



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 08:22 AM EST

PDB ID : 3JC8
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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

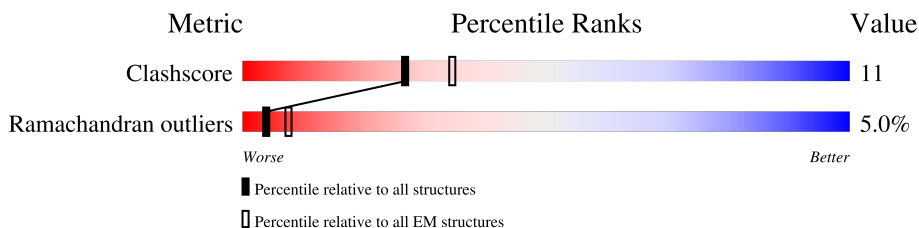
1 Overall quality at a glance

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.



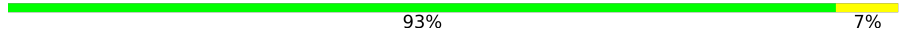
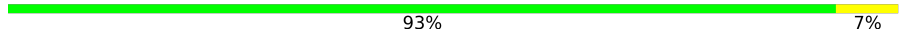
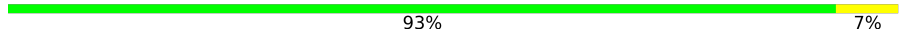
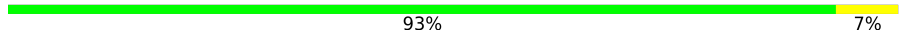
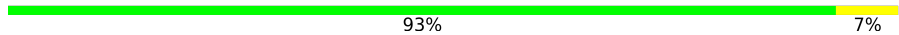
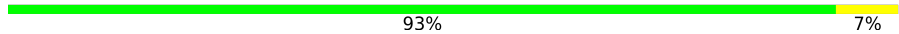
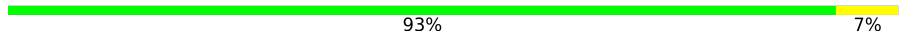
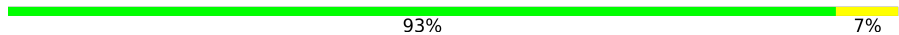
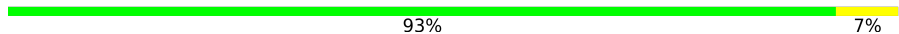
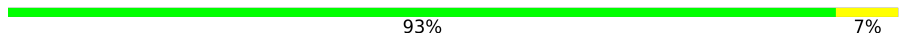
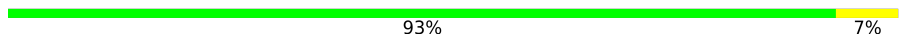
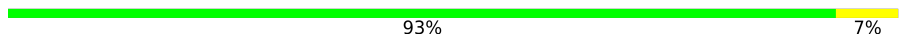

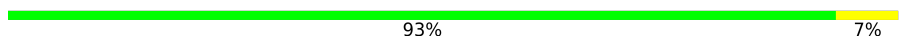










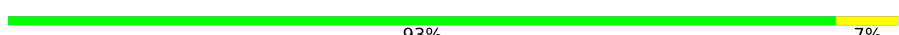
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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	 89% 8% .
1	A2	158	 89% 8% .
1	A3	158	 89% 8% .
1	A4	158	 89% 8% .
1	A5	158	 89% 8% .
1	A6	158	 91% 7% .
1	A7	158	 89% 8% .
1	A8	158	 91% 7% .
1	A9	158	 90% 7% .
1	Aa	158	 93% 7%


























Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Ab	158	 93% 7%
1	Ac	158	 93% 7%
1	Ad	158	 93% 7%
1	Ae	158	 93% 7%
1	Af	158	 93% 7%
1	Ag	158	 93% 7%
1	Ah	158	 93% 7%
1	Ai	158	 93% 7%
1	Aj	158	 93% 7%
1	Ak	158	 93% 7%
1	Al	158	 93% 7%
1	Am	158	 93% 7%
1	An	158	 92% 8%
1	Ao	158	 93% 7%
1	Ap	158	 93% 7%
1	Aq	158	 93% 7%
1	Ar	158	 93% 7%
1	As	158	 93% 7%
1	At	158	 93% 7%
1	Au	158	 93% 7%
1	Av	158	 93% 7%
1	Aw	158	 93% 7%
1	Ax	158	 93% 7%
1	Ay	158	 93% 7%
1	Az	158	 93% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	Ba	566	 75% 5% 20%
2	Bb	566	 74% 5% 20%
2	Bc	566	 75% 5% 20%
2	Bd	566	 74% 5% 20%
2	Be	566	 75% 5% 20%
2	Bf	566	 74% 6% 20%
3	Ca	417	 71% 5% 24%
3	Cb	417	 71% 5% 24%
4	Na	225	 91% 8%
4	Nb	225	 90% 8%
4	Nc	225	 91% 8%
4	Nd	225	 91% 8%
4	Ne	225	 91% 8%
4	Nf	225	 91% 8%
4	Ng	225	 91% 8%
4	Nh	225	 91% 8%
4	Ni	225	 91% 8%
4	Nj	225	 91% 8%
4	Nk	225	 91% 8%
4	Nl	225	 91% 8%
5	Oa	205	 91% 8%
5	Ob	205	 91% 8%
5	Oc	205	 91% 8%
5	Od	205	 91% 8%
5	Oe	205	 91% 8%


























Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
5	Of	205	91%	8%
5	Og	205	91%	8%
5	Oh	205	91%	8%
5	Oi	205	91%	8%
5	Oj	205	91%	8%
5	Ok	205	91%	8%
5	Ol	205	91%	8%
6	Ma	395	88%	10%
6	Mb	395	88%	10%
6	Mc	395	88%	10%
6	Md	395	87%	10%
6	Me	395	88%	10%
6	Mf	395	88%	10%
6	Mg	395	88%	10%
6	Mh	395	88%	10%
6	Mi	395	88%	10%
6	Mj	395	88%	10%
6	Mk	395	88%	10%
6	Ml	395	88%	10%
7	Qa	901	43%	54%
7	Qb	901	42%	54%
7	Qc	901	43%	54%
7	Qd	901	42%	54%
7	Qe	901	42%	54%
7	Qf	901	43%	54%






Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	Qg	901	 42% 54%
7	Qh	901	 43% 54%
7	Qi	901	 42% 54%
7	Qj	901	 42% 54%
7	Qk	901	 43% 54%
7	Ql	901	 42% 54%
8	Pa	172	 70% 12% 8% 10%
8	Pb	172	 69% 12% 9% 10%
8	Pc	172	 73% 10% 6% 10%
8	Pd	172	 70% 12% 7% 10%
8	Pe	172	 73% 11% 6% 10%
8	Pf	172	 74% 9% 6% 10%
8	Pg	172	 73% 12% 5% 10%
8	Ph	172	 70% 13% 6% 10%
8	Pi	172	 74% 9% 6% 10%
8	Pj	172	 76% 8% 5% 10%
8	Pk	172	 75% 9% 5% 10%
8	Pl	172	 73% 9% 7% 10%
9	Ta	411	 35% 5% 60%
9	Tb	411	 35% 5% 60%
9	Tc	411	 35% 5% 60%
9	Td	411	 35% 60%
9	Te	411	 36% 60%
9	Tf	411	 36% 60%
9	Tg	411	 35% 60%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	Th	411	 35% 5% 60%
9	Ti	411	 35% 5% 60%
9	Tj	411	 35% 5% 60%
9	Tk	411	 35% 5% 60%
9	Tl	411	 35% 5% 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
			Total	C	N	O		
1	Aa	158	632	316	158	158	0	0
1	Ab	158	632	316	158	158	0	0
1	Ac	158	632	316	158	158	0	0
1	Ad	158	632	316	158	158	0	0
1	Ae	158	632	316	158	158	0	0
1	Af	158	632	316	158	158	0	0
1	Ag	158	632	316	158	158	0	0
1	Ah	158	632	316	158	158	0	0
1	Ai	158	632	316	158	158	0	0
1	Aj	158	632	316	158	158	0	0
1	Ak	158	632	316	158	158	0	0
1	Al	158	632	316	158	158	0	0
1	Am	158	632	316	158	158	0	0
1	An	158	632	316	158	158	0	0
1	Ao	158	632	316	158	158	0	0
1	Ap	158	632	316	158	158	0	0
1	Aq	158	632	316	158	158	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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

- Molecule 7 is a protein called PilQ.

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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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

Chain Aa:  93% 7%



- Molecule 1: PilA

Chain Ab:  93% 7%



- Molecule 1: PilA

Chain Ac:  93% 7%



- Molecule 1: PilA

Chain Ad:  93% 7%



- Molecule 1: PilA

Chain Ae:  93% 7%



- Molecule 1: PilA

Chain Af:  93% 7%



• 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





• Molecule 1: PilA



• Molecule 1: PilA



• Molecule 1: PilA



• Molecule 1: PilA



• Molecule 1: PilA



• Molecule 1: PilA

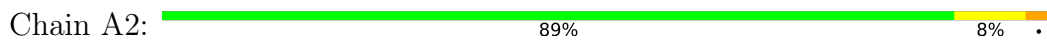


• Molecule 1: PilA

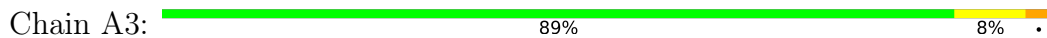




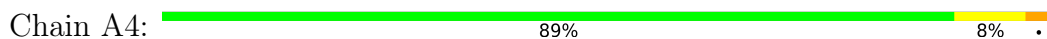
• Molecule 1: PilA



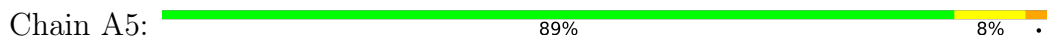
• Molecule 1: PilA



• Molecule 1: PilA



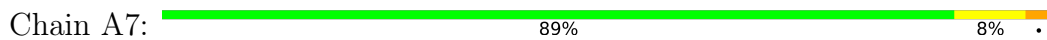
• Molecule 1: PilA



• Molecule 1: PilA



• Molecule 1: PilA



• Molecule 1: PilA

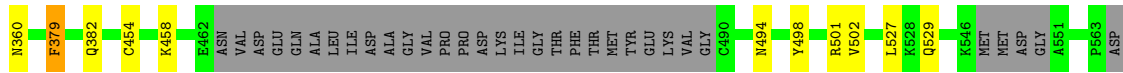
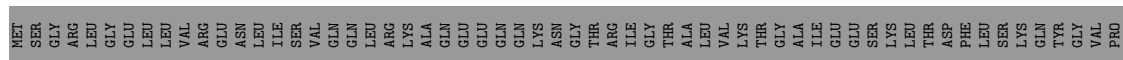
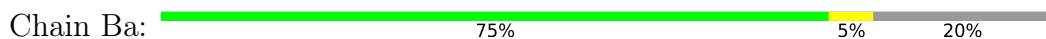




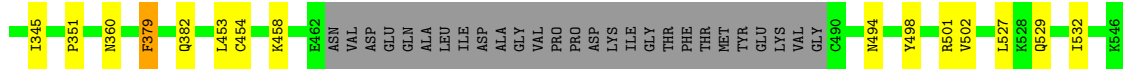
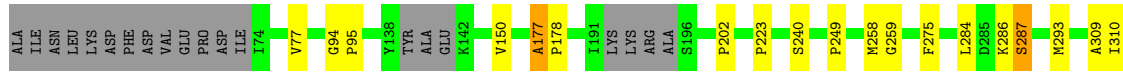
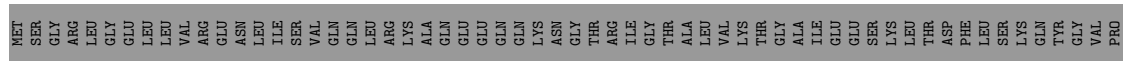
• Molecule 1: PilA



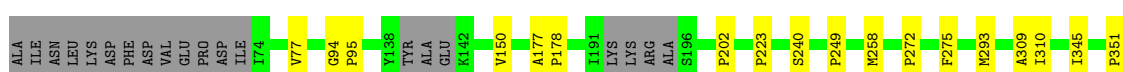
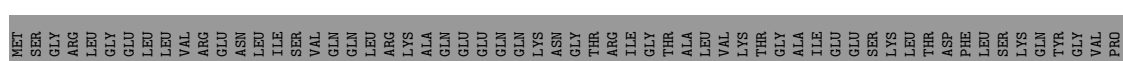
• Molecule 2: Type IV-A pilus assembly ATPase PilB

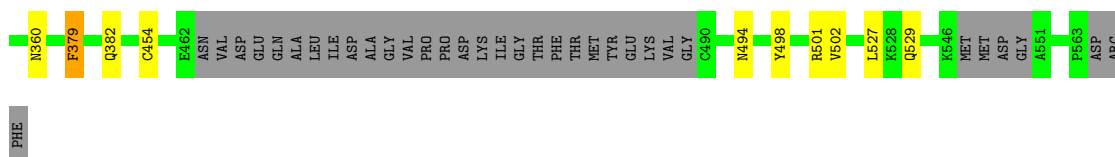


• Molecule 2: Type IV-A pilus assembly ATPase PilB



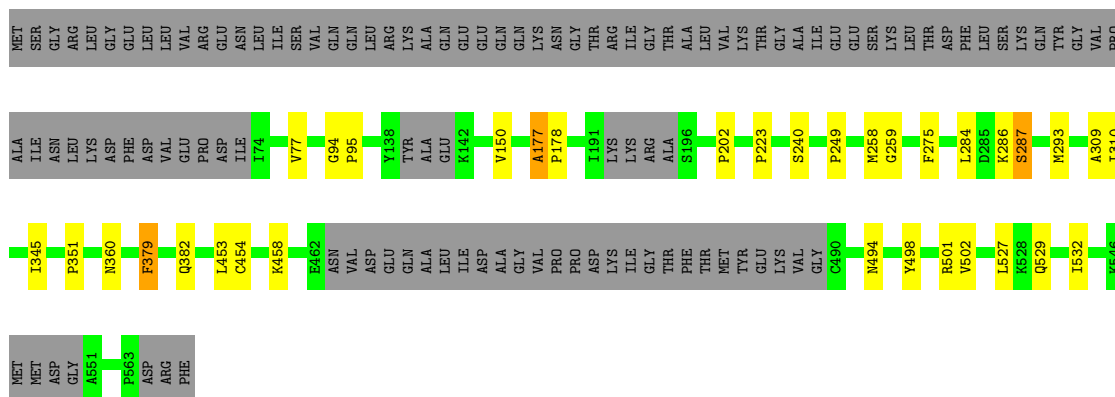
• Molecule 2: Type IV-A pilus assembly ATPase PilB





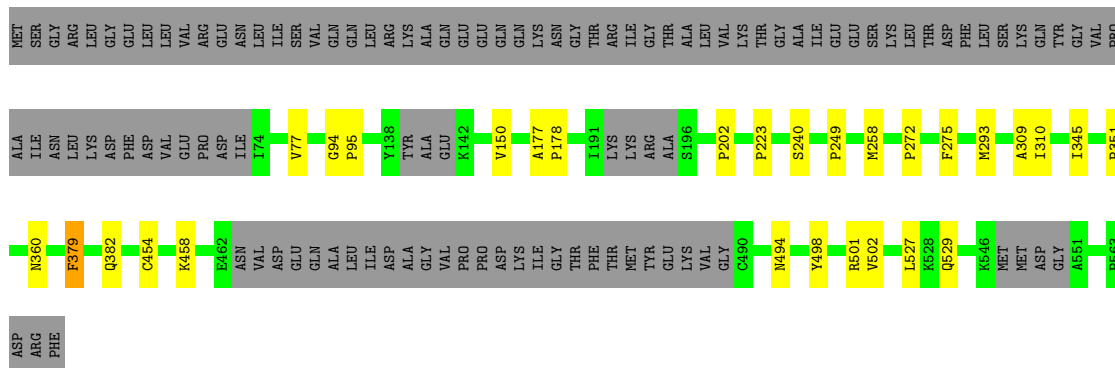
- Molecule 2: Type IV-A pilus assembly ATPase PilB

Chain Bd: 74% 5% 20%



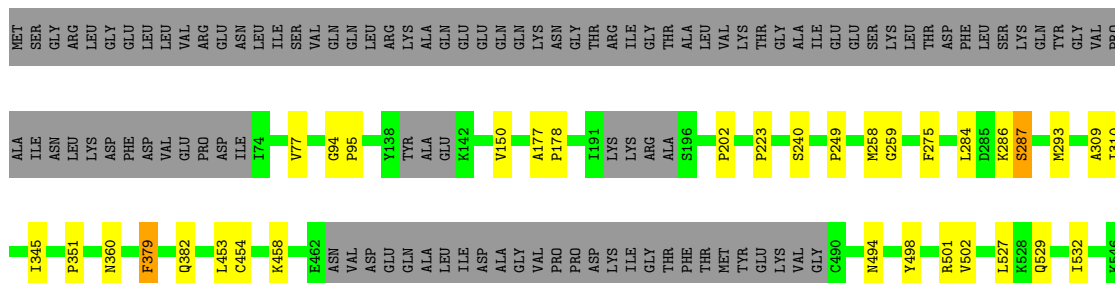
- Molecule 2: Type IV-A pilus assembly ATPase PilB

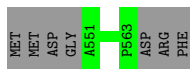
Chain Be: 75% 5% 20%



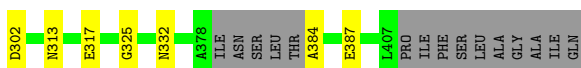
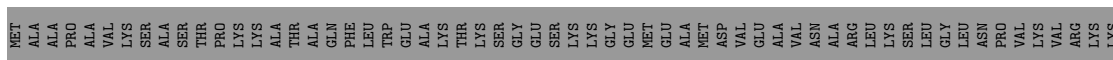
- Molecule 2: Type IV-A pilus assembly ATPase PilB

Chain Bf: 74% 6% 20%

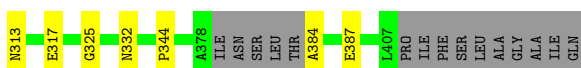
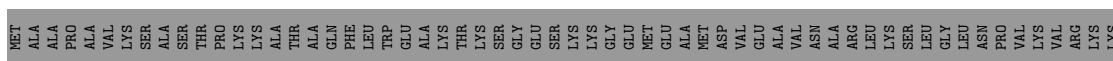




• Molecule 3: Type 4 fimbrial assembly protein PilC



• Molecule 3: Type 4 fimbrial assembly protein PilC



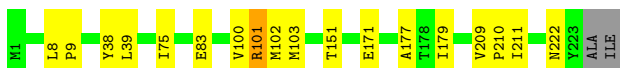
• Molecule 4: PilN




• Molecule 4: PilN



• Molecule 4: PilN



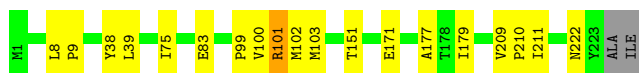
• Molecule 4: PilN

Chain Nd:  91% 8%



• Molecule 4: Pi1N

Chain Ne:  91% 8%



• Molecule 4: Pi1N

Chain Nf:  91% 8%



• Molecule 4: Pi1N

Chain Ng:  91% 8%



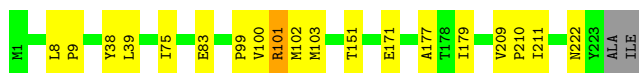
• Molecule 4: Pi1N

Chain Nh:  91% 8%



• Molecule 4: Pi1N

Chain Ni:  91% 8%



• Molecule 4: Pi1N

Chain Nj:  91% 8%



• Molecule 4: Pi1N

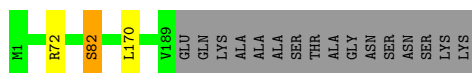
Chain Nk:  91% 8%



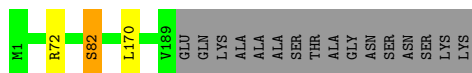
• Molecule 4: PiIN



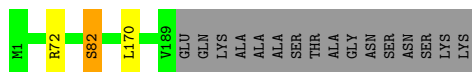
• Molecule 5: PiIO



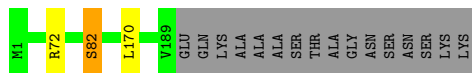
• Molecule 5: PiIO



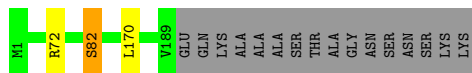
• Molecule 5: PiIO



• Molecule 5: PiIO

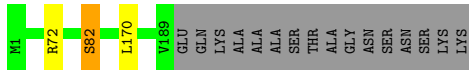


• Molecule 5: PiIO

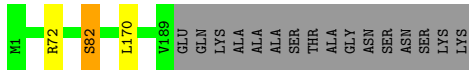


• Molecule 5: PiIO

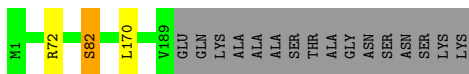
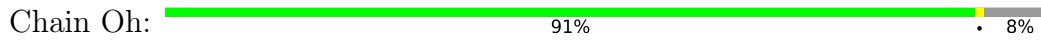




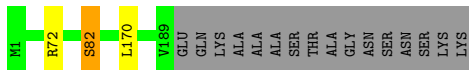
- Molecule 5: PilO



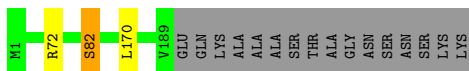
- Molecule 5: PilO



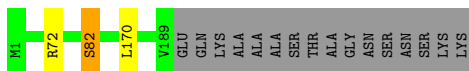
- Molecule 5: PilO



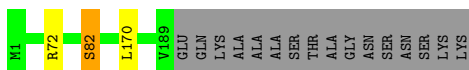
- Molecule 5: PilO



- Molecule 5: PilO

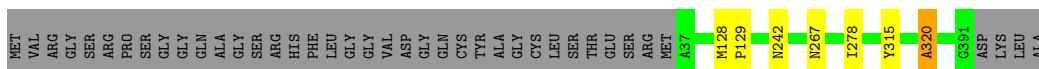


- Molecule 5: PilO

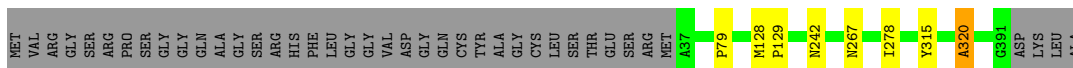


- Molecule 6: Type IV pilus biogenesis protein PilM

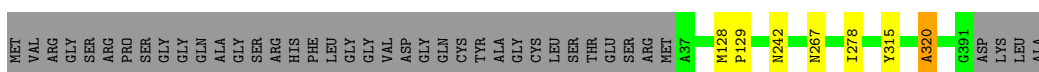
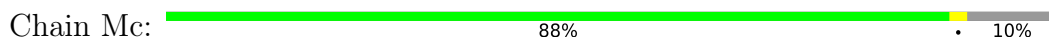




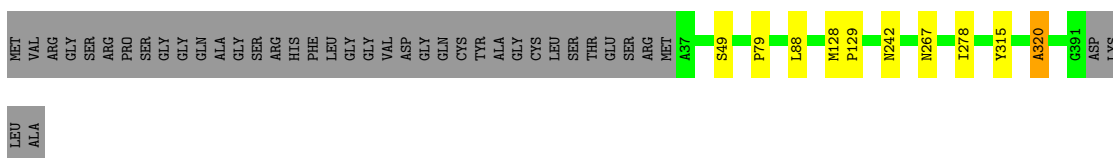
• Molecule 6: Type IV pilus biogenesis protein PilM



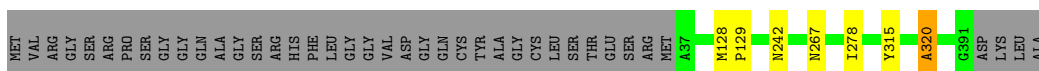
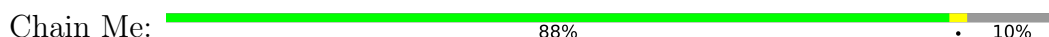
• Molecule 6: Type IV pilus biogenesis protein PilM



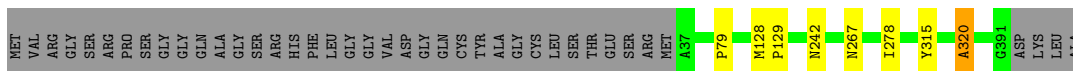
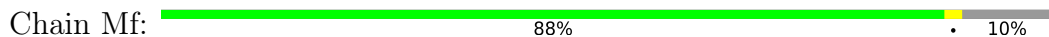
• Molecule 6: Type IV pilus biogenesis protein PilM



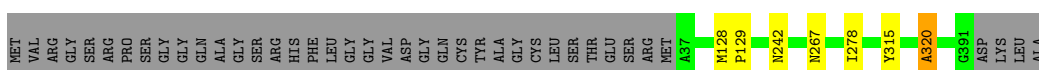
• Molecule 6: Type IV pilus biogenesis protein PilM



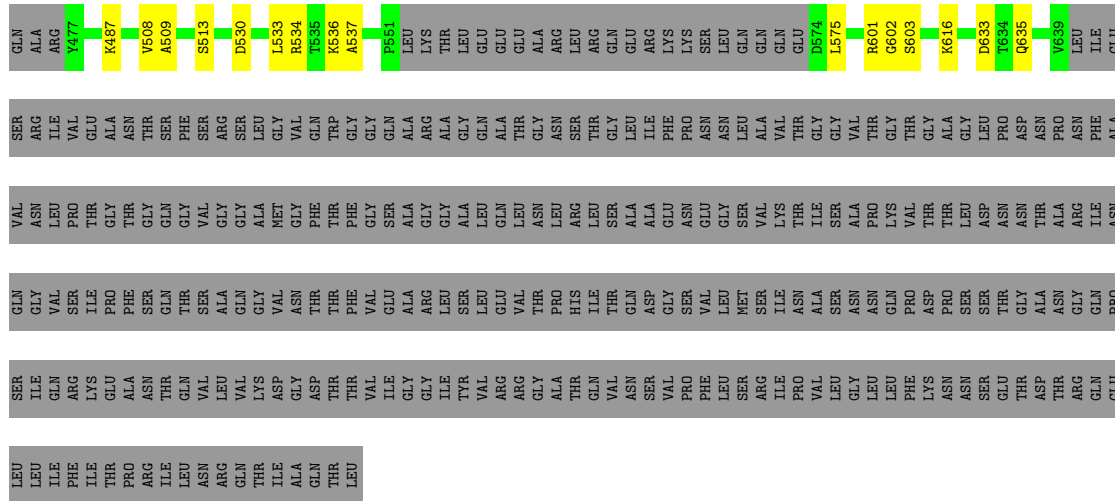
• Molecule 6: Type IV pilus biogenesis protein PilM



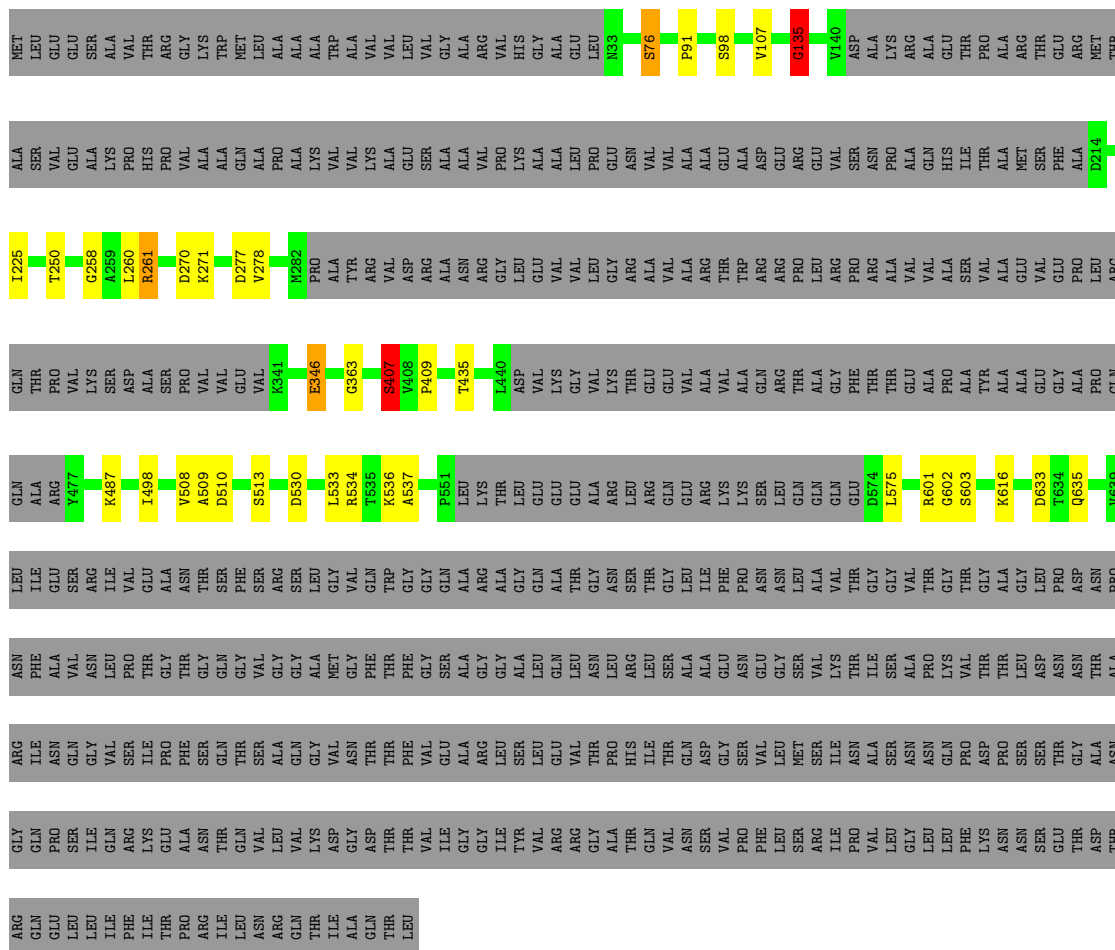
• Molecule 6: Type IV pilus biogenesis protein PilM



• Molecule 6: Type IV pilus biogenesis protein PilM

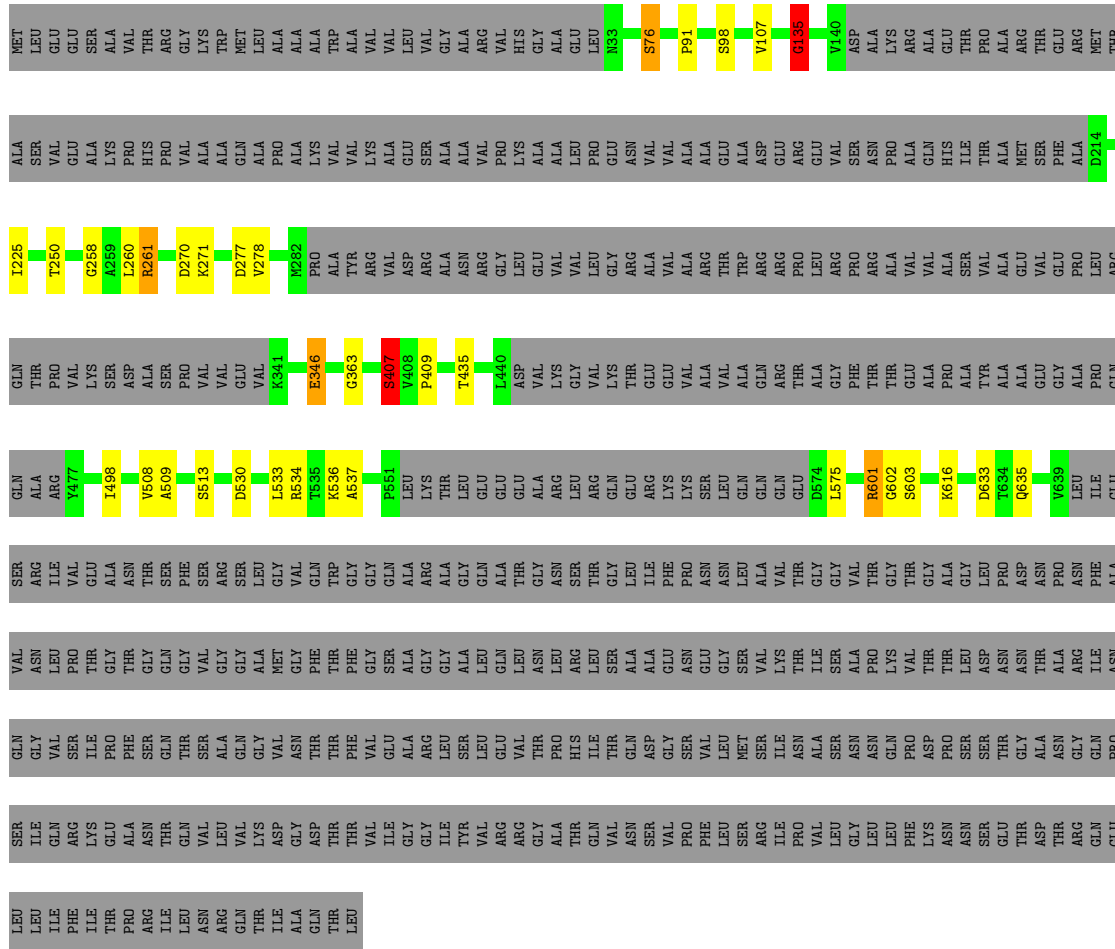


• Molecule 7: PilQ

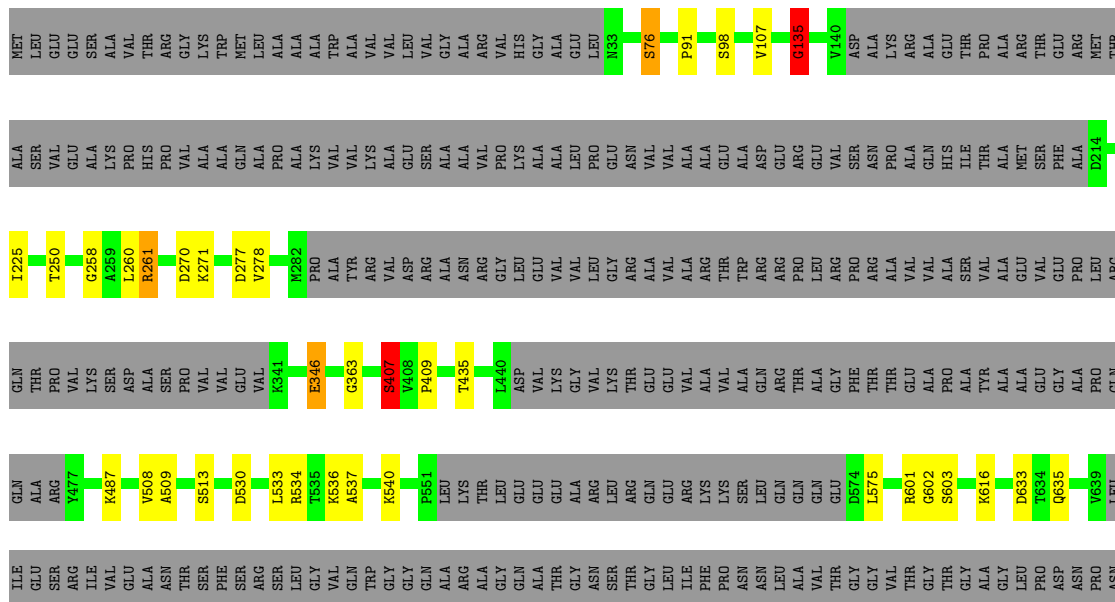


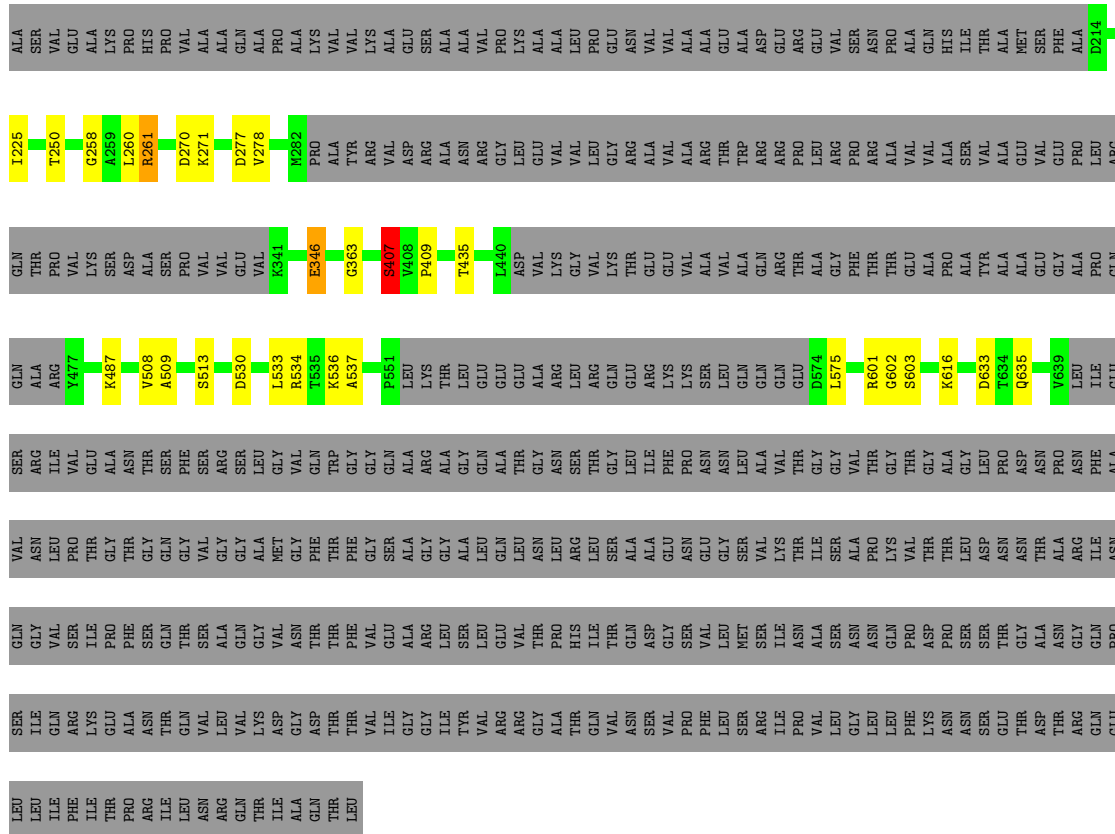
• Molecule 7: PilQ



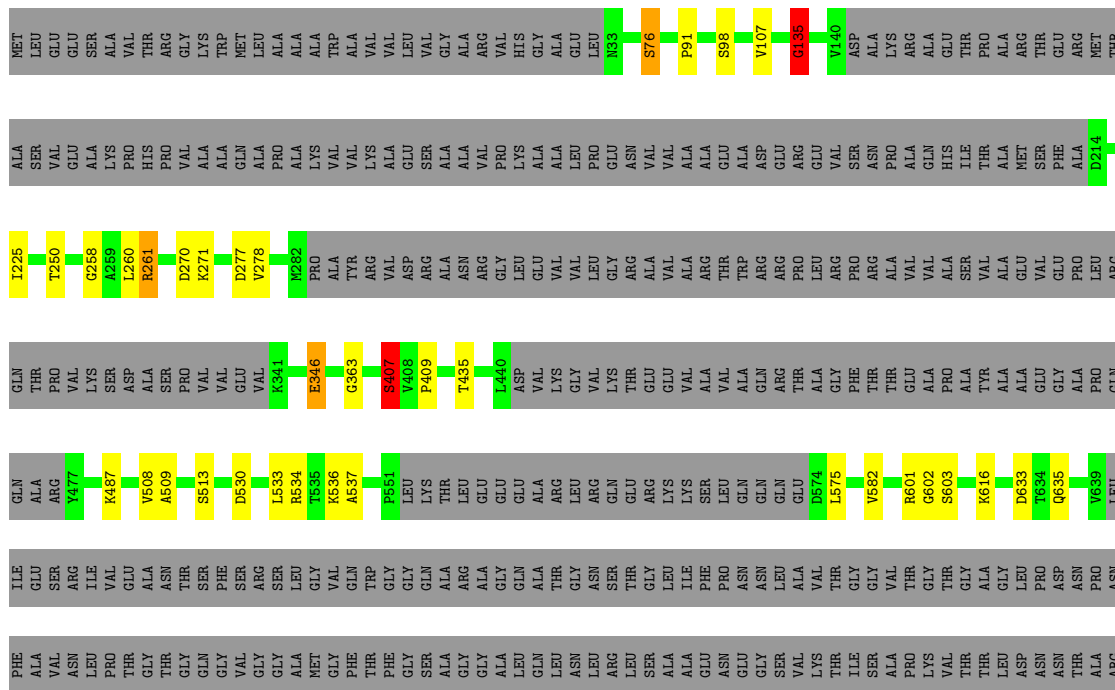


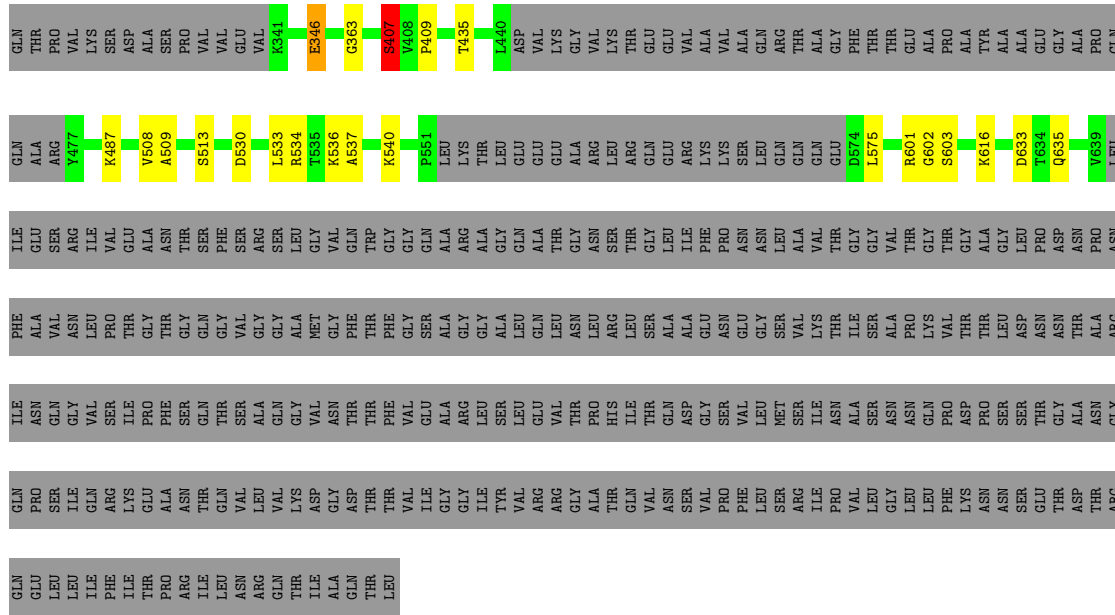
● Molecule 7: PilQ



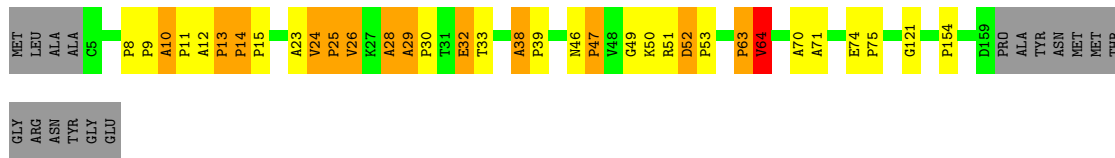


● Molecule 7: PilQ

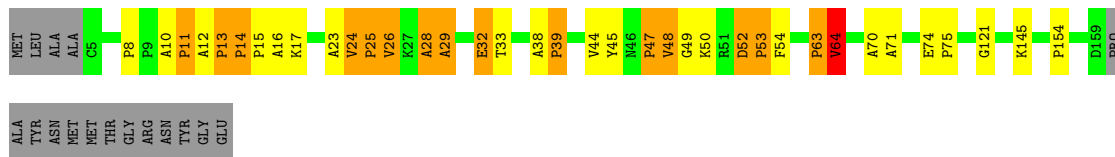




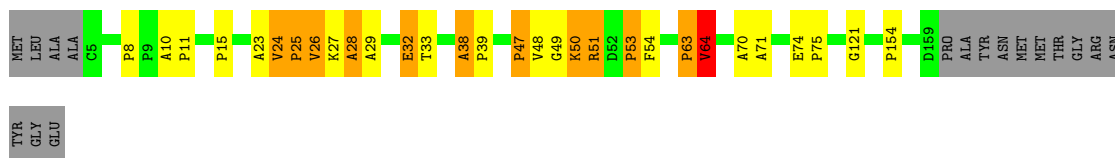
• Molecule 8: PiIP



• Molecule 8: PiIP

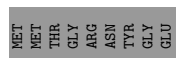


• Molecule 8: PiIP

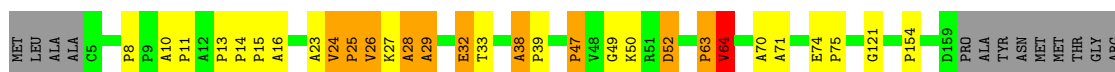


• Molecule 8: PiIP

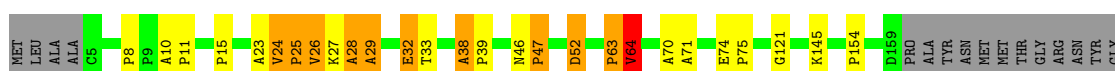




• Molecule 8: PiIP



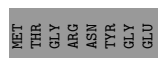
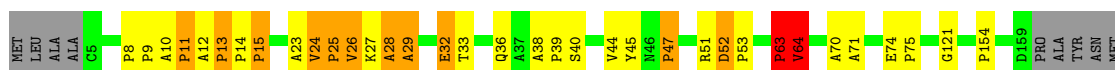
• Molecule 8: PiIP



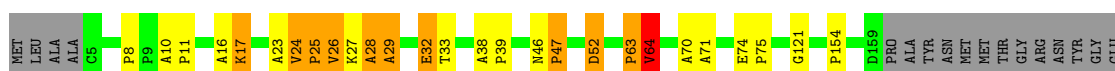
• Molecule 8: PiIP

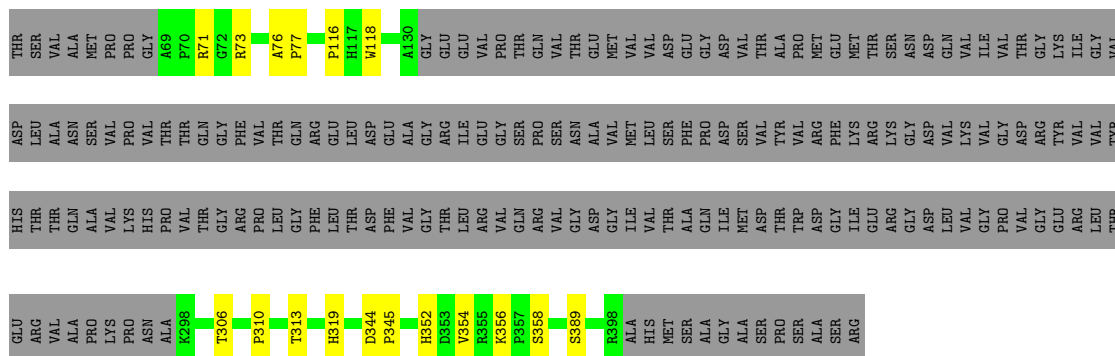


• Molecule 8: PiIP

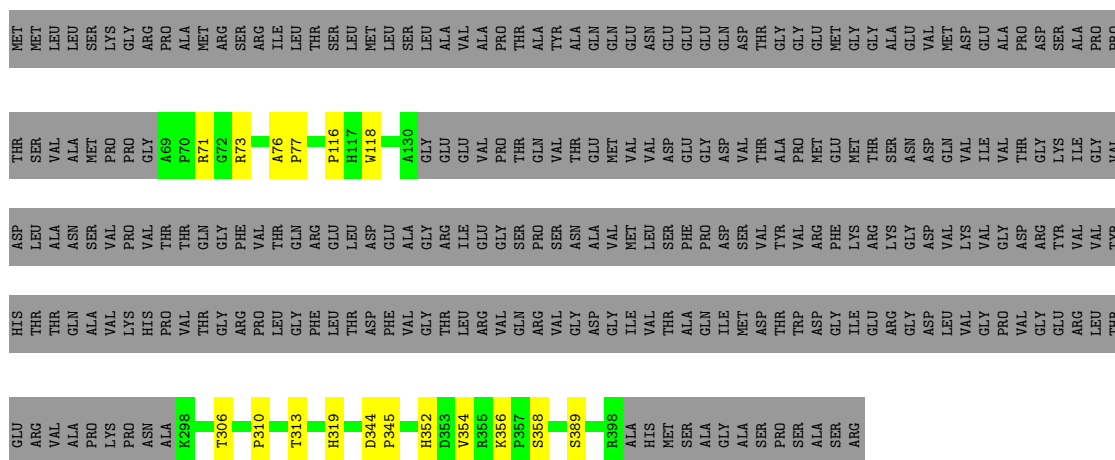


• Molecule 8: PiIP

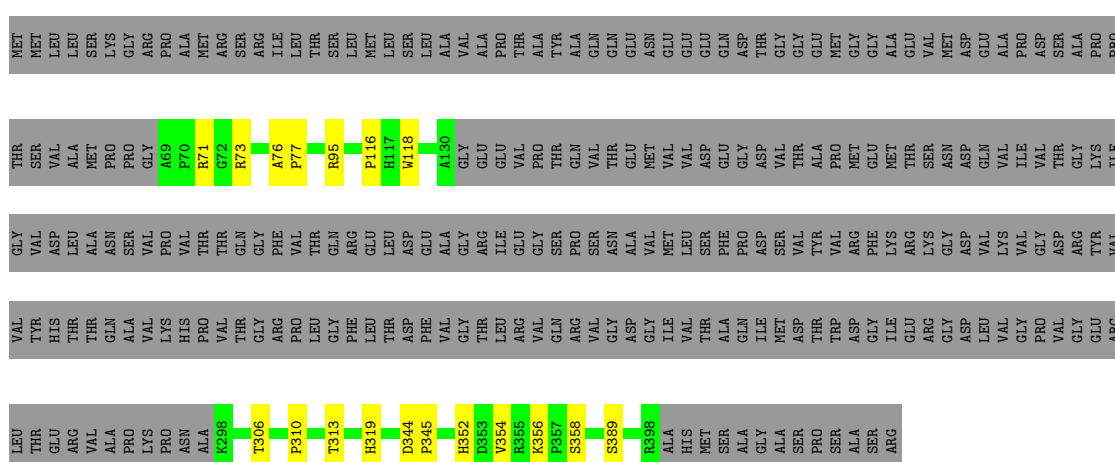




● Molecule 9: LysM domain protein

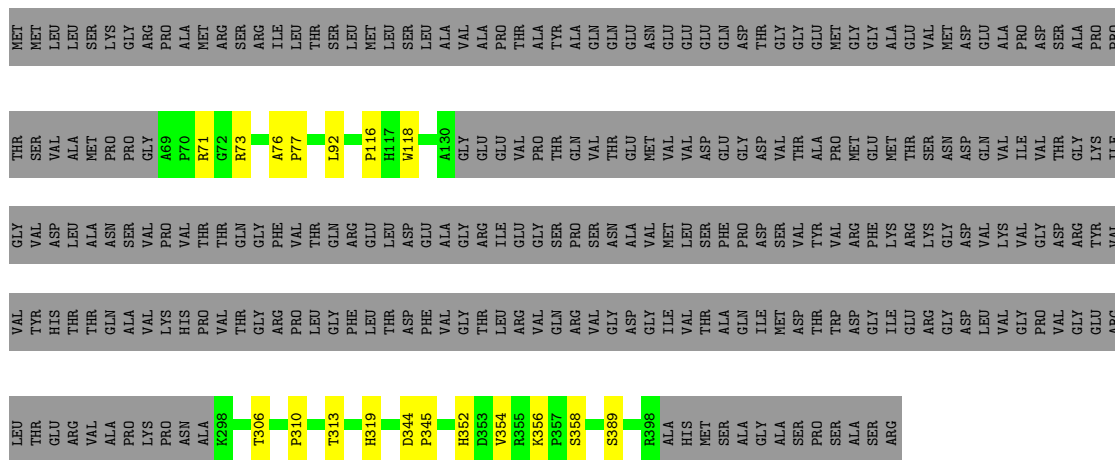


● Molecule 9: LysM domain protein

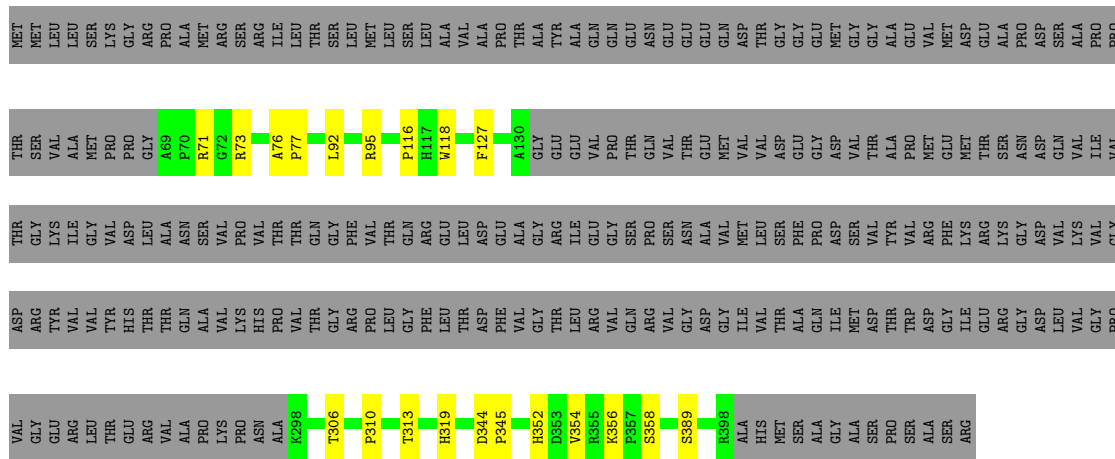


● Molecule 9: LysM domain protein

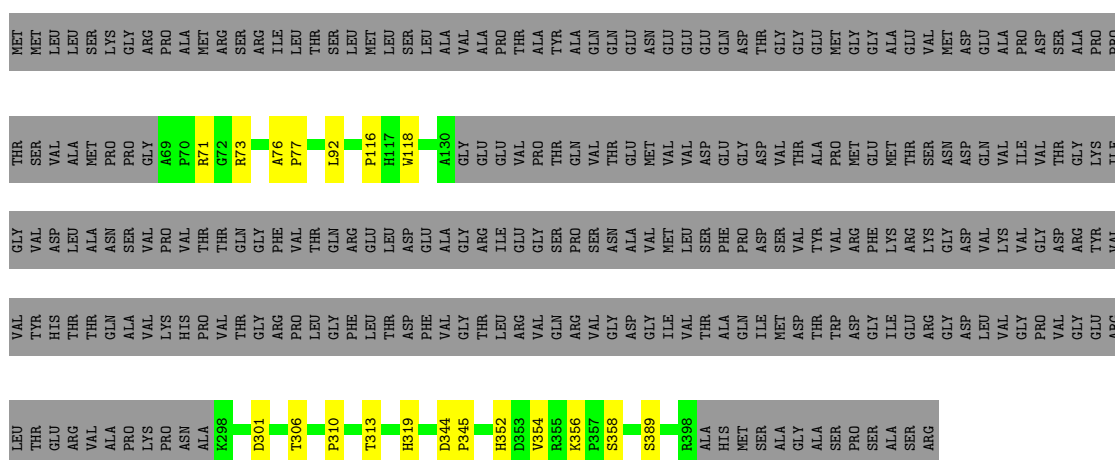
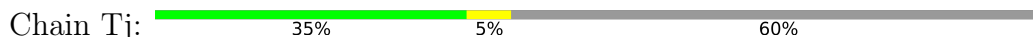




• Molecule 9: LysM domain protein



• Molecule 9: LysM domain protein



• Molecule 9: LysM domain protein

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 i

5.1 Standard geometry i

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	0.70	1/627 (0.2%)	0.72	1/782 (0.1%)
1	A2	0.70	1/627 (0.2%)	0.72	1/782 (0.1%)
1	A3	0.70	1/627 (0.2%)	0.72	1/782 (0.1%)
1	A4	0.70	1/627 (0.2%)	0.72	1/782 (0.1%)
1	A5	0.70	1/627 (0.2%)	0.72	1/782 (0.1%)
1	A6	0.69	1/627 (0.2%)	0.72	1/782 (0.1%)
1	A7	0.70	1/627 (0.2%)	0.72	1/782 (0.1%)
1	A8	0.70	1/627 (0.2%)	0.72	1/782 (0.1%)
1	A9	0.71	1/627 (0.2%)	0.72	1/782 (0.1%)
1	Aa	0.71	1/627 (0.2%)	0.72	1/782 (0.1%)
1	Ab	0.71	1/627 (0.2%)	0.72	1/782 (0.1%)
1	Ac	0.70	1/627 (0.2%)	0.71	1/782 (0.1%)
1	Ad	0.71	1/627 (0.2%)	0.72	1/782 (0.1%)
1	Ae	0.71	1/627 (0.2%)	0.72	1/782 (0.1%)
1	Af	0.70	1/627 (0.2%)	0.71	1/782 (0.1%)
1	Ag	0.71	1/627 (0.2%)	0.72	1/782 (0.1%)
1	Ah	0.70	1/627 (0.2%)	0.72	1/782 (0.1%)
1	Ai	0.70	1/627 (0.2%)	0.72	1/782 (0.1%)
1	Aj	0.70	1/627 (0.2%)	0.72	1/782 (0.1%)
1	Ak	0.71	1/627 (0.2%)	0.72	1/782 (0.1%)
1	Al	0.70	1/627 (0.2%)	0.72	1/782 (0.1%)
1	Am	0.70	1/627 (0.2%)	0.71	1/782 (0.1%)
1	An	0.69	1/627 (0.2%)	0.70	1/782 (0.1%)
1	Ao	0.70	1/627 (0.2%)	0.72	1/782 (0.1%)
1	Ap	0.70	1/627 (0.2%)	0.72	1/782 (0.1%)
1	Aq	0.71	1/627 (0.2%)	0.72	1/782 (0.1%)
1	Ar	0.70	1/627 (0.2%)	0.72	1/782 (0.1%)
1	As	0.71	1/627 (0.2%)	0.72	1/782 (0.1%)
1	At	0.70	1/627 (0.2%)	0.72	1/782 (0.1%)
1	Au	0.70	1/627 (0.2%)	0.72	1/782 (0.1%)
1	Av	0.71	1/627 (0.2%)	0.72	1/782 (0.1%)
1	Aw	0.71	1/627 (0.2%)	0.72	1/782 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Ax	0.70	1/627 (0.2%)	0.72	1/782 (0.1%)
1	Ay	0.71	1/627 (0.2%)	0.72	1/782 (0.1%)
1	Az	0.70	1/627 (0.2%)	0.72	1/782 (0.1%)
2	Ba	0.44	0/1803	0.77	1/2245 (0.0%)
2	Bb	0.49	2/1803 (0.1%)	0.78	1/2245 (0.0%)
2	Bc	0.44	0/1803	0.77	0/2245
2	Bd	0.47	1/1803 (0.1%)	0.79	1/2245 (0.0%)
2	Be	0.45	0/1803	0.77	1/2245 (0.0%)
2	Bf	0.47	0/1803	0.79	1/2245 (0.0%)
3	Ca	0.62	0/1260	0.93	1/1568 (0.1%)
3	Cb	0.62	0/1260	0.92	1/1568 (0.1%)
4	Na	0.32	0/891	0.61	0/1112
4	Nb	0.34	0/891	0.62	0/1112
4	Nc	0.33	0/891	0.62	0/1112
4	Nd	0.33	0/891	0.62	0/1112
4	Ne	0.33	0/891	0.62	0/1112
4	Nf	0.33	0/891	0.62	0/1112
4	Ng	0.33	0/891	0.62	0/1112
4	Nh	0.33	0/891	0.62	0/1112
4	Ni	0.32	0/891	0.62	0/1112
4	Nj	0.33	0/891	0.62	0/1112
4	Nk	0.33	0/891	0.62	0/1112
4	Nl	0.32	0/891	0.62	0/1112
5	Oa	0.29	0/755	0.55	0/942
5	Ob	0.30	0/755	0.54	0/942
5	Oc	0.29	0/755	0.55	0/942
5	Od	0.30	0/755	0.55	0/942
5	Oe	0.29	0/755	0.55	0/942
5	Of	0.29	0/755	0.55	0/942
5	Og	0.30	0/755	0.55	0/942
5	Oh	0.29	0/755	0.55	0/942
5	Oi	0.30	0/755	0.55	0/942
5	Oj	0.30	0/755	0.55	0/942
5	Ok	0.30	0/755	0.55	0/942
5	Ol	0.30	0/755	0.55	0/942
6	Ma	0.33	0/1419	0.60	0/1772
6	Mb	0.32	0/1419	0.60	0/1772
6	Mc	0.33	0/1419	0.61	0/1772
6	Md	0.33	0/1419	0.60	0/1772
6	Me	0.32	0/1419	0.61	0/1772
6	Mf	0.32	0/1419	0.60	0/1772
6	Mg	0.33	0/1419	0.60	0/1772
6	Mh	0.32	0/1419	0.60	0/1772

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	Mi	0.33	0/1419	0.61	0/1772
6	Mj	0.33	0/1419	0.60	0/1772
6	Mk	0.32	0/1419	0.60	0/1772
6	Ml	0.33	0/1419	0.60	0/1772
7	Qa	0.63	1/1667 (0.1%)	1.72	10/2075 (0.5%)
7	Qb	0.63	1/1667 (0.1%)	1.71	10/2075 (0.5%)
7	Qc	0.63	1/1667 (0.1%)	1.72	11/2075 (0.5%)
7	Qd	0.63	1/1667 (0.1%)	1.72	10/2075 (0.5%)
7	Qe	0.63	1/1667 (0.1%)	1.72	10/2075 (0.5%)
7	Qf	0.63	1/1667 (0.1%)	1.72	10/2075 (0.5%)
7	Qg	0.63	1/1667 (0.1%)	1.72	10/2075 (0.5%)
7	Qh	0.63	1/1667 (0.1%)	1.72	10/2075 (0.5%)
7	Qi	0.63	1/1667 (0.1%)	1.71	10/2075 (0.5%)
7	Qj	0.63	1/1667 (0.1%)	1.72	10/2075 (0.5%)
7	Qk	0.63	1/1667 (0.1%)	1.72	10/2075 (0.5%)
7	Ql	0.63	1/1667 (0.1%)	1.71	10/2075 (0.5%)
8	Pa	0.76	1/619 (0.2%)	1.05	4/772 (0.5%)
8	Pb	0.75	1/619 (0.2%)	1.00	4/772 (0.5%)
8	Pc	0.78	1/619 (0.2%)	1.07	4/772 (0.5%)
8	Pd	0.79	1/619 (0.2%)	1.06	4/772 (0.5%)
8	Pe	0.77	1/619 (0.2%)	1.08	4/772 (0.5%)
8	Pf	0.81	1/619 (0.2%)	1.14	4/772 (0.5%)
8	Pg	0.78	1/619 (0.2%)	1.06	4/772 (0.5%)
8	Ph	0.74	1/619 (0.2%)	1.02	4/772 (0.5%)
8	Pi	0.81	1/619 (0.2%)	1.16	4/772 (0.5%)
8	Pj	0.79	1/619 (0.2%)	1.15	4/772 (0.5%)
8	Pk	0.81	1/619 (0.2%)	1.13	4/772 (0.5%)
8	Pl	0.78	1/619 (0.2%)	1.08	4/772 (0.5%)
9	Ta	0.64	0/650	0.96	1/809 (0.1%)
9	Tb	0.64	0/650	0.96	1/809 (0.1%)
9	Tc	0.65	0/650	0.97	2/809 (0.2%)
9	Td	0.64	0/650	0.97	1/809 (0.1%)
9	Te	0.65	0/650	0.97	1/809 (0.1%)
9	Tf	0.64	0/650	0.97	1/809 (0.1%)
9	Tg	0.64	0/650	0.96	1/809 (0.1%)
9	Th	0.64	0/650	0.96	1/809 (0.1%)
9	Ti	0.65	0/650	0.97	1/809 (0.1%)
9	Tj	0.65	0/650	0.96	1/809 (0.1%)
9	Tk	0.64	0/650	0.96	2/809 (0.2%)
9	Tl	0.65	0/650	0.96	1/809 (0.1%)
All	All	0.56	62/107295 (0.1%)	1.00	225/133760 (0.2%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
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

Continued on next page...

Continued from previous page...

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 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Ay	26	ASP	N-CA	15.27	1.76	1.46
1	Ae	26	ASP	N-CA	15.21	1.76	1.46
1	Ad	26	ASP	N-CA	15.21	1.76	1.46
1	Aa	26	ASP	N-CA	15.17	1.76	1.46
1	Ag	26	ASP	N-CA	15.16	1.76	1.46

The worst 5 of 225 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Qi	407	SER	O-C-N	-54.05	36.22	122.70
7	Qj	407	SER	O-C-N	-54.05	36.22	122.70
7	Qb	407	SER	O-C-N	-54.05	36.23	122.70
7	Qk	407	SER	O-C-N	-54.04	36.23	122.70
7	Qe	407	SER	O-C-N	-54.04	36.23	122.70

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	10	0
1	A2	632	0	174	9	0
1	A3	632	0	174	10	0
1	A4	632	0	174	11	0
1	A5	632	0	174	10	0
1	A6	632	0	174	8	0
1	A7	632	0	174	11	0
1	A8	632	0	174	8	0
1	A9	632	0	174	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Aa	632	0	174	0	0
1	Ab	632	0	174	0	0
1	Ac	632	0	174	0	0
1	Ad	632	0	174	0	0
1	Ae	632	0	174	0	0
1	Af	632	0	174	0	0
1	Ag	632	0	174	0	0
1	Ah	632	0	174	0	0
1	Ai	632	0	174	0	0
1	Aj	632	0	174	0	0
1	Ak	632	0	174	0	0
1	Al	632	0	174	0	0
1	Am	632	0	174	0	0
1	An	632	0	174	0	0
1	Ao	632	0	174	0	0
1	Ap	632	0	174	0	0
1	Aq	632	0	174	0	0
1	Ar	632	0	174	0	0
1	As	632	0	174	0	0
1	At	632	0	174	0	0
1	Au	632	0	174	0	0
1	Av	632	0	174	0	0
1	Aw	632	0	174	0	0
1	Ax	632	0	174	0	0
1	Ay	632	0	174	0	0
1	Az	632	0	174	0	0
2	Ba	1808	0	487	0	0
2	Bb	1808	0	487	0	0
2	Bc	1808	0	487	0	0
2	Bd	1808	0	487	0	0
2	Be	1808	0	487	0	0
2	Bf	1808	0	487	0	0
3	Ca	1264	0	354	0	0
3	Cb	1264	0	354	0	0
4	Na	892	0	248	0	0
4	Nb	892	0	248	0	0
4	Nc	892	0	248	0	0
4	Nd	892	0	248	0	0
4	Ne	892	0	248	0	0
4	Nf	892	0	248	0	0
4	Ng	892	0	248	0	0
4	Nh	892	0	248	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Ni	892	0	248	0	0
4	Nj	892	0	248	0	0
4	Nk	892	0	248	0	0
4	Nl	892	0	248	0	0
5	Oa	756	0	207	0	0
5	Ob	756	0	207	0	0
5	Oc	756	0	207	0	0
5	Od	756	0	207	0	0
5	Oe	756	0	207	0	0
5	Of	756	0	207	0	0
5	Og	756	0	207	0	0
5	Oh	756	0	207	0	0
5	Oi	756	0	207	0	0
5	Oj	756	0	207	0	0
5	Ok	756	0	207	0	0
5	Ol	756	0	207	0	0
6	Ma	1420	0	396	0	0
6	Mb	1420	0	396	0	0
6	Mc	1420	0	396	0	0
6	Md	1420	0	396	0	0
6	Me	1420	0	396	0	0
6	Mf	1420	0	396	0	0
6	Mg	1420	0	396	0	0
6	Mh	1420	0	396	0	0
6	Mi	1420	0	396	0	0
6	Mj	1420	0	396	0	0
6	Mk	1420	0	396	0	0
6	Ml	1420	0	396	0	0
7	Qa	1672	0	462	0	0
7	Qb	1672	0	462	0	0
7	Qc	1672	0	462	0	0
7	Qd	1672	0	462	0	0
7	Qe	1672	0	462	0	0
7	Qf	1672	0	462	0	0
7	Qg	1672	0	462	0	0
7	Qh	1672	0	462	0	0
7	Qi	1672	0	462	0	0
7	Qj	1672	0	462	0	0
7	Qk	1672	0	462	0	0
7	Ql	1672	0	462	0	0
8	Pa	620	0	155	0	0
8	Pb	620	0	155	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	Pc	620	0	155	0	0
8	Pd	620	0	155	0	0
8	Pe	620	0	155	0	0
8	Pf	620	0	155	0	0
8	Pg	620	0	155	0	0
8	Ph	620	0	155	0	0
8	Pi	620	0	155	0	0
8	Pj	620	0	155	0	0
8	Pk	620	0	155	0	0
8	Pl	620	0	155	0	0
9	Ta	652	0	177	0	0
9	Tb	652	0	177	0	0
9	Tc	652	0	177	0	0
9	Td	652	0	177	0	0
9	Te	652	0	177	0	0
9	Tf	652	0	177	0	0
9	Tg	652	0	177	0	0
9	Th	652	0	177	0	0
9	Ti	652	0	177	0	0
9	Tj	652	0	177	0	0
9	Tk	652	0	177	0	0
9	Tl	652	0	177	0	0
All	All	107640	0	29460	82	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 11.

The worst 5 of 82 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:A2:26:ASP:N	1:A2:26:ASP:CA	1.76	1.49
1:A5:26:ASP:N	1:A5:26:ASP:CA	1.76	1.49
1:A4:26:ASP:N	1:A4:26:ASP:CA	1.76	1.48
1:A3:26:ASP:N	1:A3:26:ASP:CA	1.76	1.47
1:A6:26:ASP:N	1:A6:26:ASP:CA	1.76	1.47

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

Continued on next page...

Continued from previous page...

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%)	6	6
3	Cb	308/417 (74%)	292 (95%)	10 (3%)	6 (2%)	8	8
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%)	9	9

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	Qi	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	4	4
7	Qj	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	4	4
7	Qk	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	4	4
7	Ql	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	4	4
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%)	1	1
9	Tb	159/411 (39%)	114 (72%)	32 (20%)	13 (8%)	1	1
9	Tc	159/411 (39%)	114 (72%)	32 (20%)	13 (8%)	1	1
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%)	1	1
9	Tj	159/411 (39%)	114 (72%)	33 (21%)	12 (8%)	1	1
9	Tk	159/411 (39%)	114 (72%)	32 (20%)	13 (8%)	1	1
9	Tl	159/411 (39%)	114 (72%)	32 (20%)	13 (8%)	1	1
All	All	26500/37468 (71%)	22659 (86%)	2521 (10%)	1320 (5%)	4	2

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	Az	1	1	3,3,13	0.87	0	0,2,16	-	-
1	MEA	Ar	1	1	3,3,13	0.84	0	0,2,16	-	-
1	MEA	Am	1	1	3,3,13	0.79	0	0,2,16	-	-
1	MEA	Aq	1	1	3,3,13	0.87	0	0,2,16	-	-
1	MEA	Ah	1	1	3,3,13	0.85	0	0,2,16	-	-
1	MEA	Av	1	1	3,3,13	0.87	0	0,2,16	-	-
1	MEA	Ag	1	1	3,3,13	0.85	0	0,2,16	-	-
1	MEA	Ad	1	1	3,3,13	0.90	0	0,2,16	-	-
1	MEA	Ax	1	1	3,3,13	0.91	0	0,2,16	-	-
1	MEA	A2	1	1	3,3,13	0.83	0	0,2,16	-	-
1	MEA	Ay	1	1	3,3,13	0.87	0	0,2,16	-	-
1	MEA	A4	1	1	3,3,13	0.84	0	0,2,16	-	-
1	MEA	A5	1	1	3,3,13	0.86	0	0,2,16	-	-
1	MEA	Ai	1	1	3,3,13	0.90	0	0,2,16	-	-
1	MEA	Ak	1	1	3,3,13	0.86	0	0,2,16	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MEA	Aa	1	1	3,3,13	0.88	0	0,2,16	-	-
1	MEA	A6	1	1	3,3,13	0.82	0	0,2,16	-	-
1	MEA	Au	1	1	3,3,13	0.86	0	0,2,16	-	-
1	MEA	Ao	1	1	3,3,13	0.85	0	0,2,16	-	-
1	MEA	As	1	1	3,3,13	0.89	0	0,2,16	-	-
1	MEA	Ap	1	1	3,3,13	0.87	0	0,2,16	-	-
1	MEA	Ab	1	1	3,3,13	0.84	0	0,2,16	-	-
1	MEA	A7	1	1	3,3,13	0.90	0	0,2,16	-	-
1	MEA	Ae	1	1	3,3,13	0.89	0	0,2,16	-	-
1	MEA	Aj	1	1	3,3,13	0.87	0	0,2,16	-	-
1	MEA	At	1	1	3,3,13	0.86	0	0,2,16	-	-
1	MEA	An	1	1	3,3,13	0.85	0	0,2,16	-	-
1	MEA	Al	1	1	3,3,13	0.89	0	0,2,16	-	-
1	MEA	A8	1	1	3,3,13	0.84	0	0,2,16	-	-
1	MEA	Af	1	1	3,3,13	0.86	0	0,2,16	-	-
1	MEA	Aw	1	1	3,3,13	0.85	0	0,2,16	-	-
1	MEA	A3	1	1	3,3,13	0.80	0	0,2,16	-	-
1	MEA	Ac	1	1	3,3,13	0.85	0	0,2,16	-	-
1	MEA	A9	1	1	3,3,13	0.89	0	0,2,16	-	-
1	MEA	A1	1	1	3,3,13	0.90	0	0,2,16	-	-

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	Az	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	Aq	1	1	-	0/0/1/10	-
1	MEA	Ah	1	1	-	0/0/1/10	-
1	MEA	Av	1	1	-	0/0/1/10	-
1	MEA	Ag	1	1	-	0/0/1/10	-
1	MEA	Ad	1	1	-	0/0/1/10	-
1	MEA	Ax	1	1	-	0/0/1/10	-
1	MEA	A2	1	1	-	0/0/1/10	-
1	MEA	Ay	1	1	-	0/0/1/10	-
1	MEA	A4	1	1	-	0/0/1/10	-
1	MEA	A5	1	1	-	0/0/1/10	-
1	MEA	Ai	1	1	-	0/0/1/10	-
1	MEA	Ak	1	1	-	0/0/1/10	-
1	MEA	Aa	1	1	-	0/0/1/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MEA	A6	1	1	-	0/0/1/10	-
1	MEA	Au	1	1	-	0/0/1/10	-
1	MEA	Ao	1	1	-	0/0/1/10	-
1	MEA	As	1	1	-	0/0/1/10	-
1	MEA	Ap	1	1	-	0/0/1/10	-
1	MEA	Ab	1	1	-	0/0/1/10	-
1	MEA	A7	1	1	-	0/0/1/10	-
1	MEA	Ae	1	1	-	0/0/1/10	-
1	MEA	Aj	1	1	-	0/0/1/10	-
1	MEA	At	1	1	-	0/0/1/10	-
1	MEA	An	1	1	-	0/0/1/10	-
1	MEA	Al	1	1	-	0/0/1/10	-
1	MEA	A8	1	1	-	0/0/1/10	-
1	MEA	Af	1	1	-	0/0/1/10	-
1	MEA	Aw	1	1	-	0/0/1/10	-
1	MEA	A3	1	1	-	0/0/1/10	-
1	MEA	Ac	1	1	-	0/0/1/10	-
1	MEA	A9	1	1	-	0/0/1/10	-
1	MEA	A1	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.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides 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

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 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.