)	7	7
5	Oc	187/205 (91%)	169 (90%)	15 (8%)	3 (2%)	7	7
5	Od	187/205 (91%)	169 (90%)	15 (8%)	3 (2%)	7	7
5	Oe	187/205 (91%)	169 (90%)	15 (8%)	3 (2%)	7	7
5	Of	187/205 (91%)	169 (90%)	15 (8%)	3 (2%)	7	7
5	Og	187/205 (91%)	169 (90%)	15 (8%)	3 (2%)	7	7
5	Oh	187/205 (91%)	169 (90%)	15 (8%)	3 (2%)	7	7
5	Oi	187/205 (91%)	169 (90%)	15 (8%)	3 (2%)	7	7
5	Oj	187/205 (91%)	169 (90%)	15 (8%)	3 (2%)	7	7
5	Ok	187/205 (91%)	169 (90%)	15 (8%)	3 (2%)	7	7
5	Ol	187/205 (91%)	170 (91%)	14 (8%)	3 (2%)	7	7
6	Ma	353/395 (89%)	320 (91%)	27 (8%)	6 (2%)	7	7
6	Mb	353/395 (89%)	320 (91%)	26 (7%)	7 (2%)	6	6
6	Mc	353/395 (89%)	321 (91%)	26 (7%)	6 (2%)	7	7
6	Md	353/395 (89%)	320 (91%)	24 (7%)	9 (2%)	4	4
6	Me	353/395 (89%)	321 (91%)	26 (7%)	6 (2%)	7	7
6	Mf	353/395 (89%)	318 (90%)	28 (8%)	7 (2%)	6	6
6	Mg	353/395 (89%)	320 (91%)	27 (8%)	6 (2%)	7	7
6	Mh	353/395 (89%)	317 (90%)	29 (8%)	7 (2%)	6	6
6	Mi	353/395 (89%)	321 (91%)	26 (7%)	6 (2%)	7	7
6	Mj	353/395 (89%)	319 (90%)	26 (7%)	8 (2%)	5	5
6	Mk	353/395 (89%)	319 (90%)	28 (8%)	6 (2%)	7	7
6	Ml	353/395 (89%)	319 (90%)	28 (8%)	6 (2%)	7	7
7	Qa	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
7	Qb	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
7	Qc	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
7	Qd	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
7	Qe	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
7	Qf	408/901 (45%)	359 (88%)	36 (9%)	13 (3%)	3	3
7	Qg	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
7	Qh	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	Qi	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
7	Qj	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
7	Qk	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
7	Ql	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
8	Pa	153/172 (89%)	110 (72%)	21 (14%)	22 (14%)	0	0
8	Pb	153/172 (89%)	106 (69%)	22 (14%)	25 (16%)	0	0
8	Pc	153/172 (89%)	108 (71%)	24 (16%)	21 (14%)	0	0
8	Pd	153/172 (89%)	109 (71%)	22 (14%)	22 (14%)	0	0
8	Pe	153/172 (89%)	111 (72%)	23 (15%)	19 (12%)	0	0
8	Pf	153/172 (89%)	115 (75%)	20 (13%)	18 (12%)	0	0
8	Pg	153/172 (89%)	112 (73%)	25 (16%)	16 (10%)	0	0
8	Ph	153/172 (89%)	110 (72%)	21 (14%)	22 (14%)	0	0
8	Pi	153/172 (89%)	116 (76%)	19 (12%)	18 (12%)	0	0
8	Pj	153/172 (89%)	116 (76%)	20 (13%)	17 (11%)	0	0
8	Pk	153/172 (89%)	115 (75%)	20 (13%)	18 (12%)	0	0
8	Pl	153/172 (89%)	115 (75%)	16 (10%)	22 (14%)	0	0
9	Ta	159/411 (39%)	114 (72%)	32 (20%)	13 (8%)	0	0
9	Tb	159/411 (39%)	114 (72%)	32 (20%)	13 (8%)	0	0
9	Tc	159/411 (39%)	114 (72%)	32 (20%)	13 (8%)	0	0
9	Td	159/411 (39%)	114 (72%)	33 (21%)	12 (8%)	1	1
9	Te	159/411 (39%)	114 (72%)	34 (21%)	11 (7%)	1	1
9	Tf	159/411 (39%)	114 (72%)	34 (21%)	11 (7%)	1	1
9	Tg	159/411 (39%)	114 (72%)	33 (21%)	12 (8%)	1	1
9	Th	159/411 (39%)	114 (72%)	33 (21%)	12 (8%)	1	1
9	Ti	159/411 (39%)	114 (72%)	32 (20%)	13 (8%)	0	0
9	Tj	159/411 (39%)	114 (72%)	33 (21%)	12 (8%)	1	1
9	Tk	159/411 (39%)	114 (72%)	32 (20%)	13 (8%)	0	0
9	Tl	159/411 (39%)	114 (72%)	32 (20%)	13 (8%)	0	0
All	All	26500/37468 (71%)	22659 (86%)	2521 (10%)	1320 (5%)	3	1

5 of 1320 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Aa	93	LEU
1	Aa	98	ASN
1	Ab	93	LEU
1	Ab	98	ASN
1	Ac	93	LEU

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

35 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	MEA	An	1	1	3,3,13	0.97	0	1,2,16	0.34	0
1	MEA	Aq	1	1	3,3,13	1.01	0	1,2,16	0.32	0
1	MEA	Aj	1	1	3,3,13	0.96	0	1,2,16	0.35	0
1	MEA	Av	1	1	3,3,13	0.98	0	1,2,16	0.34	0
1	MEA	A5	1	1	3,3,13	0.96	0	1,2,16	0.33	0
1	MEA	At	1	1	3,3,13	0.95	0	1,2,16	0.35	0
1	MEA	Ay	1	1	3,3,13	0.98	0	1,2,16	0.32	0
1	MEA	Al	1	1	3,3,13	0.97	0	1,2,16	0.33	0
1	MEA	Ao	1	1	3,3,13	0.91	0	1,2,16	0.35	0
1	MEA	Ad	1	1	3,3,13	1.01	0	1,2,16	0.33	0
1	MEA	Ag	1	1	3,3,13	0.97	0	1,2,16	0.33	0
1	MEA	Ai	1	1	3,3,13	0.99	0	1,2,16	0.32	0
1	MEA	A3	1	1	3,3,13	0.92	0	1,2,16	0.34	0
1	MEA	Aa	1	1	3,3,13	0.94	0	1,2,16	0.34	0
1	MEA	Ah	1	1	3,3,13	0.95	0	1,2,16	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MEA	A6	1	1	3,3,13	0.96	0	1,2,16	0.33	0
1	MEA	A1	1	1	3,3,13	1.01	0	1,2,16	0.32	0
1	MEA	Aw	1	1	3,3,13	0.97	0	1,2,16	0.34	0
1	MEA	A2	1	1	3,3,13	0.97	0	1,2,16	0.35	0
1	MEA	Ac	1	1	3,3,13	0.98	0	1,2,16	0.32	0
1	MEA	Ae	1	1	3,3,13	0.98	0	1,2,16	0.34	0
1	MEA	A7	1	1	3,3,13	1.01	0	1,2,16	0.34	0
1	MEA	Ap	1	1	3,3,13	0.98	0	1,2,16	0.33	0
1	MEA	As	1	1	3,3,13	0.97	0	1,2,16	0.34	0
1	MEA	Ab	1	1	3,3,13	0.97	0	1,2,16	0.35	0
1	MEA	Au	1	1	3,3,13	0.98	0	1,2,16	0.34	0
1	MEA	Ax	1	1	3,3,13	0.98	0	1,2,16	0.33	0
1	MEA	Az	1	1	3,3,13	1.00	0	1,2,16	0.32	0
1	MEA	A9	1	1	3,3,13	0.97	0	1,2,16	0.33	0
1	MEA	Af	1	1	3,3,13	0.96	0	1,2,16	0.33	0
1	MEA	Ar	1	1	3,3,13	0.99	0	1,2,16	0.33	0
1	MEA	Am	1	1	3,3,13	0.90	0	1,2,16	0.36	0
1	MEA	Ak	1	1	3,3,13	0.93	0	1,2,16	0.34	0
1	MEA	A8	1	1	3,3,13	0.98	0	1,2,16	0.34	0
1	MEA	A4	1	1	3,3,13	0.96	0	1,2,16	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MEA	An	1	1	-	0/0/1/10	-
1	MEA	Aq	1	1	-	0/0/1/10	-
1	MEA	Aj	1	1	-	0/0/1/10	-
1	MEA	Av	1	1	-	0/0/1/10	-
1	MEA	A5	1	1	-	0/0/1/10	-
1	MEA	At	1	1	-	0/0/1/10	-
1	MEA	Ay	1	1	-	0/0/1/10	-
1	MEA	Al	1	1	-	0/0/1/10	-
1	MEA	Ao	1	1	-	0/0/1/10	-
1	MEA	Ad	1	1	-	0/0/1/10	-
1	MEA	Ag	1	1	-	0/0/1/10	-
1	MEA	Ai	1	1	-	0/0/1/10	-
1	MEA	A3	1	1	-	0/0/1/10	-
1	MEA	Aa	1	1	-	0/0/1/10	-
1	MEA	Ah	1	1	-	0/0/1/10	-
1	MEA	A6	1	1	-	0/0/1/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MEA	A1	1	1	-	0/0/1/10	-
1	MEA	Aw	1	1	-	0/0/1/10	-
1	MEA	A2	1	1	-	0/0/1/10	-
1	MEA	Ac	1	1	-	0/0/1/10	-
1	MEA	Ae	1	1	-	0/0/1/10	-
1	MEA	A7	1	1	-	0/0/1/10	-
1	MEA	Ap	1	1	-	0/0/1/10	-
1	MEA	As	1	1	-	0/0/1/10	-
1	MEA	Ab	1	1	-	0/0/1/10	-
1	MEA	Au	1	1	-	0/0/1/10	-
1	MEA	Ax	1	1	-	0/0/1/10	-
1	MEA	Az	1	1	-	0/0/1/10	-
1	MEA	A9	1	1	-	0/0/1/10	-
1	MEA	Af	1	1	-	0/0/1/10	-
1	MEA	Ar	1	1	-	0/0/1/10	-
1	MEA	Am	1	1	-	0/0/1/10	-
1	MEA	Ak	1	1	-	0/0/1/10	-
1	MEA	A8	1	1	-	0/0/1/10	-
1	MEA	A4	1	1	-	0/0/1/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	Aa	1	MEA	4	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	Pb	1
8	Pc	1
8	Pd	1
8	Pi	1
8	Pk	1
8	Pa	1
8	Pe	1
8	Pf	1
8	Pg	1
8	Ph	1
8	Pj	1
8	Pl	1

The worst 5 of 12 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Pb	63:PRO	C	64:VAL	N	1.66
1	Pc	63:PRO	C	64:VAL	N	1.66
1	Pd	63:PRO	C	64:VAL	N	1.66
1	Pi	63:PRO	C	64:VAL	N	1.66
1	Pk	63:PRO	C	64:VAL	N	1.66

6 Tomogram visualisation

This section contains visualisations of the EMDB entry EMD-3247. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Mask visualisation

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

7 Tomogram analysis

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

7.1 Map-value distribution

This section was not generated.

8 Map-model fit

This section was not generated.