Full wwPDB EM Validation 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ 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:

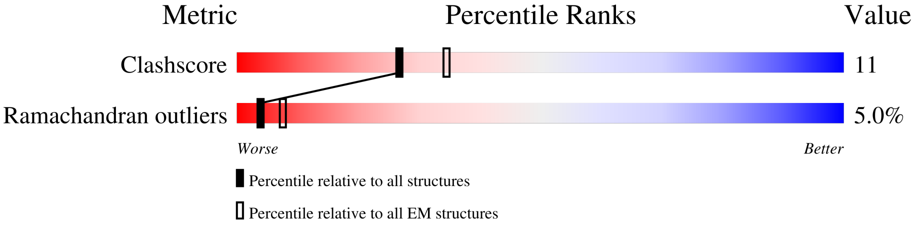
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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

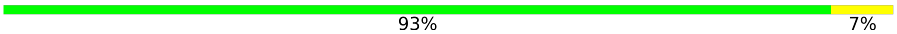
The reported resolution of this entry is unknown.

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 <=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%

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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%

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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%

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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%

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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%

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Mol	Chain	Length	Quality of chain
9	Th	411	
9	Ti	411	
9	Tj	411	
9	Tk	411	
9	Tl	411	

2 Entry composition ⓘ

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

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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 1808 904 452 452	0	0
2	Bc	452	Total C N O 1808 904 452 452	0	0
2	Bd	452	Total C N O 1808 904 452 452	0	0
2	Be	452	Total C N O 1808 904 452 452	0	0
2	Bf	452	Total C N O 1808 904 452 452	0	0

- 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 1264 632 316 316	0	0
3	Cb	316	Total C N O 1264 632 316 316	0	0

- Molecule 4 is a protein called PilN.

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

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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 1420	C 710	N 355	O 355	0	0
6	Me	355	Total 1420	C 710	N 355	O 355	0	0
6	Mf	355	Total 1420	C 710	N 355	O 355	0	0
6	Mg	355	Total 1420	C 710	N 355	O 355	0	0
6	Mh	355	Total 1420	C 710	N 355	O 355	0	0
6	Mi	355	Total 1420	C 710	N 355	O 355	0	0
6	Mj	355	Total 1420	C 710	N 355	O 355	0	0
6	Mk	355	Total 1420	C 710	N 355	O 355	0	0
6	Ml	355	Total 1420	C 710	N 355	O 355	0	0

- Molecule 7 is a protein called PilQ.

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

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

- Molecule 8 is a protein called PilP.

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

- Molecule 9 is a protein called LysM domain protein.

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

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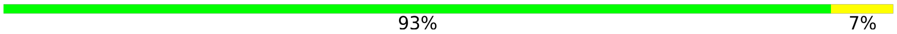
Mol	**Chain**	**Residues**	**Atoms**	**AltConf**	**Trace**
9	Td	163	Total C N O 652 326 163 163	0	0
9	Te	163	Total C N O 652 326 163 163	0	0
9	Tf	163	Total C N O 652 326 163 163	0	0
9	Tg	163	Total C N O 652 326 163 163	0	0
9	Th	163	Total C N O 652 326 163 163	0	0
9	Ti	163	Total C N O 652 326 163 163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

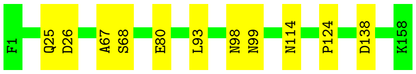
3 Residue-property plots ⓘ

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

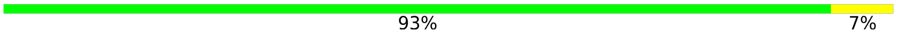
Chain Aa:

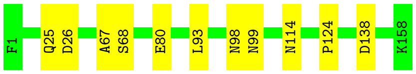




- Molecule 1: PilA

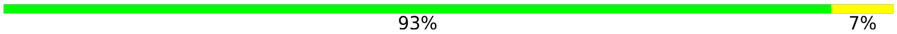
Chain Ab:

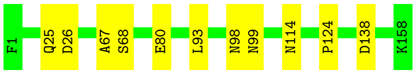




- Molecule 1: PilA

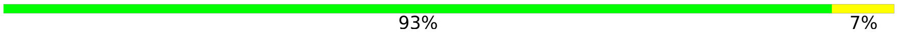
Chain Ac:

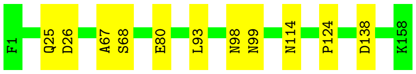




- Molecule 1: PilA

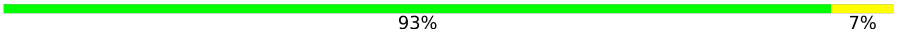
Chain Ad:

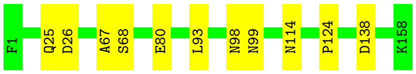




- Molecule 1: PilA

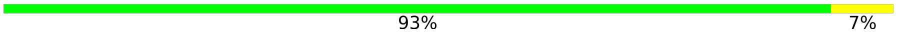
Chain Ae:

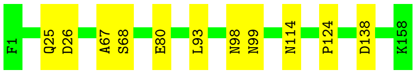




- Molecule 1: PilA

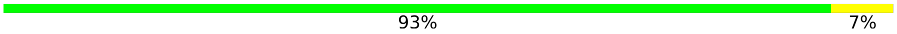
Chain Af:

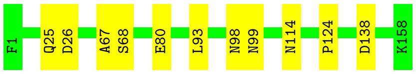




- Molecule 1: PilA

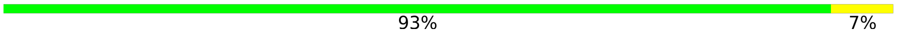
Chain Ag:

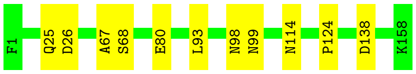




- Molecule 1: PilA

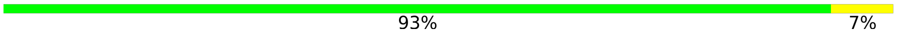
Chain Ah:

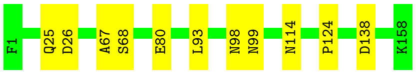




- Molecule 1: PilA

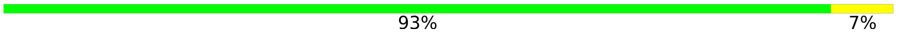
Chain Ai:

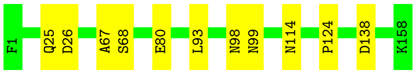




- Molecule 1: PilA

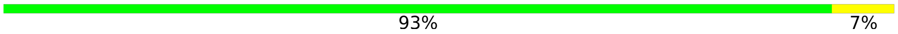
Chain Aj:

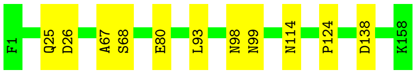




- Molecule 1: PilA

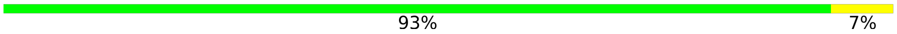
Chain Ak:

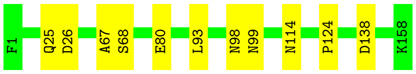




- Molecule 1: PilA

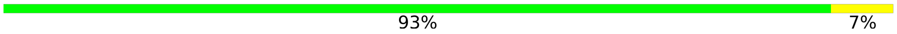
Chain Al:

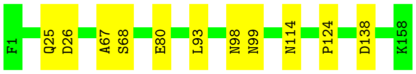




- Molecule 1: PilA

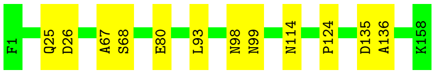
Chain Am:





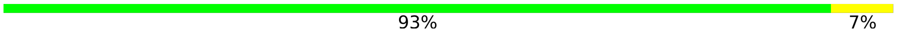
- Molecule 1: PilA

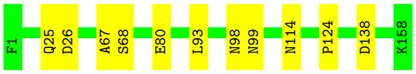
Chain An:



- Molecule 1: PilA

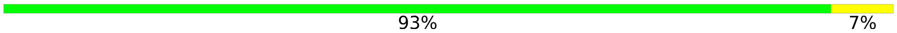
Chain Ao:

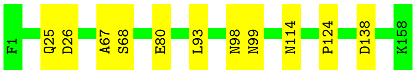




- Molecule 1: PilA

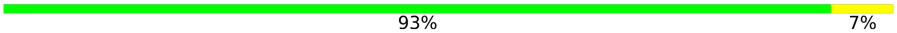
Chain Ap:

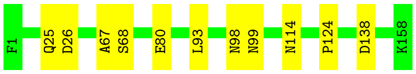




- Molecule 1: PilA

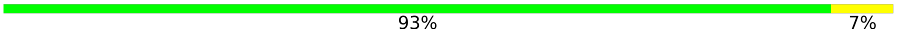
Chain Aq:

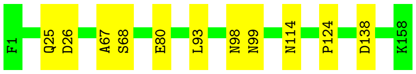




- Molecule 1: PilA

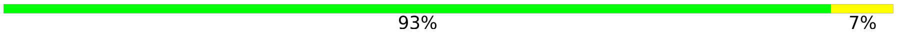
Chain Ar:

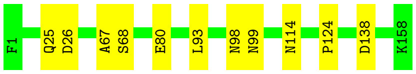




- Molecule 1: PilA

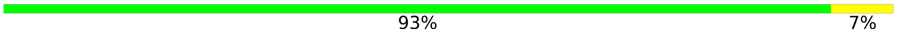
Chain As:

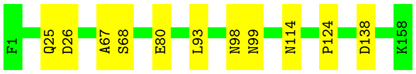




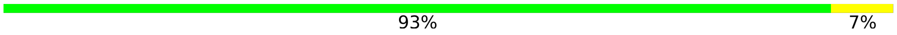
- Molecule 1: PilA

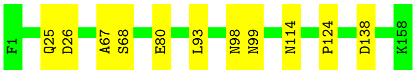
Chain At:



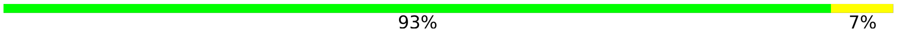


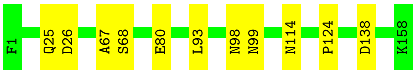
- Molecule 1: PilA

Chain Au:


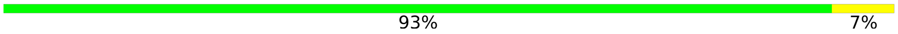


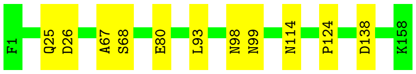
- Molecule 1: PilA

Chain Av:


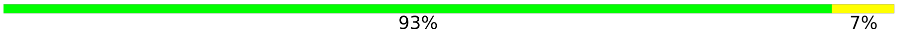


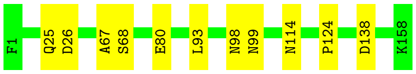
- Molecule 1: PilA

Chain Aw:


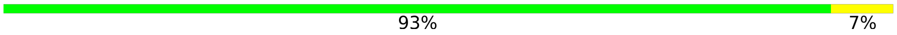


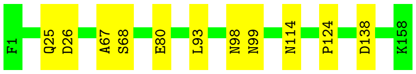
- Molecule 1: PilA

Chain Ax:


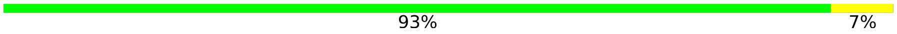


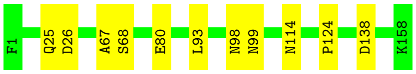
- Molecule 1: PilA

Chain Ay:




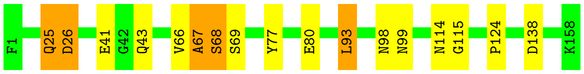
- Molecule 1: PilA

Chain Az:




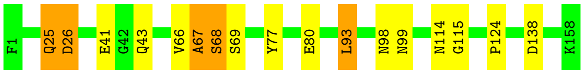
- Molecule 1: PilA

Chain A1:

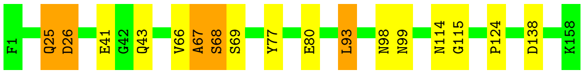
- Molecule 1: PilA

Chain A2:



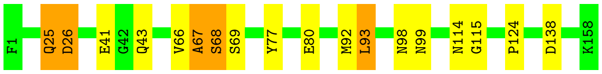
- Molecule 1: PilA

Chain A3:



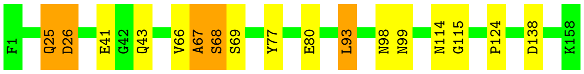
- Molecule 1: PilA

Chain A4:



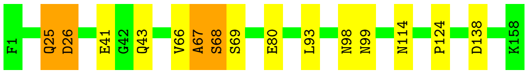
- Molecule 1: PilA

Chain A5:



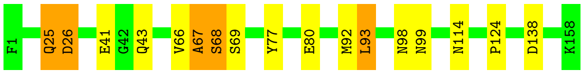
- Molecule 1: PilA

Chain A6:



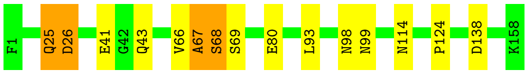
- Molecule 1: PilA

Chain A7:



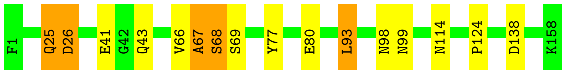
- Molecule 1: PilA

Chain A8:



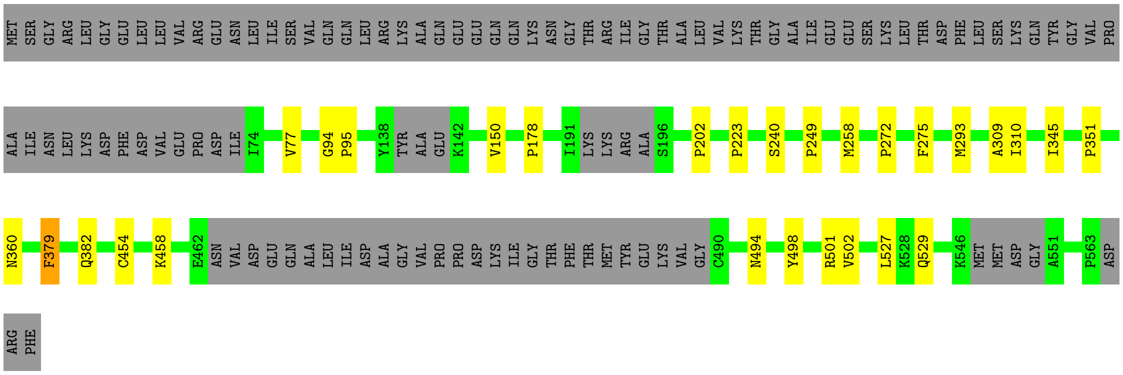
- Molecule 1: PilA

Chain A9:



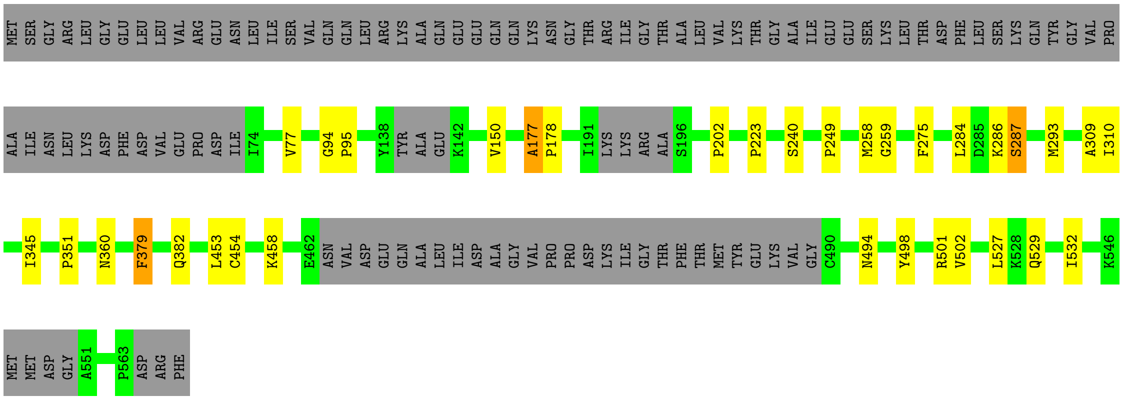
- Molecule 2: Type IV-A pilus assembly ATPase PilB

Chain Ba:



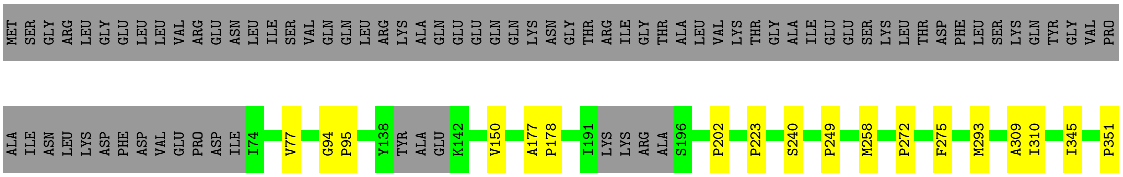
- Molecule 2: Type IV-A pilus assembly ATPase PilB

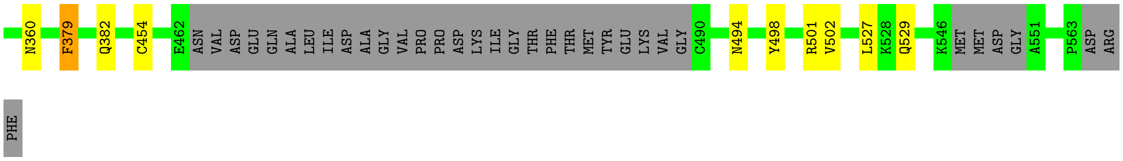
Chain Bb:



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

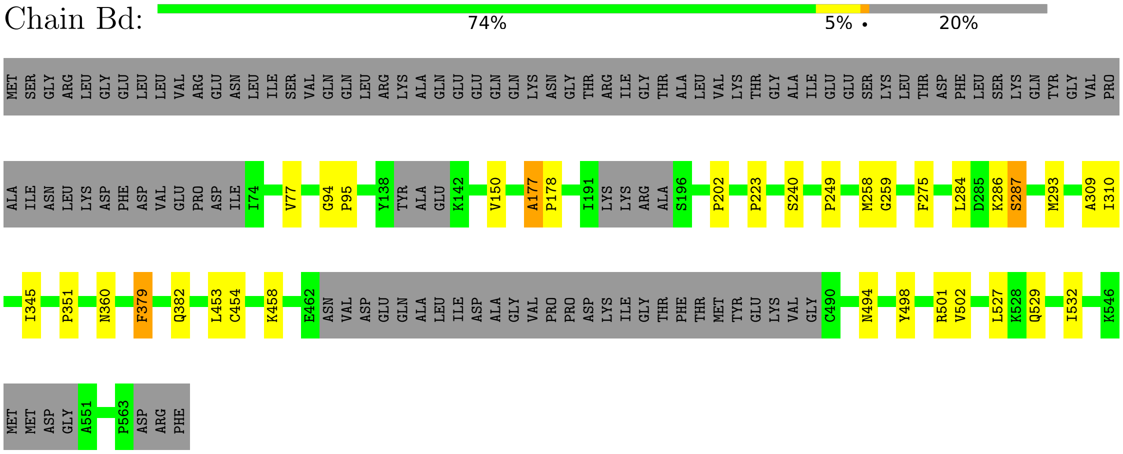
Chain Bc:





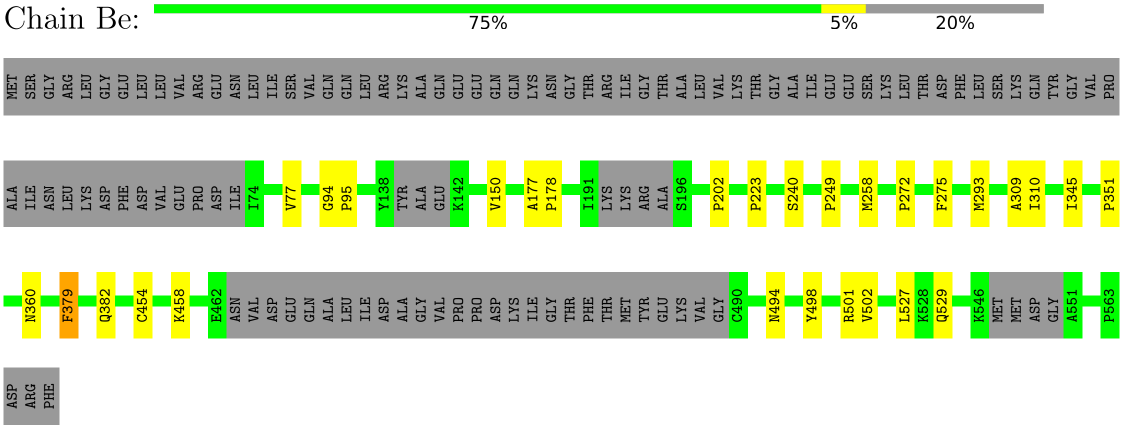
- Molecule 2: Type IV-A pilus assembly ATPase PilB

Chain Bd:



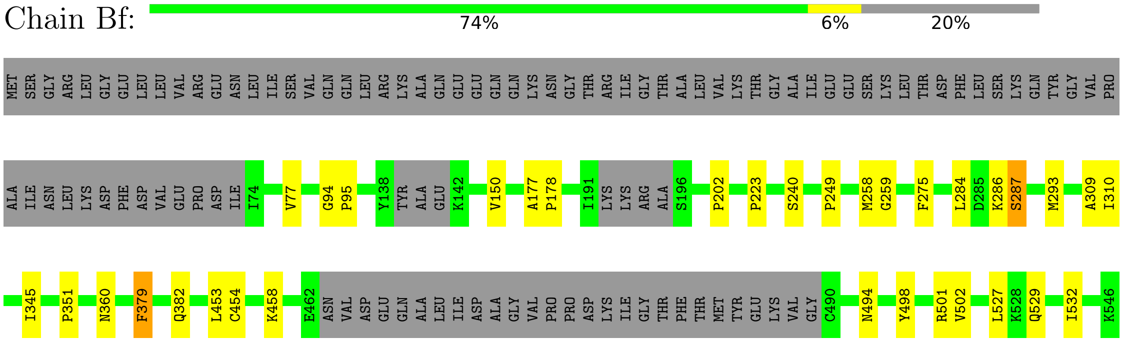
- Molecule 2: Type IV-A pilus assembly ATPase PilB

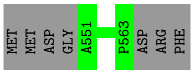
Chain Be:



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

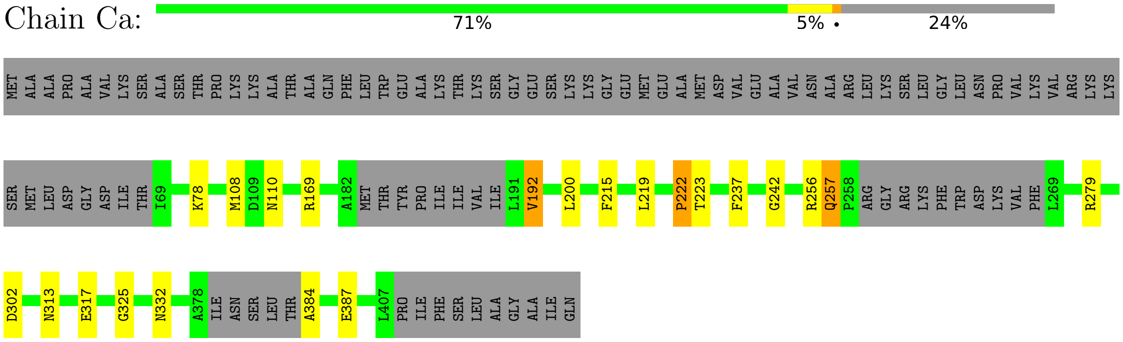
Chain Bf:





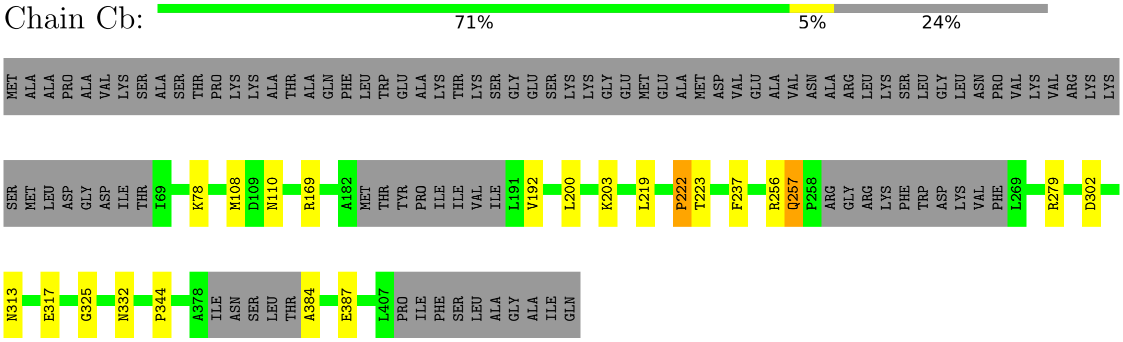
- Molecule 3: Type 4 fimbrial assembly protein PilC

Chain Ca:



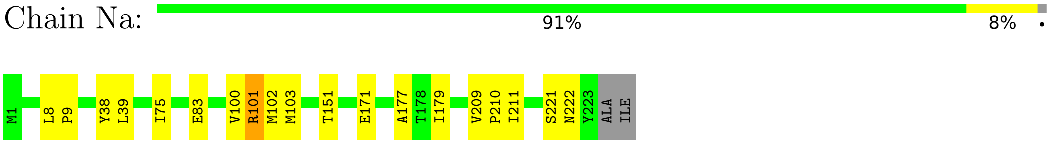
- Molecule 3: Type 4 fimbrial assembly protein PilC

Chain Cb:



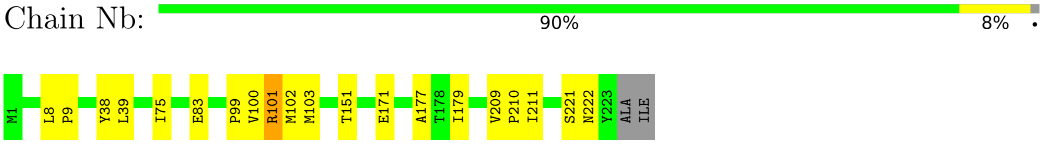
- Molecule 4: PilN

Chain Na:



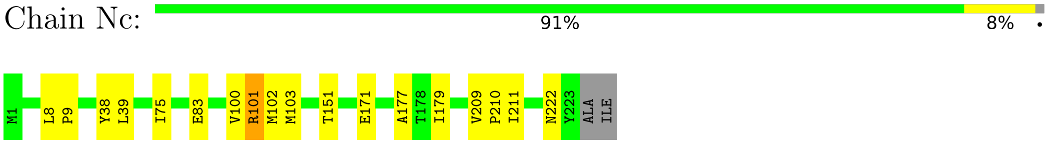
- Molecule 4: PilN

Chain Nb:



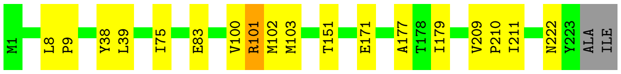
- Molecule 4: PilN

Chain Nc:



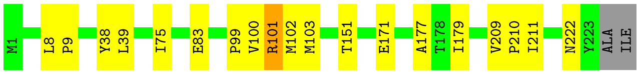
- Molecule 4: PilN

Chain Nd:



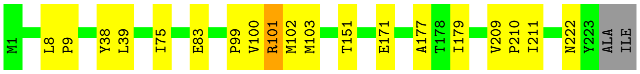
- Molecule 4: PilN

Chain Ne:



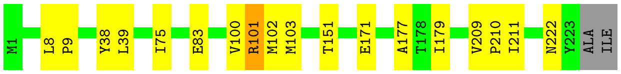
- Molecule 4: PilN

Chain Nf:



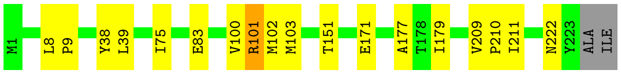
- Molecule 4: PilN

Chain Ng:



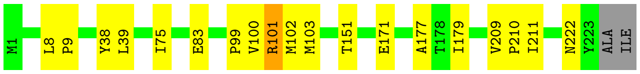
- Molecule 4: PilN

Chain Nh:



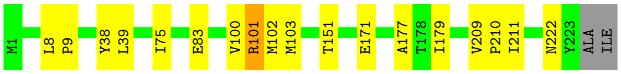
- Molecule 4: PilN

Chain Ni:



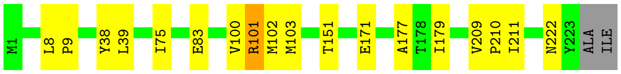
- Molecule 4: PilN

Chain Nj:



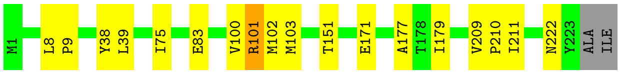
- Molecule 4: PilN

Chain Nk:



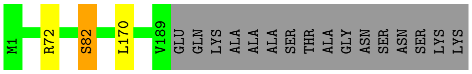
- Molecule 4: PilN

Chain Nl:



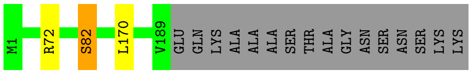
- Molecule 5: PilO

Chain Oa:



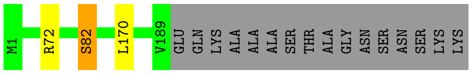
- Molecule 5: PilO

Chain Ob:



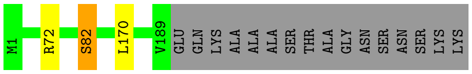
- Molecule 5: PilO

Chain Oc:



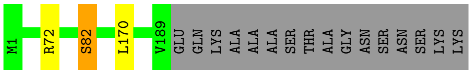
- Molecule 5: PilO

Chain Od:



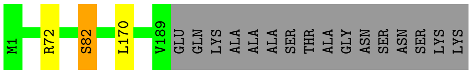
- Molecule 5: PilO

Chain Oe:



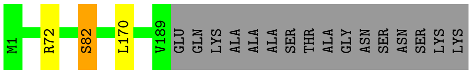
- Molecule 5: PilO

Chain Of:



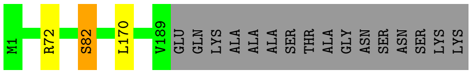
- Molecule 5: PilO

Chain Og:



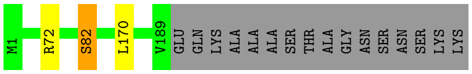
- Molecule 5: PilO

Chain Oh:



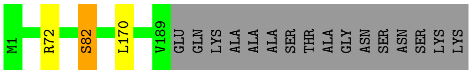
- Molecule 5: PilO

Chain Oi:



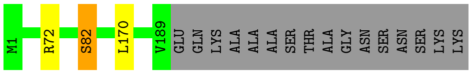
- Molecule 5: PilO

Chain Oj:



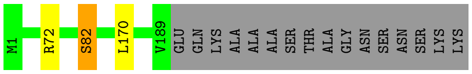
- Molecule 5: PilO

Chain Ok:



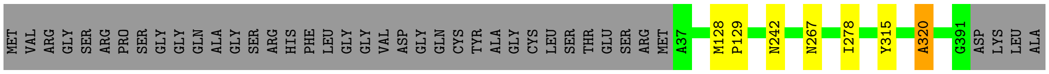
- Molecule 5: PilO

Chain Ol:



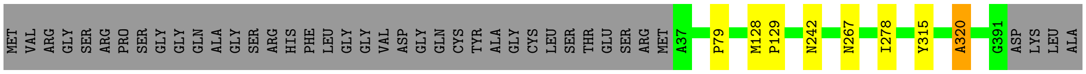
- Molecule 6: Type IV pilus biogenesis protein PilM

Chain Ma:



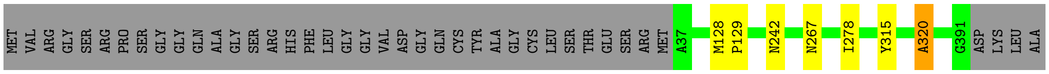
- Molecule 6: Type IV pilus biogenesis protein PilM

Chain Mb:



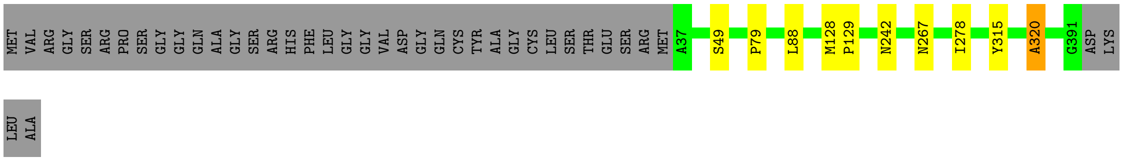
- Molecule 6: Type IV pilus biogenesis protein PilM

Chain Mc:



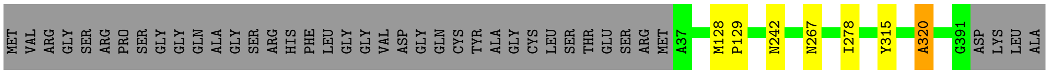
- Molecule 6: Type IV pilus biogenesis protein PilM

Chain Md:



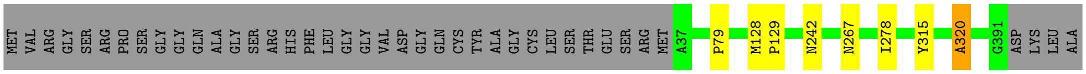
- Molecule 6: Type IV pilus biogenesis protein PilM

Chain Me:



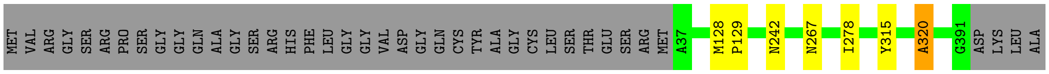
- Molecule 6: Type IV pilus biogenesis protein PilM

Chain Mf:

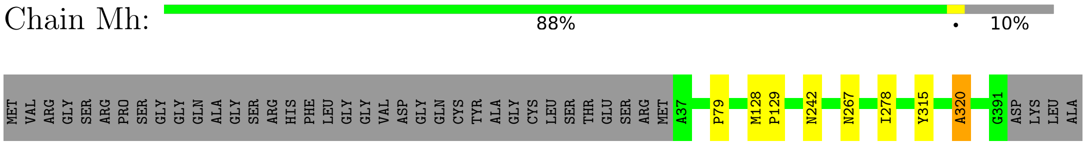


- Molecule 6: Type IV pilus biogenesis protein PilM

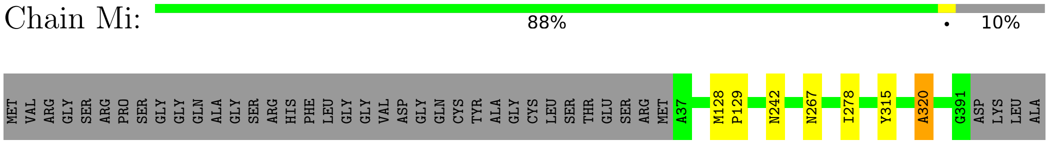
Chain Mg:



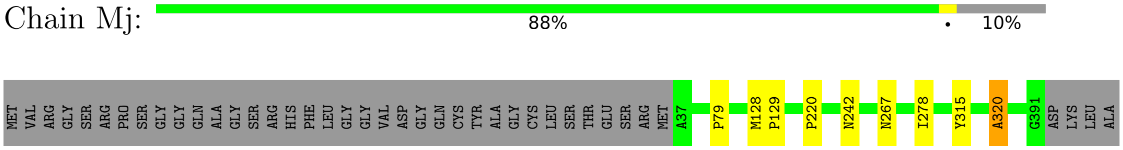
- Molecule 6: Type IV pilus biogenesis protein PilM



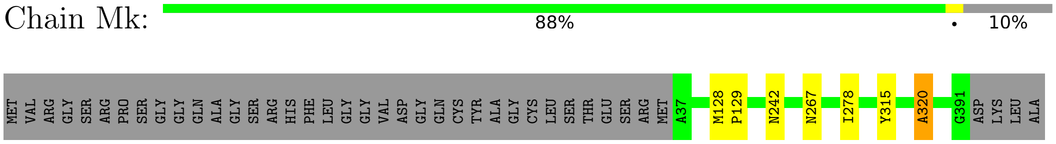
- Molecule 6: Type IV pilus biogenesis protein PilM



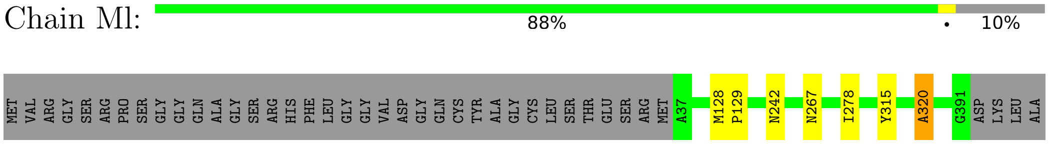
- Molecule 6: Type IV pilus biogenesis protein PilM



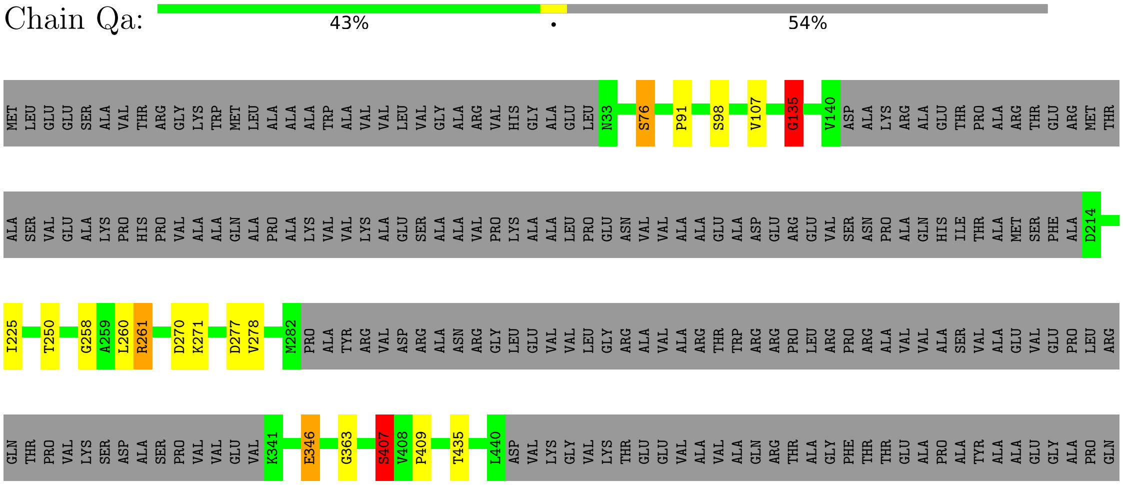
- Molecule 6: Type IV pilus biogenesis protein PilM

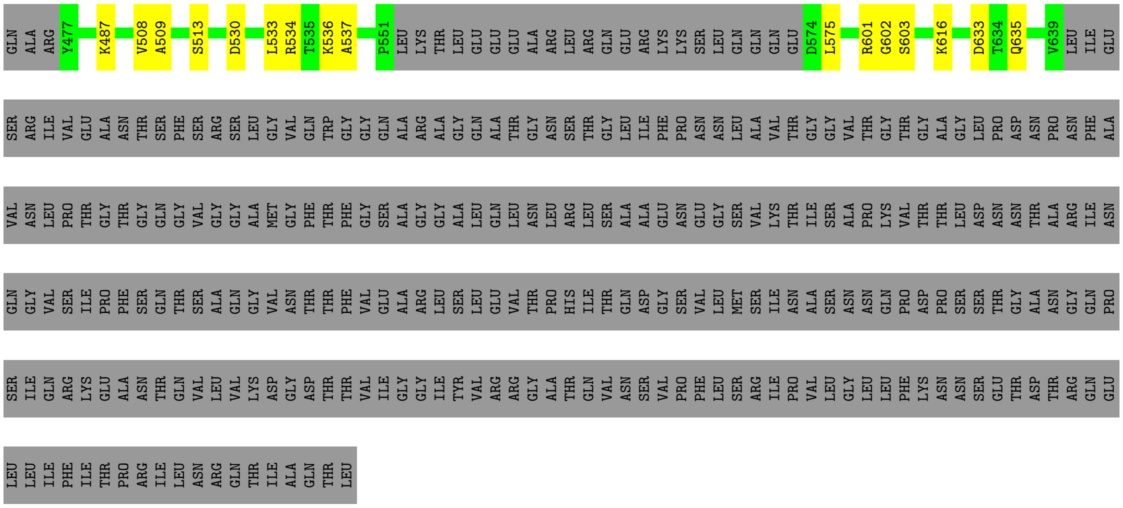


- Molecule 6: Type IV pilus biogenesis protein PilM



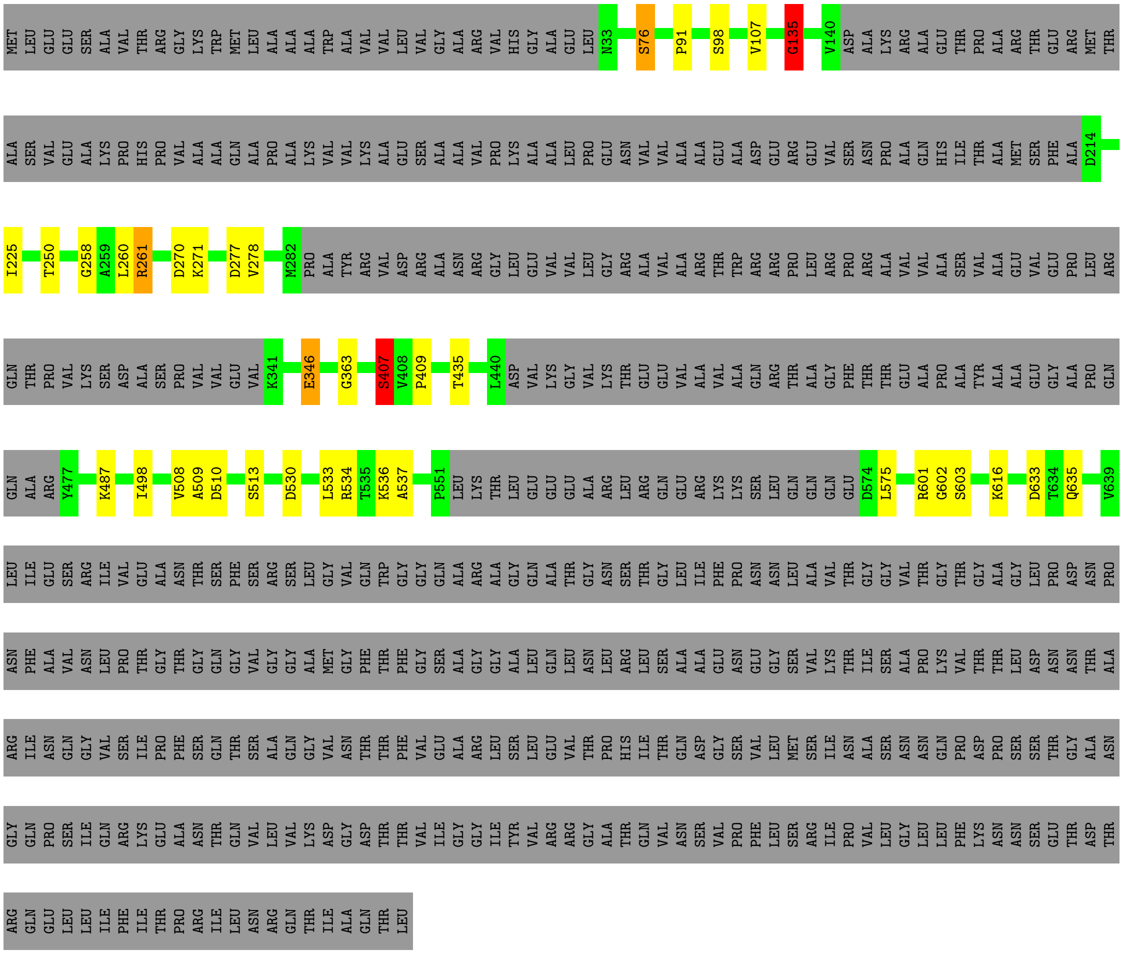
- Molecule 7: PilQ





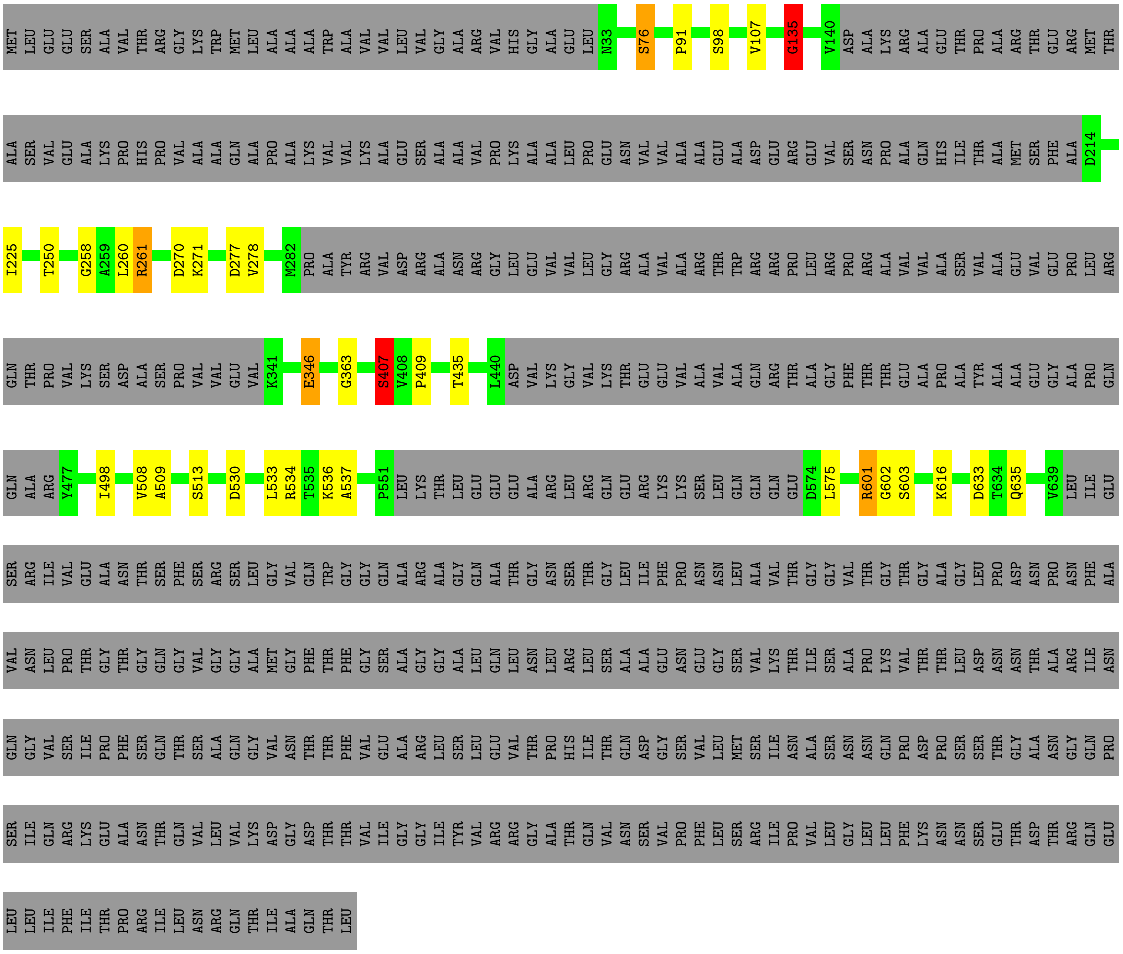
- Molecule 7: PilQ

Chain Qb:



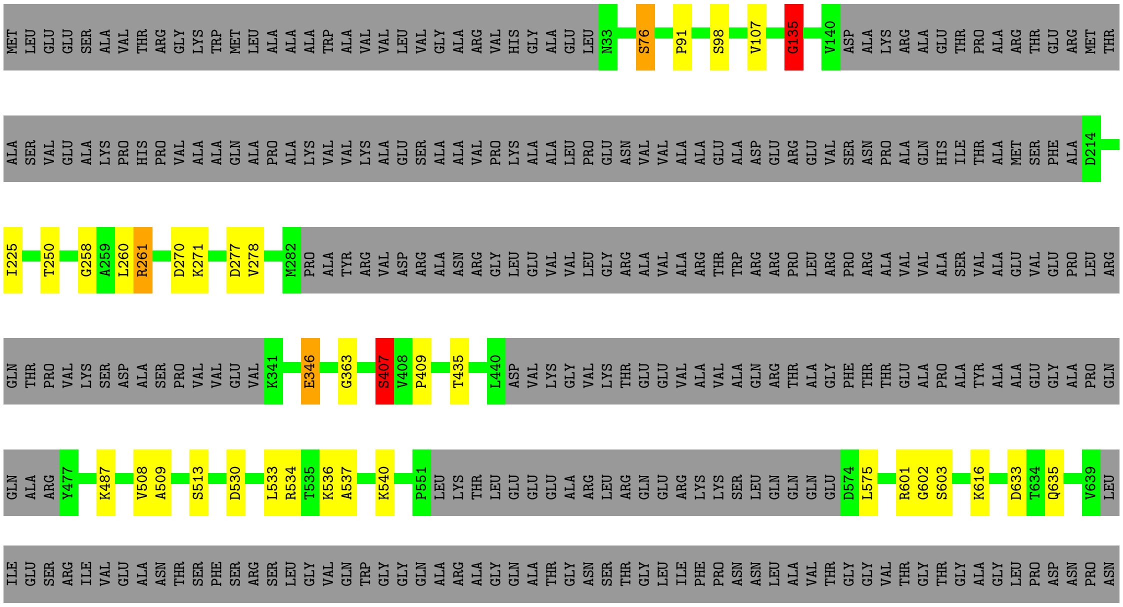
- Molecule 7: PilQ

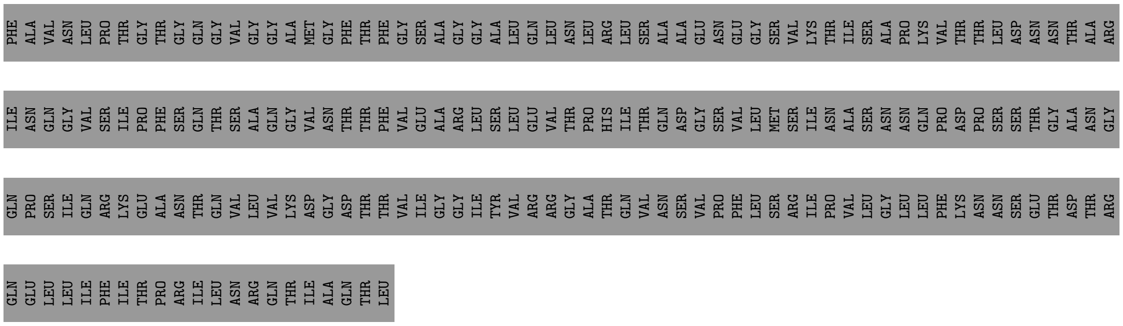
Chain Qc:



- Molecule 7: PilQ

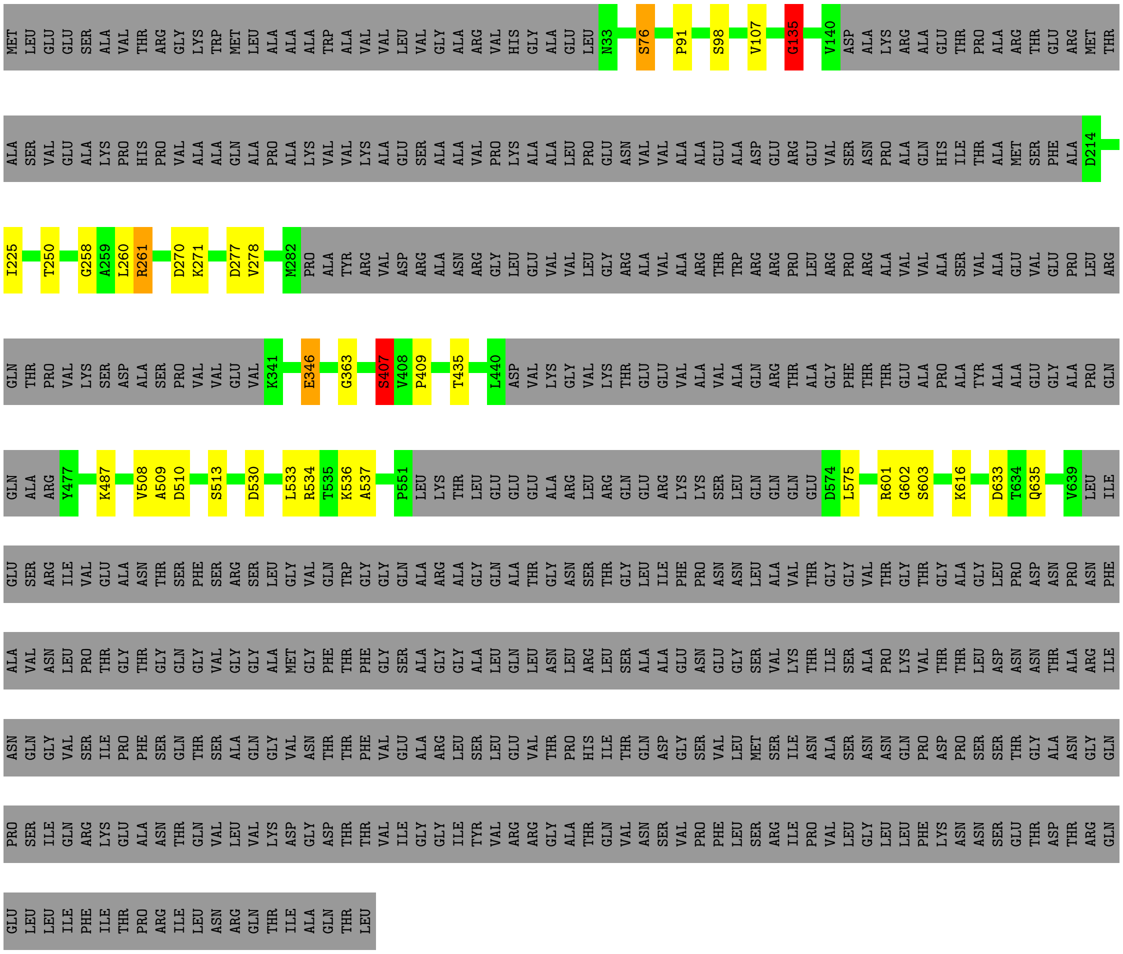
Chain Qd:





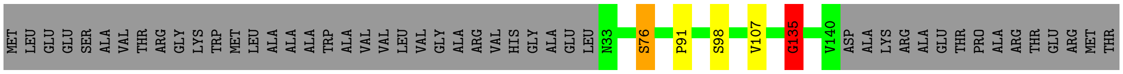
- Molecule 7: PilQ

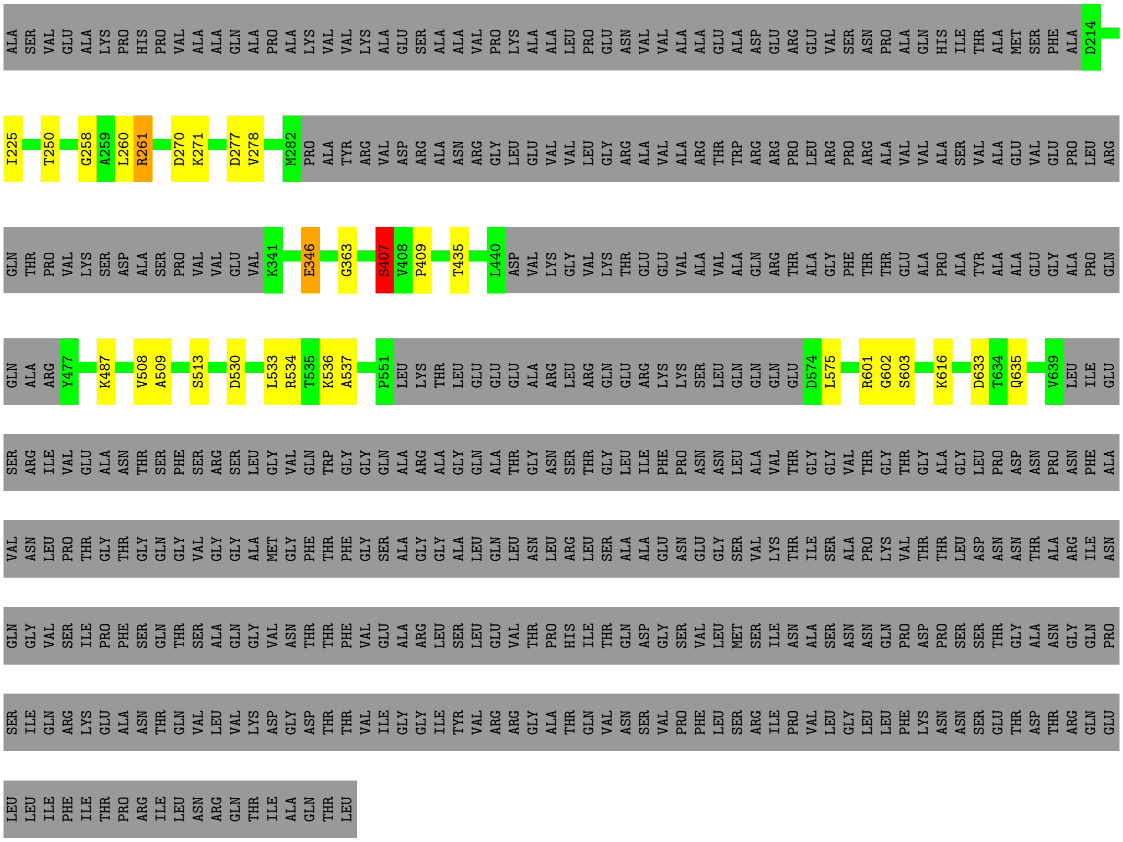
Chain Qe:



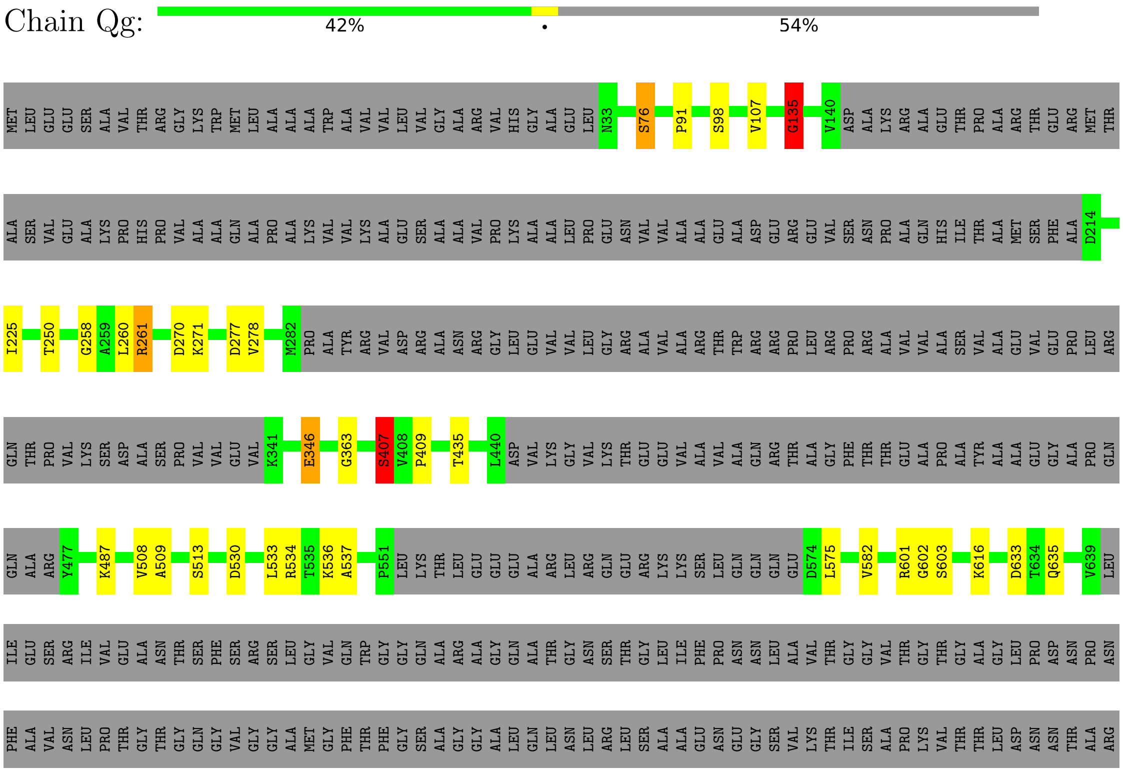
- Molecule 7: PilQ

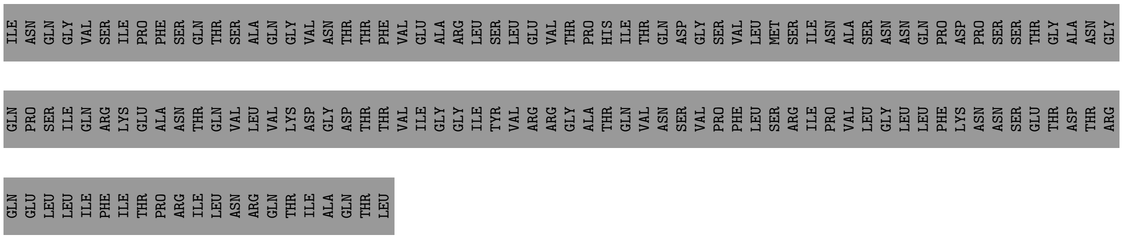
Chain Qf:





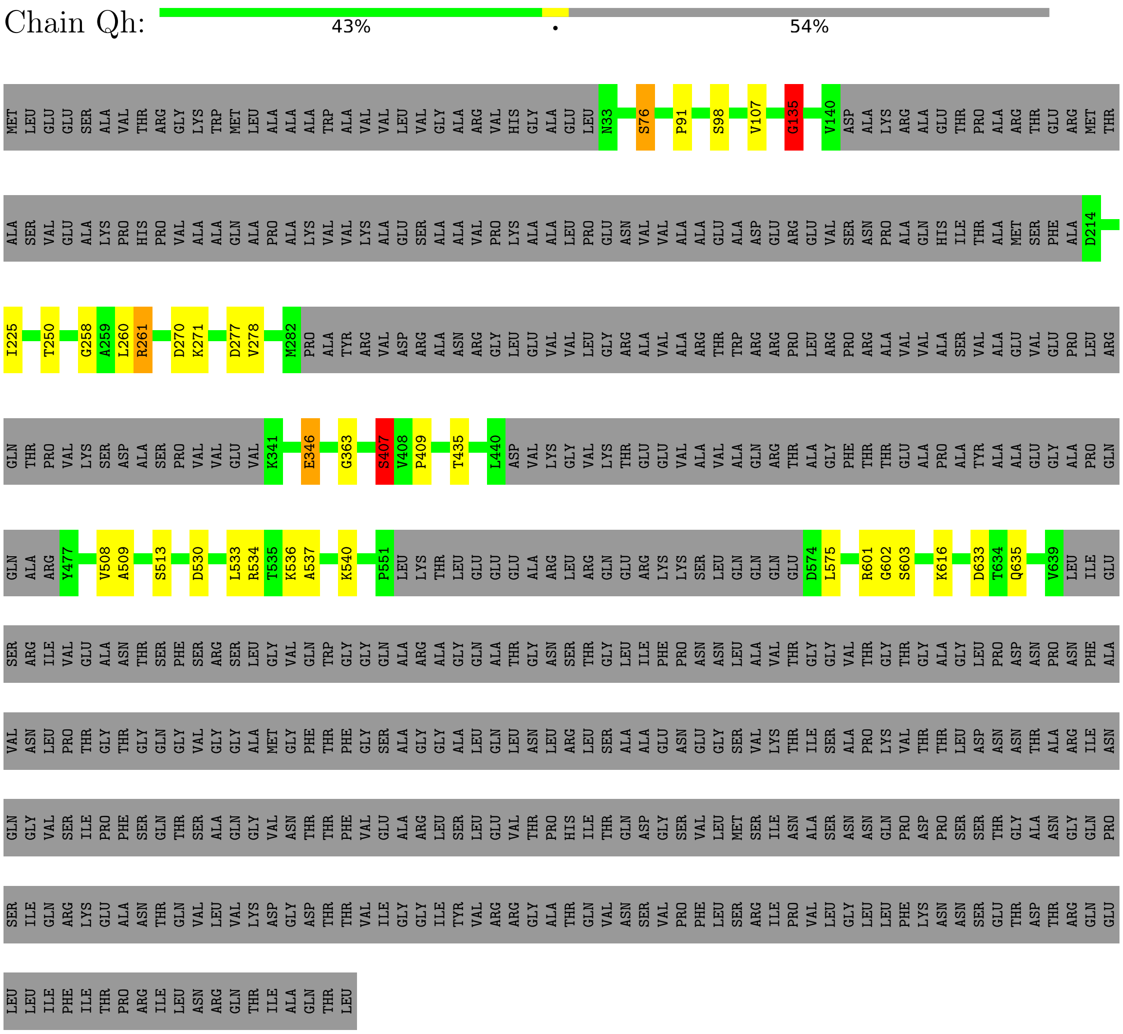
- Molecule 7: PilQ





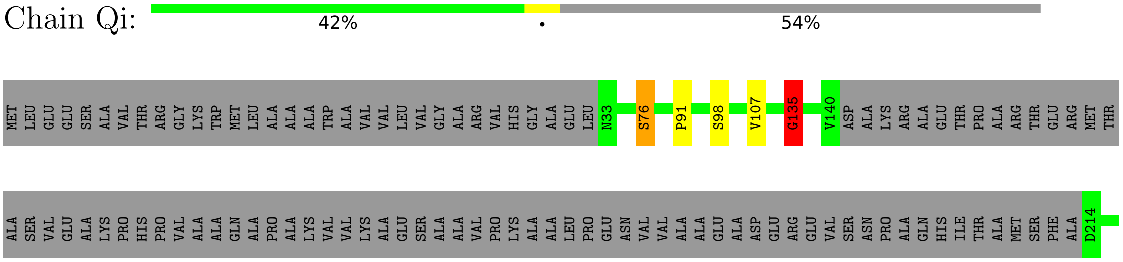
- Molecule 7: PilQ

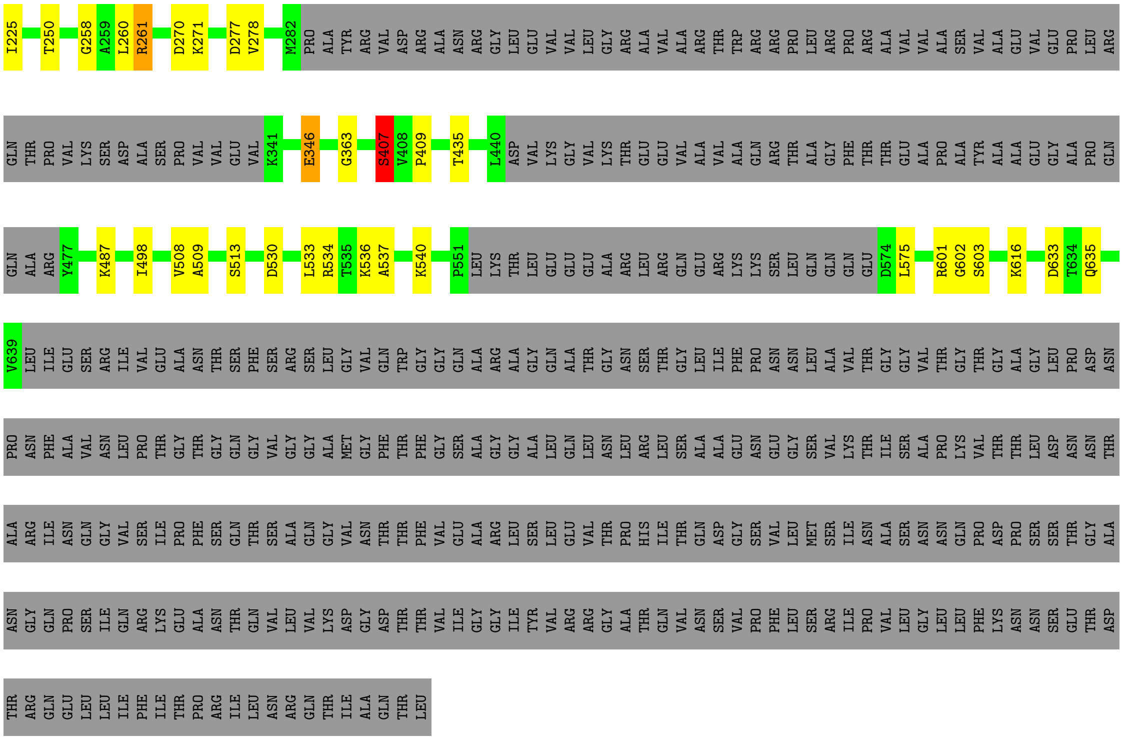
Chain Qh:



- Molecule 7: PilQ

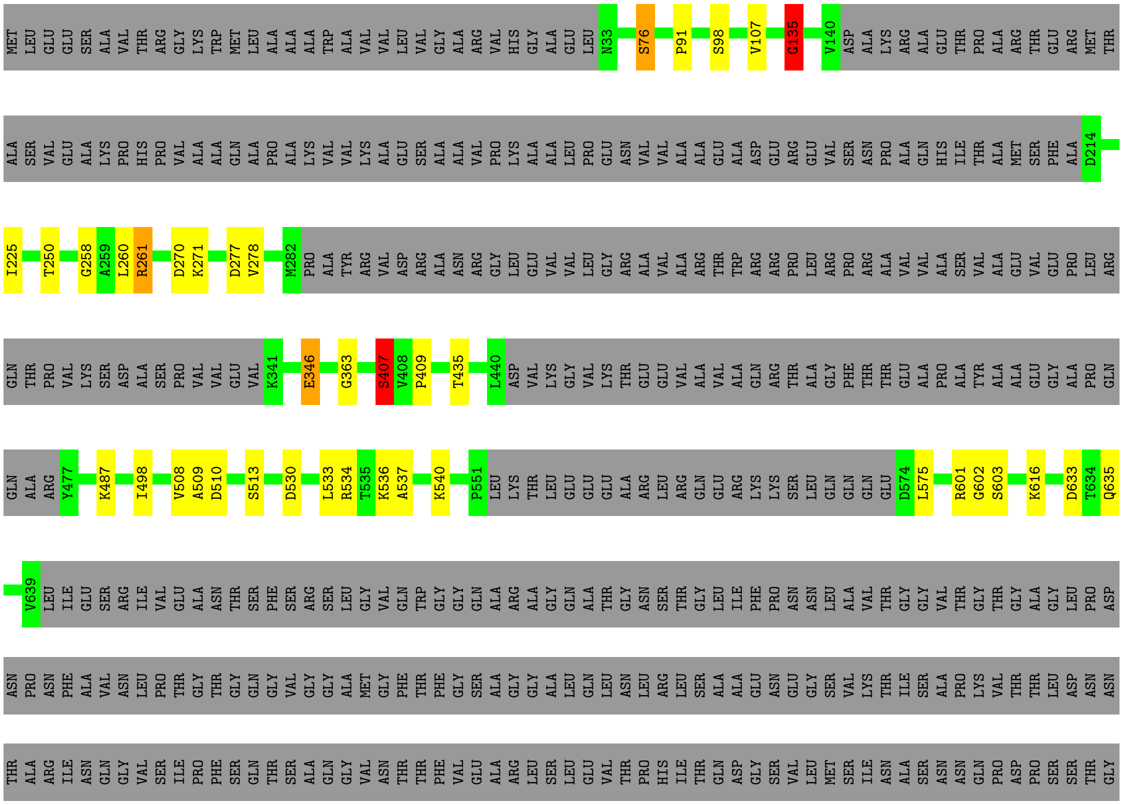
Chain Qi:

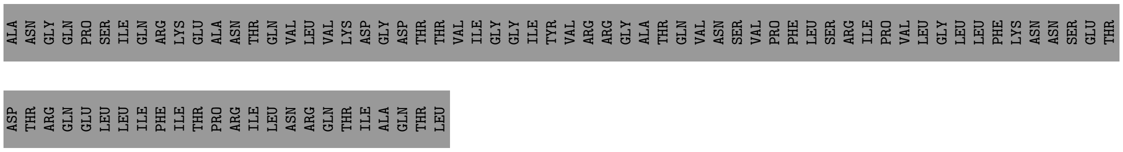




- Molecule 7: PilQ

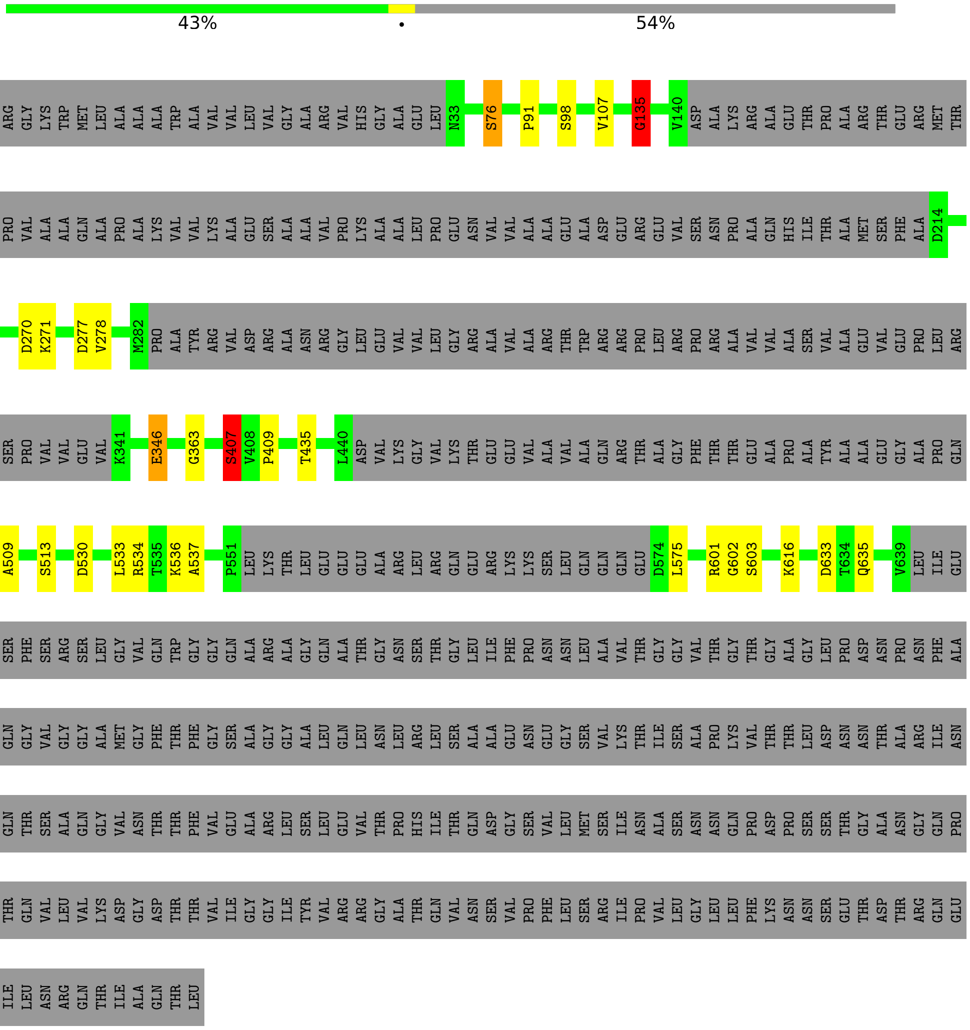
Chain Qj:





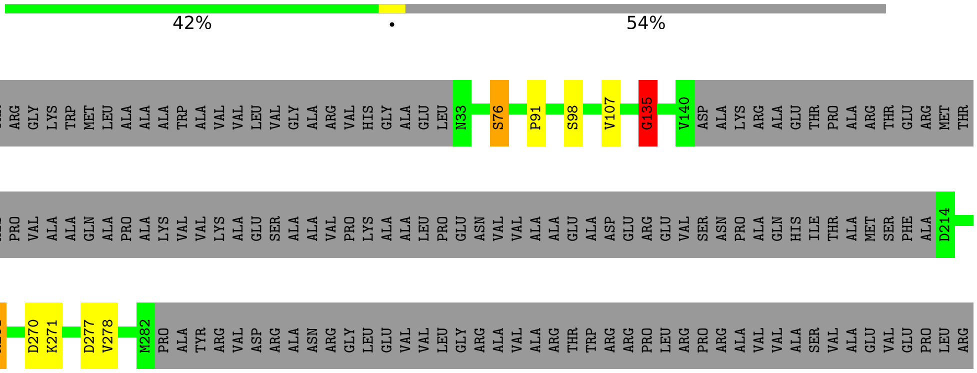
- Molecule 7: PilQ

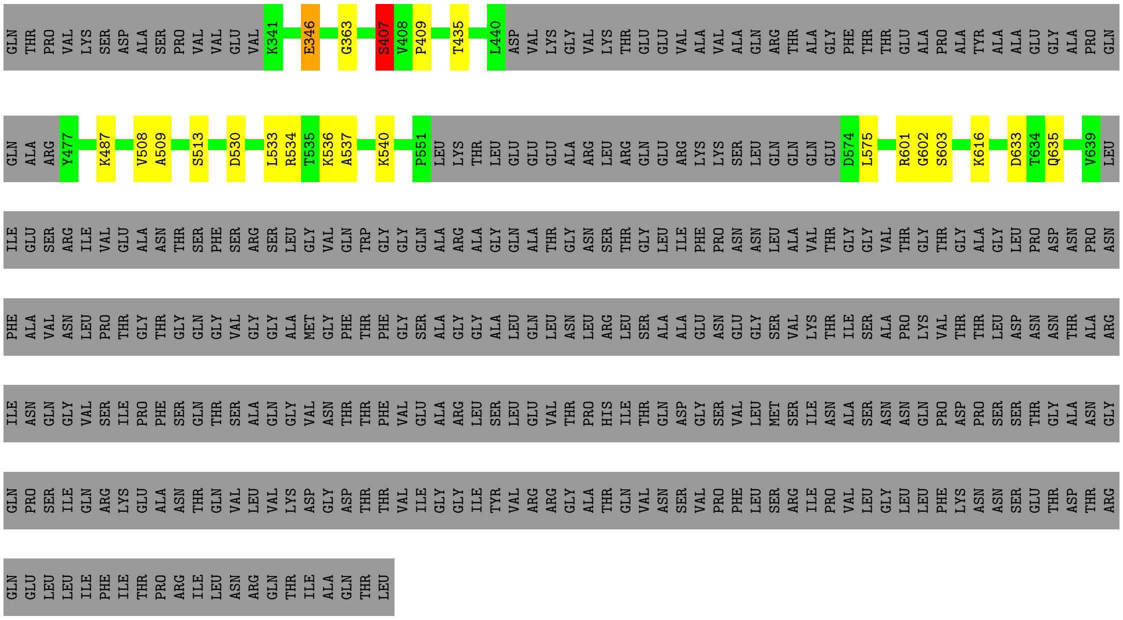
Chain Qk:



- Molecule 7: PilQ

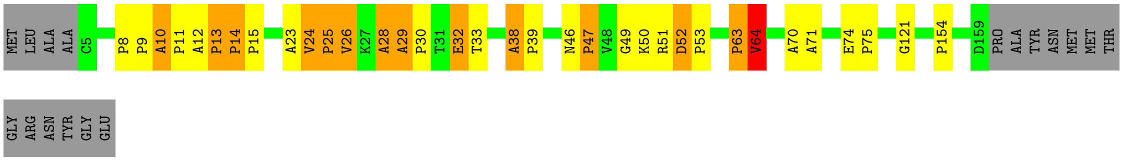
Chain Ql:





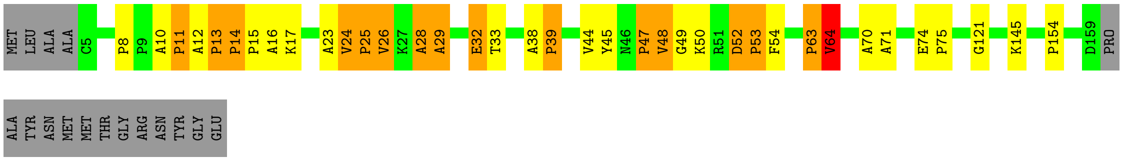
- Molecule 8: PilP

Chain Pa:



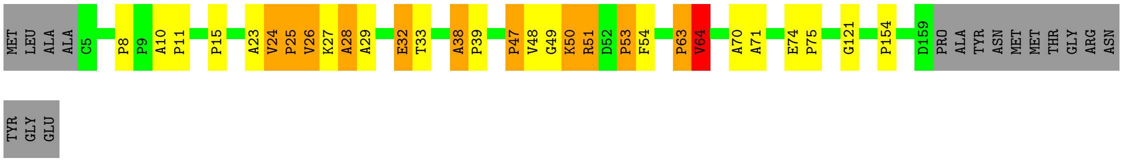
- Molecule 8: PilP

Chain Pb:



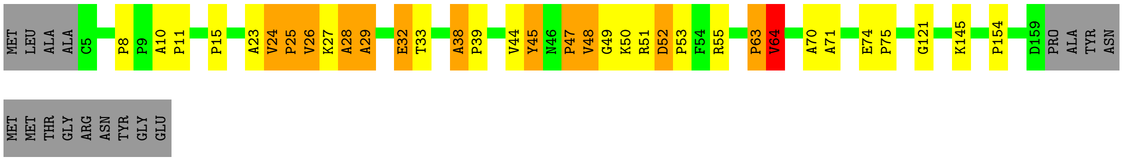
- Molecule 8: PilP

Chain Pc:



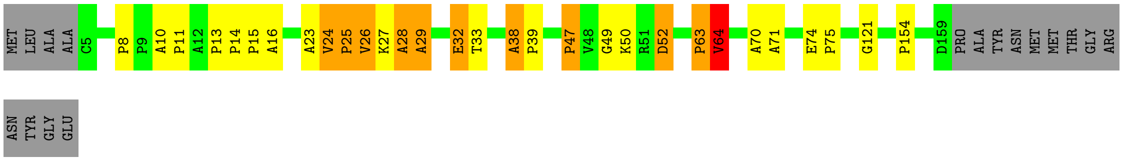
- Molecule 8: PilP

Chain Pd:



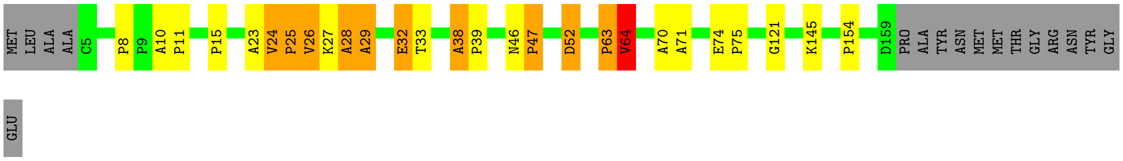
- Molecule 8: PilP

Chain Pe:



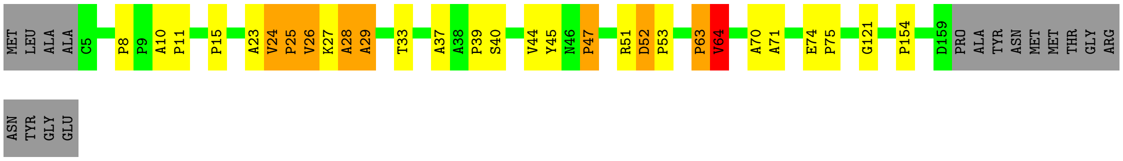
- Molecule 8: PilP

Chain Pf:



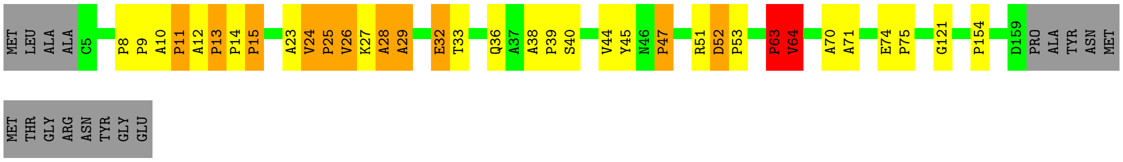
- Molecule 8: PilP

Chain Pg:



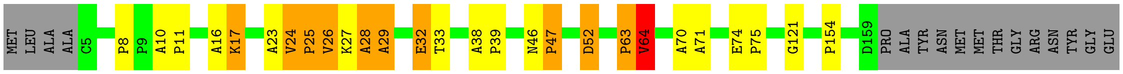
- Molecule 8: PilP

Chain Ph:



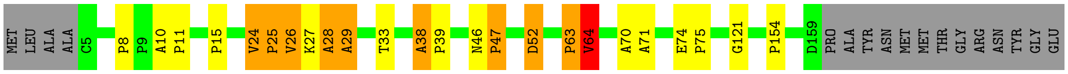
- Molecule 8: PilP

Chain Pi:



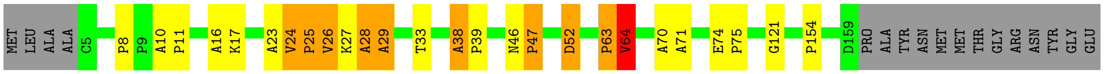
- Molecule 8: PilP

Chain Pj:



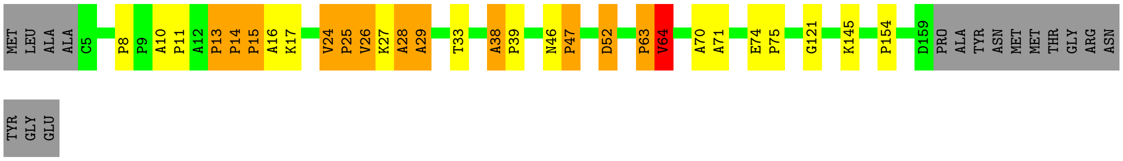
- Molecule 8: PilP

Chain Pk:



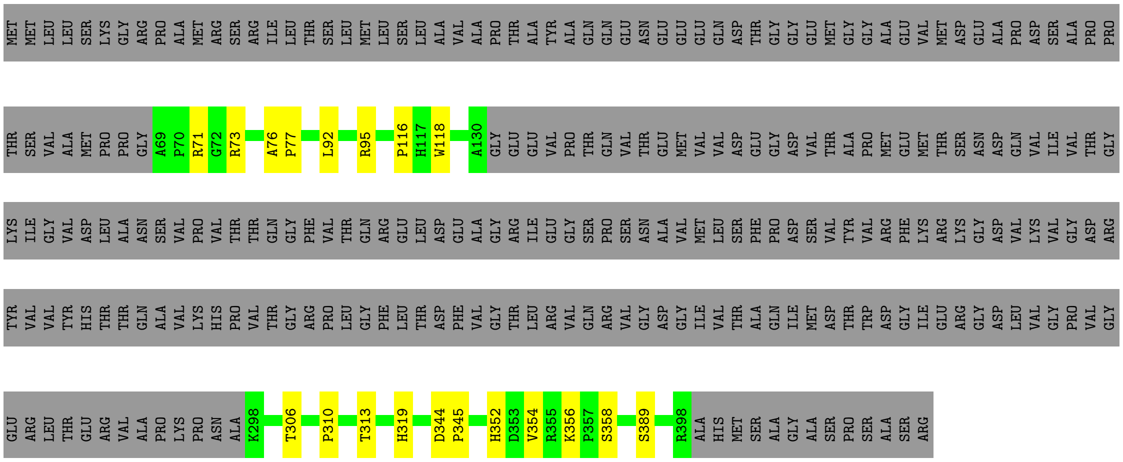
- Molecule 8: PilP

Chain Pl:



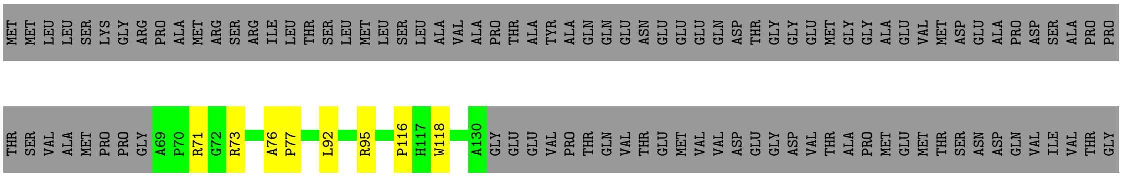
- Molecule 9: LysM domain protein

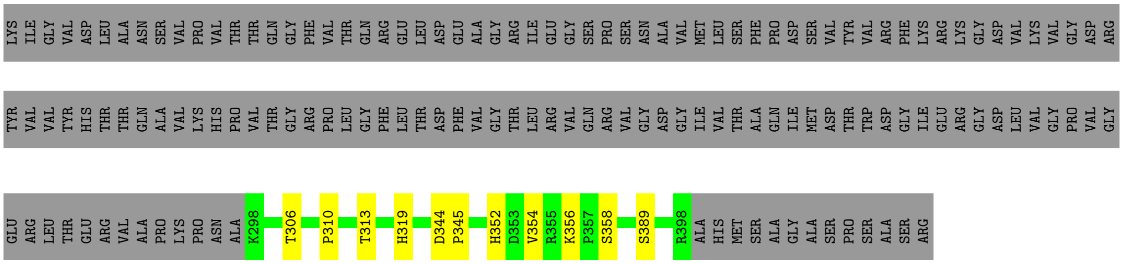
Chain Ta:



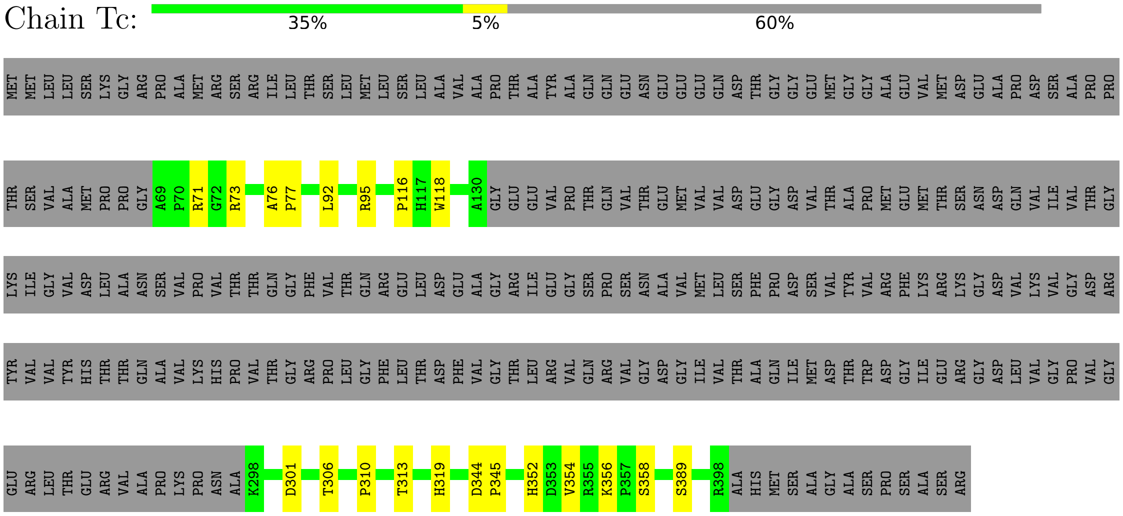
- Molecule 9: LysM domain protein

Chain Tb:

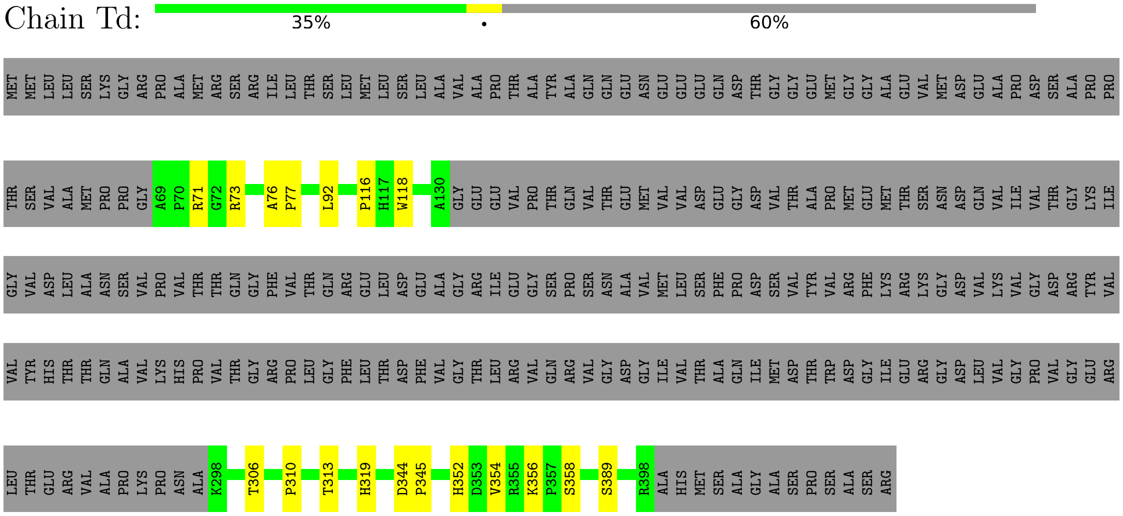




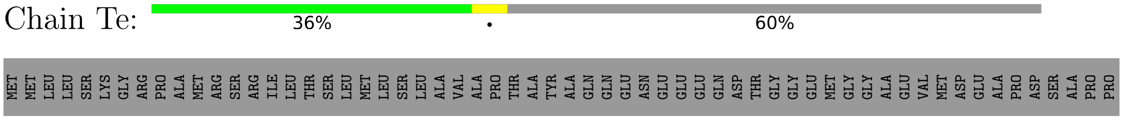
- Molecule 9: LysM domain protein

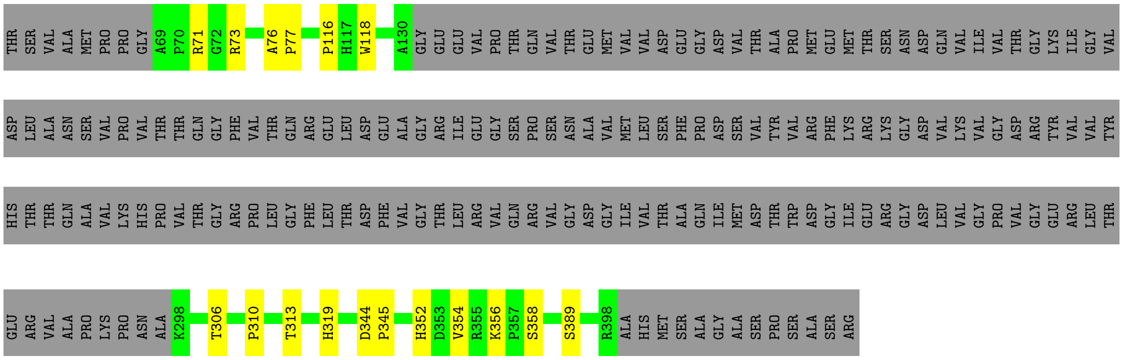


- Molecule 9: LysM domain protein



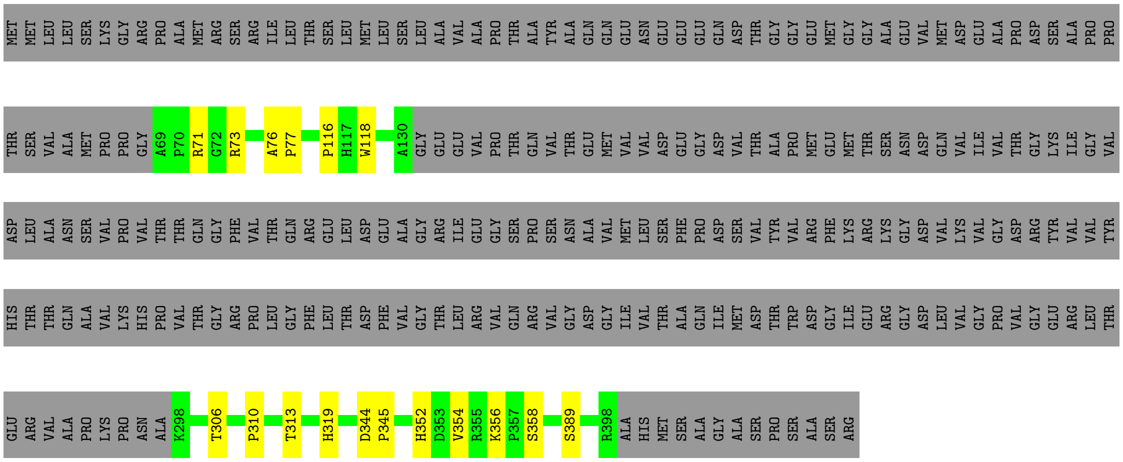
- Molecule 9: LysM domain protein





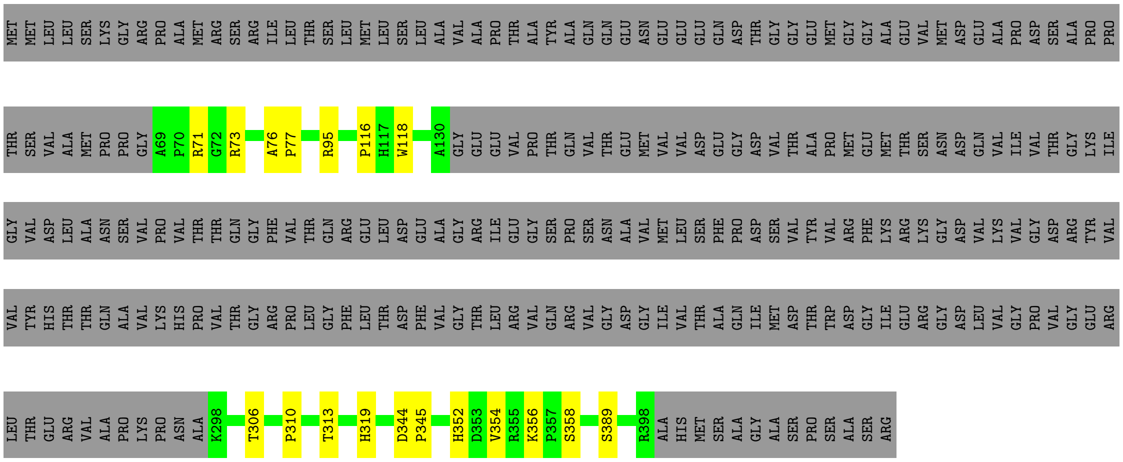
- Molecule 9: LysM domain protein

Chain Tf:



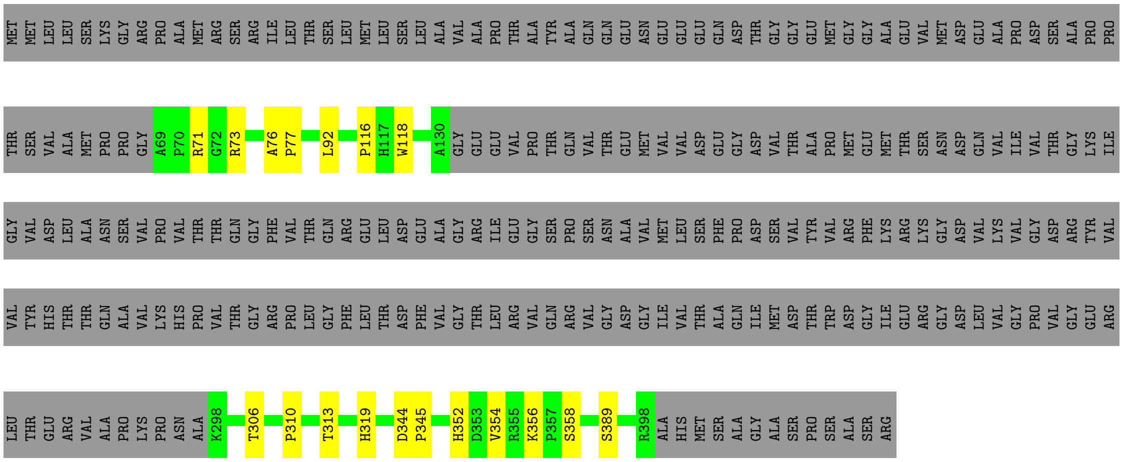
- Molecule 9: LysM domain protein

Chain Tg:



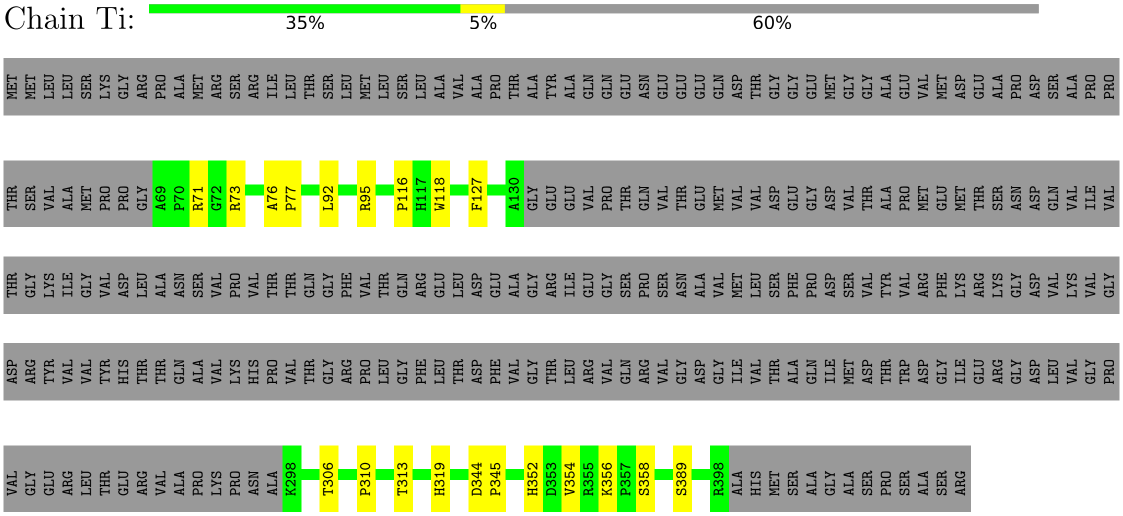
- Molecule 9: LysM domain protein

Chain Th:



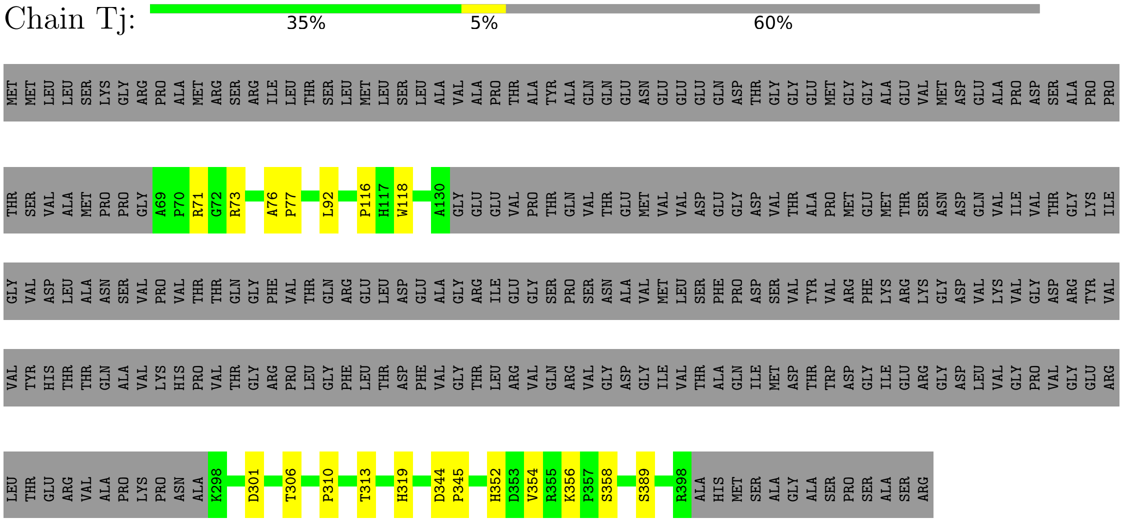
- Molecule 9: LysM domain protein

Chain Ti:



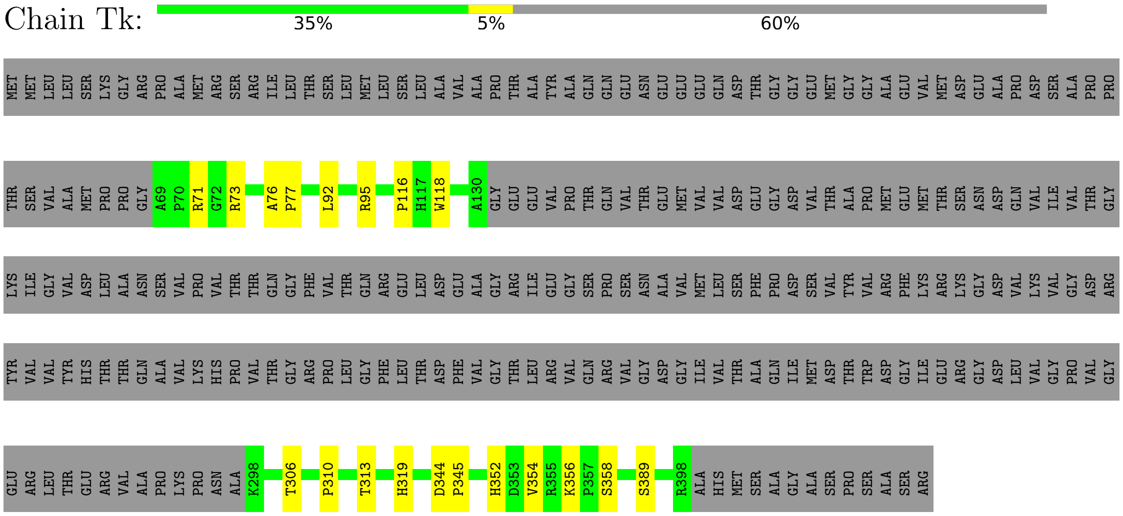
- Molecule 9: LysM domain protein

Chain Tj:



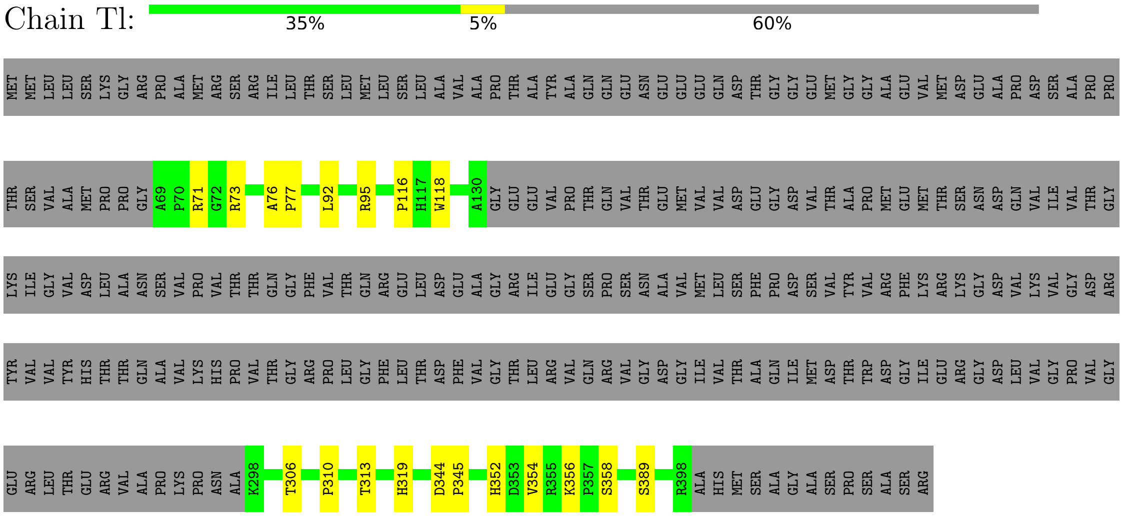
- Molecule 9: LysM domain protein

Chain Tk:



- Molecule 9: LysM domain protein

Chain Tl:



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 $(e^-/\text{Å}^2)$	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	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

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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

All (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
1	Ak	26	ASP	N-CA	15.15	1.76	1.46
1	Av	26	ASP	N-CA	15.14	1.76	1.46
1	As	26	ASP	N-CA	15.12	1.76	1.46
1	Aw	26	ASP	N-CA	15.12	1.76	1.46
1	Aj	26	ASP	N-CA	15.11	1.76	1.46
1	Aq	26	ASP	N-CA	15.11	1.76	1.46
1	Ah	26	ASP	N-CA	15.09	1.76	1.46
1	Au	26	ASP	N-CA	15.09	1.76	1.46
1	A7	26	ASP	N-CA	15.09	1.76	1.46
1	Ab	26	ASP	N-CA	15.09	1.76	1.46
1	A9	26	ASP	N-CA	15.09	1.76	1.46
1	A8	26	ASP	N-CA	15.08	1.76	1.46
1	A5	26	ASP	N-CA	15.07	1.76	1.46
1	At	26	ASP	N-CA	15.06	1.76	1.46
1	A2	26	ASP	N-CA	15.06	1.76	1.46
1	Ax	26	ASP	N-CA	15.06	1.76	1.46
1	A3	26	ASP	N-CA	15.05	1.76	1.46
1	Af	26	ASP	N-CA	15.04	1.76	1.46
1	Ao	26	ASP	N-CA	15.04	1.76	1.46
1	A1	26	ASP	N-CA	15.03	1.76	1.46
1	Ac	26	ASP	N-CA	15.02	1.76	1.46
1	Ap	26	ASP	N-CA	15.02	1.76	1.46
1	Az	26	ASP	N-CA	15.01	1.76	1.46
1	A4	26	ASP	N-CA	15.01	1.76	1.46
1	Ar	26	ASP	N-CA	15.00	1.76	1.46
1	Al	26	ASP	N-CA	14.99	1.76	1.46
1	Am	26	ASP	N-CA	14.98	1.76	1.46
1	An	26	ASP	N-CA	14.93	1.76	1.46
1	A6	26	ASP	N-CA	14.93	1.76	1.46
1	Ai	26	ASP	N-CA	14.87	1.76	1.46
8	Pc	63	PRO	C-N	14.28	1.66	1.34
8	Pk	63	PRO	C-N	14.18	1.66	1.34
8	Pi	63	PRO	C-N	14.16	1.66	1.34
8	Pb	63	PRO	C-N	14.04	1.66	1.34
8	Pd	63	PRO	C-N	13.96	1.66	1.34
8	Pl	63	PRO	C-N	13.80	1.65	1.34
8	Pf	63	PRO	C-N	13.80	1.65	1.34
8	Pg	63	PRO	C-N	13.69	1.65	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Pe	63	PRO	C-N	13.65	1.65	1.34
8	Pj	63	PRO	C-N	13.65	1.65	1.34
8	Ph	63	PRO	C-N	13.64	1.65	1.34
8	Pa	63	PRO	C-N	13.55	1.65	1.34
7	Qk	107	VAL	C-N	6.19	1.44	1.33
7	Qe	107	VAL	C-N	6.18	1.44	1.33
7	Qb	107	VAL	C-N	6.17	1.44	1.33
7	Qf	107	VAL	C-N	6.17	1.44	1.33
7	Qi	107	VAL	C-N	6.17	1.44	1.33
7	Qh	107	VAL	C-N	6.16	1.44	1.33
7	Qc	107	VAL	C-N	6.16	1.44	1.33
7	Qa	107	VAL	C-N	6.14	1.44	1.33
7	Qd	107	VAL	C-N	6.14	1.44	1.33
7	Qg	107	VAL	C-N	6.13	1.44	1.33
7	Ql	107	VAL	C-N	6.13	1.44	1.33
7	Qj	107	VAL	C-N	6.12	1.44	1.33
2	Bb	177	ALA	C-N	5.17	1.44	1.34
2	Bb	177	ALA	CA-C	-5.14	1.39	1.52
2	Bd	177	ALA	C-N	5.01	1.43	1.34

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
7	Qd	407	SER	O-C-N	-54.04	36.24	122.70
7	Qg	407	SER	O-C-N	-54.03	36.24	122.70
7	Qc	407	SER	O-C-N	-54.03	36.25	122.70
7	Qh	407	SER	O-C-N	-54.03	36.25	122.70
7	Ql	407	SER	O-C-N	-54.02	36.26	122.70
7	Qa	407	SER	O-C-N	-54.02	36.26	122.70
7	Qf	407	SER	O-C-N	-54.02	36.28	122.70
7	Qc	135	GLY	O-C-N	-31.62	72.11	122.70
7	Qk	135	GLY	O-C-N	-31.62	72.11	122.70
7	Qh	135	GLY	O-C-N	-31.61	72.12	122.70
7	Ql	135	GLY	O-C-N	-31.61	72.13	122.70
7	Qg	135	GLY	O-C-N	-31.60	72.14	122.70
7	Qa	135	GLY	O-C-N	-31.59	72.15	122.70
7	Qe	135	GLY	O-C-N	-31.59	72.16	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Qi	135	GLY	O-C-N	-31.59	72.16	122.70
7	Qd	135	GLY	O-C-N	-31.58	72.17	122.70
7	Qj	135	GLY	O-C-N	-31.58	72.17	122.70
7	Qb	135	GLY	O-C-N	-31.58	72.18	122.70
7	Qf	135	GLY	O-C-N	-31.57	72.18	122.70
7	Qa	76	SER	O-C-N	-13.44	101.20	122.70
7	Qf	76	SER	O-C-N	-13.43	101.21	122.70
7	Qh	76	SER	O-C-N	-13.43	101.21	122.70
7	Qd	76	SER	O-C-N	-13.41	101.24	122.70
7	Qc	76	SER	O-C-N	-13.41	101.24	122.70
7	Qj	76	SER	O-C-N	-13.41	101.24	122.70
7	Qk	76	SER	O-C-N	-13.41	101.24	122.70
7	Ql	76	SER	O-C-N	-13.41	101.24	122.70
7	Qb	76	SER	O-C-N	-13.40	101.26	122.70
7	Qg	76	SER	O-C-N	-13.40	101.26	122.70
7	Qi	76	SER	O-C-N	-13.40	101.26	122.70
7	Qe	76	SER	O-C-N	-13.39	101.28	122.70
8	Pi	64	VAL	O-C-N	-9.65	107.26	122.70
8	Pg	64	VAL	O-C-N	-9.62	107.31	122.70
7	Qf	258	GLY	CA-C-O	-9.58	103.35	120.60
7	Qj	258	GLY	CA-C-O	-9.57	103.37	120.60
7	Qg	258	GLY	CA-C-O	-9.57	103.38	120.60
7	Qb	258	GLY	CA-C-O	-9.56	103.38	120.60
7	Qi	258	GLY	CA-C-O	-9.56	103.38	120.60
7	Qe	258	GLY	CA-C-O	-9.56	103.39	120.60
7	Qh	258	GLY	CA-C-O	-9.56	103.39	120.60
7	Qc	258	GLY	CA-C-O	-9.56	103.40	120.60
7	Qa	258	GLY	CA-C-O	-9.55	103.40	120.60
7	Qk	258	GLY	CA-C-O	-9.55	103.40	120.60
7	Qd	258	GLY	CA-C-O	-9.55	103.40	120.60
7	Ql	258	GLY	CA-C-O	-9.55	103.41	120.60
8	Pd	64	VAL	O-C-N	-9.52	107.47	122.70
8	Pk	64	VAL	O-C-N	-9.49	107.52	122.70
8	Pc	64	VAL	O-C-N	-9.45	107.58	122.70
8	Pf	64	VAL	O-C-N	-9.42	107.63	122.70
8	Ph	64	VAL	O-C-N	-9.39	107.67	122.70
8	Pj	64	VAL	O-C-N	-9.38	107.69	122.70
8	Pl	64	VAL	O-C-N	-9.34	107.75	122.70
8	Pa	64	VAL	O-C-N	-9.33	107.77	122.70
8	Pe	64	VAL	O-C-N	-9.32	107.79	122.70
8	Pb	64	VAL	O-C-N	-9.08	108.17	122.70
8	Pc	70	ALA	C-N-CA	8.76	143.59	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	Pb	70	ALA	C-N-CA	8.65	143.32	121.70
8	Pj	70	ALA	C-N-CA	8.52	143.01	121.70
8	Ph	63	PRO	O-C-N	-8.48	109.12	122.70
8	Pj	63	PRO	O-C-N	-8.48	109.14	122.70
8	Pk	63	PRO	O-C-N	-8.47	109.15	122.70
8	Pk	70	ALA	C-N-CA	8.46	142.85	121.70
8	Pa	70	ALA	C-N-CA	8.43	142.77	121.70
8	Pe	70	ALA	C-N-CA	8.41	142.74	121.70
8	Pl	70	ALA	C-N-CA	8.41	142.72	121.70
8	Pb	63	PRO	O-C-N	-8.40	109.25	122.70
8	Pg	70	ALA	C-N-CA	8.40	142.69	121.70
8	Pl	63	PRO	O-C-N	-8.39	109.27	122.70
8	Pc	63	PRO	O-C-N	-8.37	109.31	122.70
8	Pi	70	ALA	C-N-CA	8.34	142.55	121.70
8	Pa	63	PRO	O-C-N	-8.33	109.37	122.70
8	Ph	70	ALA	C-N-CA	8.31	142.47	121.70
7	Qg	346	GLU	O-C-N	-8.30	109.41	122.70
7	Qf	346	GLU	O-C-N	-8.29	109.43	122.70
7	Qa	346	GLU	O-C-N	-8.29	109.43	122.70
7	Qb	346	GLU	O-C-N	-8.29	109.44	122.70
7	Qc	346	GLU	O-C-N	-8.29	109.44	122.70
8	Pg	63	PRO	O-C-N	-8.28	109.45	122.70
7	Qk	346	GLU	O-C-N	-8.28	109.45	122.70
7	Qe	346	GLU	O-C-N	-8.28	109.45	122.70
7	Qh	346	GLU	O-C-N	-8.28	109.46	122.70
7	Qi	346	GLU	O-C-N	-8.28	109.46	122.70
7	Qj	346	GLU	O-C-N	-8.27	109.47	122.70
8	Pd	70	ALA	C-N-CA	8.26	142.35	121.70
7	Ql	346	GLU	O-C-N	-8.26	109.48	122.70
7	Qd	346	GLU	O-C-N	-8.25	109.50	122.70
8	Pe	63	PRO	O-C-N	-8.21	109.56	122.70
8	Pi	63	PRO	O-C-N	-8.18	109.62	122.70
8	Pd	63	PRO	O-C-N	-8.16	109.64	122.70
8	Pf	70	ALA	C-N-CA	8.16	142.10	121.70
8	Pf	63	PRO	O-C-N	-8.14	109.67	122.70
1	A6	25	GLN	C-N-CA	-7.66	102.56	121.70
1	An	25	GLN	C-N-CA	-7.63	102.63	121.70
1	Az	25	GLN	C-N-CA	-7.62	102.65	121.70
1	A9	25	GLN	C-N-CA	-7.61	102.67	121.70
1	A5	25	GLN	C-N-CA	-7.61	102.68	121.70
1	A4	25	GLN	C-N-CA	-7.60	102.69	121.70
1	A1	25	GLN	C-N-CA	-7.60	102.70	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Al	25	GLN	C-N-CA	-7.60	102.71	121.70
1	Ao	25	GLN	C-N-CA	-7.60	102.71	121.70
1	A7	25	GLN	C-N-CA	-7.60	102.71	121.70
1	A8	25	GLN	C-N-CA	-7.59	102.73	121.70
1	Ai	25	GLN	C-N-CA	-7.57	102.77	121.70
1	A2	25	GLN	C-N-CA	-7.57	102.77	121.70
1	Ad	25	GLN	C-N-CA	-7.56	102.79	121.70
1	Ac	25	GLN	C-N-CA	-7.56	102.80	121.70
1	At	25	GLN	C-N-CA	-7.56	102.81	121.70
1	Ax	25	GLN	C-N-CA	-7.55	102.82	121.70
1	Ah	25	GLN	C-N-CA	-7.55	102.82	121.70
1	Av	25	GLN	C-N-CA	-7.55	102.82	121.70
1	A3	25	GLN	C-N-CA	-7.55	102.82	121.70
1	Ar	25	GLN	C-N-CA	-7.55	102.83	121.70
1	Au	25	GLN	C-N-CA	-7.55	102.83	121.70
1	Am	25	GLN	C-N-CA	-7.55	102.83	121.70
1	Ay	25	GLN	C-N-CA	-7.54	102.84	121.70
1	Ap	25	GLN	C-N-CA	-7.54	102.84	121.70
1	Ag	25	GLN	C-N-CA	-7.54	102.85	121.70
1	Ak	25	GLN	C-N-CA	-7.52	102.89	121.70
1	Ab	25	GLN	C-N-CA	-7.52	102.90	121.70
1	Aw	25	GLN	C-N-CA	-7.52	102.90	121.70
1	Aa	25	GLN	C-N-CA	-7.51	102.93	121.70
1	Aj	25	GLN	C-N-CA	-7.49	102.97	121.70
1	Ae	25	GLN	C-N-CA	-7.48	103.00	121.70
1	Af	25	GLN	C-N-CA	-7.46	103.06	121.70
1	Aq	25	GLN	C-N-CA	-7.46	103.06	121.70
1	As	25	GLN	C-N-CA	-7.41	103.17	121.70
7	Qb	277	ASP	O-C-N	-7.38	110.89	122.70
7	Qi	277	ASP	O-C-N	-7.37	110.91	122.70
7	Qa	277	ASP	O-C-N	-7.36	110.92	122.70
7	Qf	277	ASP	O-C-N	-7.34	110.95	122.70
7	Ql	277	ASP	O-C-N	-7.33	110.97	122.70
7	Qe	277	ASP	O-C-N	-7.33	110.97	122.70
7	Qd	277	ASP	O-C-N	-7.33	110.98	122.70
7	Qh	277	ASP	O-C-N	-7.33	110.98	122.70
7	Qj	277	ASP	O-C-N	-7.32	110.99	122.70
7	Qc	277	ASP	O-C-N	-7.32	111.00	122.70
7	Qg	277	ASP	O-C-N	-7.31	111.00	122.70
7	Qk	277	ASP	O-C-N	-7.30	111.02	122.70
7	Qf	270	ASP	C-N-CA	6.51	137.97	121.70
7	Qc	270	ASP	C-N-CA	6.50	137.94	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Qk	270	ASP	C-N-CA	6.49	137.94	121.70
7	Qa	270	ASP	C-N-CA	6.49	137.93	121.70
7	Qh	270	ASP	C-N-CA	6.49	137.91	121.70
7	Qe	270	ASP	C-N-CA	6.48	137.91	121.70
7	Qj	270	ASP	C-N-CA	6.48	137.91	121.70
7	Qd	270	ASP	C-N-CA	6.47	137.89	121.70
7	Qg	270	ASP	C-N-CA	6.47	137.88	121.70
7	Ql	270	ASP	C-N-CA	6.47	137.89	121.70
7	Qb	270	ASP	C-N-CA	6.47	137.87	121.70
7	Qi	270	ASP	C-N-CA	6.47	137.88	121.70
7	Qj	258	GLY	O-C-N	6.34	132.85	122.70
7	Qb	258	GLY	O-C-N	6.33	132.84	122.70
7	Qk	258	GLY	O-C-N	6.32	132.82	122.70
7	Qd	258	GLY	O-C-N	6.32	132.81	122.70
7	Ql	258	GLY	O-C-N	6.32	132.81	122.70
7	Qa	258	GLY	O-C-N	6.32	132.81	122.70
7	Qe	258	GLY	O-C-N	6.32	132.80	122.70
7	Qh	258	GLY	O-C-N	6.31	132.79	122.70
7	Qc	258	GLY	O-C-N	6.30	132.79	122.70
7	Qf	258	GLY	O-C-N	6.30	132.79	122.70
7	Qg	258	GLY	O-C-N	6.30	132.78	122.70
7	Qi	258	GLY	O-C-N	6.29	132.76	122.70
8	Pa	63	PRO	CA-C-N	5.79	129.95	117.20
8	Pj	63	PRO	CA-C-N	5.75	129.85	117.20
8	Ph	63	PRO	CA-C-N	5.70	129.74	117.20
8	Pl	63	PRO	CA-C-N	5.62	129.56	117.20
8	Pe	63	PRO	CA-C-N	5.59	129.51	117.20
3	Ca	110	ASN	CA-C-N	5.58	132.74	117.10
8	Pf	63	PRO	CA-C-N	5.57	129.46	117.20
8	Pg	63	PRO	CA-C-N	5.55	129.41	117.20
8	Pk	63	PRO	CA-C-N	5.50	129.31	117.20
8	Pb	63	PRO	CA-C-N	5.49	129.27	117.20
8	Pd	63	PRO	CA-C-N	5.45	129.19	117.20
8	Pc	63	PRO	CA-C-N	5.45	129.18	117.20
7	Qe	261	ARG	C-N-CA	5.41	135.22	121.70
7	Qg	261	ARG	C-N-CA	5.41	135.22	121.70
7	Qd	261	ARG	C-N-CA	5.40	135.21	121.70
7	Qj	261	ARG	C-N-CA	5.40	135.21	121.70
7	Ql	261	ARG	C-N-CA	5.40	135.21	121.70
7	Qa	261	ARG	C-N-CA	5.40	135.20	121.70
7	Qk	261	ARG	C-N-CA	5.40	135.20	121.70
7	Qb	261	ARG	C-N-CA	5.40	135.20	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Qc	261	ARG	C-N-CA	5.40	135.19	121.70
7	Qf	261	ARG	C-N-CA	5.39	135.18	121.70
7	Qi	261	ARG	C-N-CA	5.39	135.17	121.70
9	Th	356	LYS	CA-C-N	5.39	132.19	117.10
7	Qh	261	ARG	C-N-CA	5.38	135.14	121.70
8	Pi	63	PRO	CA-C-N	5.37	129.02	117.20
3	Cb	110	ASN	CA-C-N	5.35	132.09	117.10
2	Bb	458	LYS	C-N-CA	-5.33	108.38	121.70
2	Bd	458	LYS	C-N-CA	-5.30	108.44	121.70
9	Ta	356	LYS	CA-C-N	5.30	131.93	117.10
9	Td	356	LYS	CA-C-N	5.29	131.91	117.10
9	Tk	356	LYS	CA-C-N	5.27	131.86	117.10
7	Qb	270	ASP	CA-C-N	5.25	128.75	117.20
7	Qd	270	ASP	CA-C-N	5.25	128.74	117.20
7	Qj	270	ASP	CA-C-N	5.24	128.73	117.20
7	Ql	270	ASP	CA-C-N	5.24	128.72	117.20
7	Qh	270	ASP	CA-C-N	5.23	128.72	117.20
7	Qe	270	ASP	CA-C-N	5.23	128.71	117.20
7	Qi	270	ASP	CA-C-N	5.23	128.71	117.20
9	Tj	356	LYS	CA-C-N	5.23	131.75	117.10
7	Qa	270	ASP	CA-C-N	5.23	128.70	117.20
7	Qg	270	ASP	CA-C-N	5.22	128.68	117.20
7	Qc	270	ASP	CA-C-N	5.21	128.66	117.20
7	Qk	270	ASP	CA-C-N	5.21	128.66	117.20
9	Tf	356	LYS	CA-C-N	5.21	131.68	117.10
2	Ba	458	LYS	C-N-CA	-5.20	108.69	121.70
7	Qf	270	ASP	CA-C-N	5.20	128.65	117.20
9	Tl	356	LYS	CA-C-N	5.20	131.65	117.10
2	Bf	458	LYS	C-N-CA	-5.19	108.73	121.70
7	Qc	601	ARG	CA-C-N	-5.19	105.82	116.20
9	Tc	356	LYS	CA-C-N	5.18	131.62	117.10
9	Tg	356	LYS	CA-C-N	5.16	131.54	117.10
2	Be	458	LYS	C-N-CA	-5.14	108.84	121.70
9	Tb	356	LYS	CA-C-N	5.12	131.43	117.10
9	Te	356	LYS	CA-C-N	5.12	131.42	117.10
9	Ti	356	LYS	CA-C-N	5.08	131.32	117.10
9	Tc	356	LYS	CA-C-O	-5.02	109.56	120.10
9	Tk	356	LYS	CA-C-O	-5.01	109.57	120.10

There are no chirality outliers.

All (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
2	Bb	286	LYS	Peptide
2	Bb	287	SER	Peptide
2	Bb	293	MET	Peptide
2	Bb	345	ILE	Peptide
2	Bb	379	PHE	Peptide
2	Bc	177	ALA	Peptide
2	Bc	293	MET	Peptide
2	Bc	345	ILE	Peptide
2	Bc	379	PHE	Peptide
2	Bd	177	ALA	Peptide
2	Bd	284	LEU	Peptide
2	Bd	286	LYS	Peptide
2	Bd	287	SER	Peptide
2	Bd	293	MET	Peptide
2	Bd	345	ILE	Peptide
2	Bd	379	PHE	Peptide
2	Be	177	ALA	Peptide
2	Be	293	MET	Peptide
2	Be	345	ILE	Peptide
2	Be	379	PHE	Peptide
2	Bf	177	ALA	Peptide
2	Bf	284	LEU	Peptide
2	Bf	286	LYS	Peptide
2	Bf	287	SER	Peptide
2	Bf	293	MET	Peptide
2	Bf	345	ILE	Peptide
2	Bf	379	PHE	Peptide
3	Ca	108	MET	Mainchain
3	Ca	169	ARG	Mainchain
3	Ca	192	VAL	Mainchain
3	Ca	200	LEU	Mainchain
3	Ca	222	PRO	Mainchain,Peptide
3	Ca	223	THR	Peptide
3	Ca	242	GLY	Mainchain
3	Ca	256	ARG	Mainchain
3	Ca	257	GLN	Mainchain
3	Ca	279	ARG	Mainchain
3	Ca	302	ASP	Mainchain

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Mol	Chain	Res	Type	Group
3	Ca	313	ASN	Mainchain
3	Ca	317	GLU	Mainchain
3	Ca	325	GLY	Mainchain
3	Ca	332	ASN	Mainchain
3	Ca	384	ALA	Mainchain
3	Ca	78	LYS	Mainchain
3	Cb	108	MET	Mainchain
3	Cb	169	ARG	Mainchain
3	Cb	200	LEU	Mainchain
3	Cb	203	LYS	Mainchain
3	Cb	222	PRO	Mainchain,Peptide
3	Cb	223	THR	Peptide
3	Cb	256	ARG	Mainchain
3	Cb	257	GLN	Mainchain
3	Cb	279	ARG	Mainchain
3	Cb	302	ASP	Mainchain
3	Cb	313	ASN	Mainchain
3	Cb	317	GLU	Mainchain
3	Cb	325	GLY	Mainchain
3	Cb	332	ASN	Mainchain
3	Cb	344	PRO	Mainchain
3	Cb	384	ALA	Mainchain
3	Cb	78	LYS	Mainchain
6	Ma	315	TYR	Peptide
6	Ma	320	ALA	Peptide
6	Mb	315	TYR	Peptide
6	Mb	320	ALA	Peptide
6	Mc	315	TYR	Peptide
6	Mc	320	ALA	Peptide
6	Md	315	TYR	Peptide
6	Md	320	ALA	Peptide
6	Me	315	TYR	Peptide
6	Me	320	ALA	Peptide
6	Mf	315	TYR	Peptide
6	Mf	320	ALA	Peptide
6	Mg	315	TYR	Peptide
6	Mg	320	ALA	Peptide
6	Mh	315	TYR	Peptide
6	Mh	320	ALA	Peptide
6	Mi	315	TYR	Peptide
6	Mi	320	ALA	Peptide
6	Mj	315	TYR	Peptide

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Mol	Chain	Res	Type	Group
6	Mj	320	ALA	Peptide
6	Mk	315	TYR	Peptide
6	Mk	320	ALA	Peptide
6	Ml	315	TYR	Peptide
6	Ml	320	ALA	Peptide
4	Na	100	VAL	Peptide
4	Na	101	ARG	Peptide
4	Na	171	GLU	Peptide
4	Na	209	VAL	Peptide
4	Na	221	SER	Peptide
4	Na	222	ASN	Peptide
4	Nb	100	VAL	Peptide
4	Nb	101	ARG	Peptide
4	Nb	171	GLU	Peptide
4	Nb	209	VAL	Peptide
4	Nb	221	SER	Peptide
4	Nb	222	ASN	Peptide
4	Nc	100	VAL	Peptide
4	Nc	101	ARG	Peptide
4	Nc	171	GLU	Peptide
4	Nc	209	VAL	Peptide
4	Nc	222	ASN	Peptide
4	Nd	100	VAL	Peptide
4	Nd	101	ARG	Peptide
4	Nd	171	GLU	Peptide
4	Nd	209	VAL	Peptide
4	Nd	222	ASN	Peptide
4	Ne	100	VAL	Peptide
4	Ne	101	ARG	Peptide
4	Ne	171	GLU	Peptide
4	Ne	209	VAL	Peptide
4	Ne	222	ASN	Peptide
4	Nf	100	VAL	Peptide
4	Nf	101	ARG	Peptide
4	Nf	171	GLU	Peptide
4	Nf	209	VAL	Peptide
4	Nf	222	ASN	Peptide
4	Ng	100	VAL	Peptide
4	Ng	101	ARG	Peptide
4	Ng	171	GLU	Peptide
4	Ng	209	VAL	Peptide
4	Ng	222	ASN	Peptide

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Mol	Chain	Res	Type	Group
4	Nh	100	VAL	Peptide
4	Nh	101	ARG	Peptide
4	Nh	171	GLU	Peptide
4	Nh	209	VAL	Peptide
4	Nh	222	ASN	Peptide
4	Ni	100	VAL	Peptide
4	Ni	101	ARG	Peptide
4	Ni	171	GLU	Peptide
4	Ni	209	VAL	Peptide
4	Ni	222	ASN	Peptide
4	Nj	100	VAL	Peptide
4	Nj	101	ARG	Peptide
4	Nj	171	GLU	Peptide
4	Nj	209	VAL	Peptide
4	Nj	222	ASN	Peptide
4	Nk	100	VAL	Peptide
4	Nk	101	ARG	Peptide
4	Nk	171	GLU	Peptide
4	Nk	209	VAL	Peptide
4	Nk	222	ASN	Peptide
4	Nl	100	VAL	Peptide
4	Nl	101	ARG	Peptide
4	Nl	171	GLU	Peptide
4	Nl	209	VAL	Peptide
4	Nl	222	ASN	Peptide
5	Oa	82	SER	Peptide
5	Ob	82	SER	Peptide
5	Oc	82	SER	Peptide
5	Od	82	SER	Peptide
5	Oe	82	SER	Peptide
5	Of	82	SER	Peptide
5	Og	82	SER	Peptide
5	Oh	82	SER	Peptide
5	Oi	82	SER	Peptide
5	Oj	82	SER	Peptide
5	Ok	82	SER	Peptide
5	Ol	82	SER	Peptide
8	Pa	10	ALA	Peptide
8	Pa	12	ALA	Peptide
8	Pa	13	PRO	Peptide
8	Pa	14	PRO	Peptide
8	Pa	23	ALA	Peptide

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Mol	Chain	Res	Type	Group
8	Pa	24	VAL	Peptide
8	Pa	25	PRO	Peptide
8	Pa	26	VAL	Peptide
8	Pa	28	ALA	Peptide
8	Pa	29	ALA	Mainchain,Peptide
8	Pa	30	PRO	Mainchain
8	Pa	32	GLU	Peptide
8	Pa	33	THR	Peptide
8	Pa	38	ALA	Peptide
8	Pa	46	ASN	Peptide
8	Pa	47	PRO	Peptide
8	Pa	49	GLY	Peptide
8	Pa	50	LYS	Peptide
8	Pa	51	ARG	Peptide
8	Pa	52	ASP	Peptide
8	Pa	53	PRO	Peptide
8	Pa	64	VAL	Mainchain
8	Pa	74	GLU	Peptide
8	Pa	8	PRO	Peptide
8	Pb	11	PRO	Peptide
8	Pb	13	PRO	Peptide
8	Pb	14	PRO	Peptide
8	Pb	145	LYS	Mainchain
8	Pb	15	PRO	Peptide
8	Pb	23	ALA	Peptide
8	Pb	24	VAL	Peptide
8	Pb	25	PRO	Peptide
8	Pb	26	VAL	Peptide
8	Pb	28	ALA	Peptide
8	Pb	29	ALA	Peptide
8	Pb	32	GLU	Peptide
8	Pb	33	THR	Peptide
8	Pb	38	ALA	Peptide
8	Pb	39	PRO	Peptide
8	Pb	44	VAL	Peptide
8	Pb	45	TYR	Peptide
8	Pb	47	PRO	Peptide
8	Pb	48	VAL	Peptide
8	Pb	49	GLY	Peptide
8	Pb	52	ASP	Peptide
8	Pb	53	PRO	Peptide
8	Pb	54	PHE	Peptide

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Mol	Chain	Res	Type	Group
8	Pb	64	VAL	Mainchain
8	Pb	74	GLU	Mainchain,Peptide
8	Pb	8	PRO	Mainchain,Peptide
8	Pc	15	PRO	Peptide
8	Pc	23	ALA	Peptide
8	Pc	24	VAL	Peptide
8	Pc	25	PRO	Peptide
8	Pc	26	VAL	Peptide
8	Pc	27	LYS	Peptide
8	Pc	28	ALA	Peptide
8	Pc	32	GLU	Peptide
8	Pc	33	THR	Peptide
8	Pc	38	ALA	Peptide
8	Pc	47	PRO	Peptide
8	Pc	49	GLY	Peptide
8	Pc	50	LYS	Peptide
8	Pc	51	ARG	Peptide
8	Pc	53	PRO	Peptide
8	Pc	54	PHE	Peptide
8	Pc	64	VAL	Mainchain
8	Pc	74	GLU	Peptide
8	Pc	8	PRO	Mainchain,Peptide
8	Pd	145	LYS	Mainchain
8	Pd	15	PRO	Peptide
8	Pd	23	ALA	Peptide
8	Pd	24	VAL	Peptide
8	Pd	25	PRO	Peptide
8	Pd	26	VAL	Peptide
8	Pd	27	LYS	Peptide
8	Pd	28	ALA	Peptide
8	Pd	29	ALA	Peptide
8	Pd	32	GLU	Peptide
8	Pd	33	THR	Peptide
8	Pd	38	ALA	Peptide
8	Pd	44	VAL	Peptide
8	Pd	45	TYR	Peptide
8	Pd	47	PRO	Peptide
8	Pd	48	VAL	Peptide
8	Pd	49	GLY	Peptide
8	Pd	51	ARG	Peptide
8	Pd	52	ASP	Peptide
8	Pd	53	PRO	Peptide

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Mol	Chain	Res	Type	Group
8	Pd	64	VAL	Mainchain
8	Pd	74	GLU	Peptide
8	Pd	8	PRO	Mainchain,Peptide
8	Pe	13	PRO	Peptide
8	Pe	14	PRO	Peptide
8	Pe	15	PRO	Peptide
8	Pe	23	ALA	Peptide
8	Pe	24	VAL	Peptide
8	Pe	25	PRO	Peptide
8	Pe	26	VAL	Peptide
8	Pe	27	LYS	Peptide
8	Pe	28	ALA	Peptide
8	Pe	29	ALA	Peptide
8	Pe	32	GLU	Peptide
8	Pe	33	THR	Peptide
8	Pe	38	ALA	Peptide
8	Pe	47	PRO	Peptide
8	Pe	49	GLY	Peptide
8	Pe	50	LYS	Peptide
8	Pe	52	ASP	Peptide
8	Pe	64	VAL	Mainchain
8	Pe	74	GLU	Mainchain,Peptide
8	Pe	8	PRO	Mainchain,Peptide
8	Pf	145	LYS	Mainchain
8	Pf	15	PRO	Peptide
8	Pf	23	ALA	Peptide
8	Pf	24	VAL	Peptide
8	Pf	25	PRO	Peptide
8	Pf	26	VAL	Peptide
8	Pf	27	LYS	Peptide
8	Pf	28	ALA	Peptide
8	Pf	29	ALA	Peptide
8	Pf	32	GLU	Peptide
8	Pf	33	THR	Peptide
8	Pf	38	ALA	Peptide
8	Pf	46	ASN	Peptide
8	Pf	47	PRO	Mainchain,Peptide
8	Pf	52	ASP	Mainchain,Peptide
8	Pf	64	VAL	Mainchain
8	Pf	74	GLU	Peptide
8	Pf	8	PRO	Mainchain,Peptide
8	Pg	15	PRO	Peptide

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Mol	Chain	Res	Type	Group
8	Pg	23	ALA	Peptide
8	Pg	24	VAL	Peptide
8	Pg	25	PRO	Peptide
8	Pg	26	VAL	Peptide
8	Pg	27	LYS	Peptide
8	Pg	28	ALA	Peptide
8	Pg	29	ALA	Peptide
8	Pg	33	THR	Peptide
8	Pg	37	ALA	Peptide
8	Pg	40	SER	Peptide
8	Pg	44	VAL	Peptide
8	Pg	45	TYR	Peptide
8	Pg	47	PRO	Peptide
8	Pg	51	ARG	Peptide
8	Pg	52	ASP	Peptide
8	Pg	53	PRO	Peptide
8	Pg	64	VAL	Mainchain
8	Pg	74	GLU	Peptide
8	Pg	8	PRO	Mainchain,Peptide
8	Ph	11	PRO	Peptide
8	Ph	13	PRO	Peptide
8	Ph	14	PRO	Peptide
8	Ph	15	PRO	Peptide
8	Ph	23	ALA	Peptide
8	Ph	24	VAL	Peptide
8	Ph	25	PRO	Peptide
8	Ph	26	VAL	Peptide
8	Ph	27	LYS	Peptide
8	Ph	28	ALA	Peptide
8	Ph	29	ALA	Peptide
8	Ph	32	GLU	Peptide
8	Ph	33	THR	Peptide
8	Ph	36	GLN	Peptide
8	Ph	38	ALA	Peptide
8	Ph	40	SER	Peptide
8	Ph	44	VAL	Peptide
8	Ph	45	TYR	Peptide
8	Ph	47	PRO	Peptide
8	Ph	51	ARG	Peptide
8	Ph	52	ASP	Peptide
8	Ph	63	PRO	Mainchain
8	Ph	64	VAL	Mainchain

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Mol	Chain	Res	Type	Group
8	Ph	74	GLU	Mainchain,Peptide
8	Ph	8	PRO	Peptide
8	Pi	16	ALA	Mainchain
8	Pi	17	LYS	Mainchain
8	Pi	23	ALA	Peptide
8	Pi	24	VAL	Peptide
8	Pi	25	PRO	Peptide
8	Pi	26	VAL	Peptide
8	Pi	27	LYS	Peptide
8	Pi	28	ALA	Peptide
8	Pi	29	ALA	Peptide
8	Pi	32	GLU	Peptide
8	Pi	33	THR	Peptide
8	Pi	38	ALA	Peptide
8	Pi	46	ASN	Peptide
8	Pi	47	PRO	Mainchain,Peptide
8	Pi	52	ASP	Mainchain,Peptide
8	Pi	64	VAL	Mainchain
8	Pi	74	GLU	Peptide
8	Pi	8	PRO	Mainchain,Peptide
8	Pj	15	PRO	Peptide
8	Pj	24	VAL	Peptide
8	Pj	25	PRO	Peptide
8	Pj	26	VAL	Peptide
8	Pj	27	LYS	Peptide
8	Pj	28	ALA	Peptide
8	Pj	29	ALA	Peptide
8	Pj	33	THR	Peptide
8	Pj	38	ALA	Peptide
8	Pj	46	ASN	Peptide
8	Pj	47	PRO	Mainchain,Peptide
8	Pj	52	ASP	Mainchain,Peptide
8	Pj	64	VAL	Mainchain
8	Pj	74	GLU	Mainchain,Peptide
8	Pj	8	PRO	Mainchain,Peptide
8	Pk	17	LYS	Peptide
8	Pk	23	ALA	Peptide
8	Pk	24	VAL	Peptide
8	Pk	25	PRO	Peptide
8	Pk	26	VAL	Peptide
8	Pk	27	LYS	Peptide
8	Pk	28	ALA	Peptide

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Mol	Chain	Res	Type	Group
8	Pk	29	ALA	Peptide
8	Pk	33	THR	Peptide
8	Pk	38	ALA	Peptide
8	Pk	46	ASN	Peptide
8	Pk	47	PRO	Mainchain,Peptide
8	Pk	52	ASP	Mainchain,Peptide
8	Pk	64	VAL	Mainchain
8	Pk	74	GLU	Peptide
8	Pk	8	PRO	Mainchain,Peptide
8	Pl	13	PRO	Peptide
8	Pl	14	PRO	Peptide
8	Pl	145	LYS	Mainchain
8	Pl	15	PRO	Peptide
8	Pl	24	VAL	Peptide
8	Pl	25	PRO	Peptide
8	Pl	26	VAL	Peptide
8	Pl	27	LYS	Peptide
8	Pl	28	ALA	Peptide
8	Pl	29	ALA	Peptide
8	Pl	33	THR	Peptide
8	Pl	38	ALA	Peptide
8	Pl	46	ASN	Peptide
8	Pl	47	PRO	Mainchain,Peptide
8	Pl	52	ASP	Mainchain,Peptide
8	Pl	64	VAL	Mainchain
8	Pl	74	GLU	Peptide
8	Pl	8	PRO	Mainchain,Peptide
7	Qa	135	GLY	Mainchain
7	Qa	250	THR	Mainchain
7	Qa	278	VAL	Mainchain
7	Qa	346	GLU	Mainchain
7	Qa	407	SER	Mainchain
7	Qa	487	LYS	Mainchain
7	Qa	508	VAL	Peptide
7	Qa	530	ASP	Mainchain
7	Qa	533	LEU	Mainchain
7	Qa	534	ARG	Mainchain
7	Qa	536	LYS	Mainchain
7	Qa	537	ALA	Mainchain
7	Qa	575	LEU	Mainchain
7	Qa	601	ARG	Mainchain
7	Qa	602	GLY	Peptide

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Mol	Chain	Res	Type	Group
7	Qa	616	LYS	Mainchain
7	Qa	633	ASP	Mainchain
7	Qa	635	GLN	Mainchain
7	Qa	76	SER	Mainchain
7	Qa	98	SER	Mainchain
7	Qb	135	GLY	Mainchain
7	Qb	250	THR	Mainchain
7	Qb	278	VAL	Mainchain
7	Qb	346	GLU	Mainchain
7	Qb	407	SER	Mainchain
7	Qb	487	LYS	Mainchain
7	Qb	498	ILE	Mainchain
7	Qb	508	VAL	Peptide
7	Qb	510	ASP	Mainchain
7	Qb	530	ASP	Mainchain
7	Qb	533	LEU	Mainchain
7	Qb	534	ARG	Mainchain
7	Qb	536	LYS	Mainchain
7	Qb	537	ALA	Mainchain
7	Qb	575	LEU	Mainchain
7	Qb	601	ARG	Mainchain
7	Qb	602	GLY	Mainchain,Peptide
7	Qb	616	LYS	Mainchain
7	Qb	633	ASP	Mainchain
7	Qb	635	GLN	Mainchain
7	Qb	76	SER	Mainchain
7	Qb	98	SER	Mainchain
7	Qc	135	GLY	Mainchain
7	Qc	250	THR	Mainchain
7	Qc	278	VAL	Mainchain
7	Qc	346	GLU	Mainchain
7	Qc	407	SER	Mainchain
7	Qc	498	ILE	Mainchain
7	Qc	508	VAL	Peptide
7	Qc	530	ASP	Mainchain
7	Qc	533	LEU	Mainchain
7	Qc	534	ARG	Mainchain
7	Qc	536	LYS	Mainchain
7	Qc	537	ALA	Mainchain
7	Qc	575	LEU	Mainchain
7	Qc	601	ARG	Mainchain
7	Qc	602	GLY	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
7	Qc	616	LYS	Mainchain
7	Qc	633	ASP	Mainchain
7	Qc	635	GLN	Mainchain
7	Qc	76	SER	Mainchain
7	Qc	98	SER	Mainchain
7	Qd	135	GLY	Mainchain
7	Qd	250	THR	Mainchain
7	Qd	278	VAL	Mainchain
7	Qd	346	GLU	Mainchain
7	Qd	407	SER	Mainchain
7	Qd	487	LYS	Mainchain
7	Qd	508	VAL	Peptide
7	Qd	530	ASP	Mainchain
7	Qd	533	LEU	Mainchain
7	Qd	534	ARG	Mainchain
7	Qd	536	LYS	Mainchain
7	Qd	537	ALA	Mainchain
7	Qd	540	LYS	Mainchain
7	Qd	575	LEU	Mainchain
7	Qd	601	ARG	Mainchain
7	Qd	602	GLY	Peptide
7	Qd	616	LYS	Mainchain
7	Qd	633	ASP	Mainchain
7	Qd	635	GLN	Mainchain
7	Qd	76	SER	Mainchain
7	Qd	98	SER	Mainchain
7	Qe	135	GLY	Mainchain
7	Qe	250	THR	Mainchain
7	Qe	278	VAL	Mainchain
7	Qe	346	GLU	Mainchain
7	Qe	407	SER	Mainchain
7	Qe	487	LYS	Mainchain
7	Qe	508	VAL	Peptide
7	Qe	510	ASP	Mainchain
7	Qe	530	ASP	Mainchain
7	Qe	533	LEU	Mainchain
7	Qe	534	ARG	Mainchain
7	Qe	536	LYS	Mainchain
7	Qe	537	ALA	Mainchain
7	Qe	575	LEU	Mainchain
7	Qe	601	ARG	Mainchain
7	Qe	602	GLY	Peptide

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Mol	Chain	Res	Type	Group
7	Qe	616	LYS	Mainchain
7	Qe	633	ASP	Mainchain
7	Qe	635	GLN	Mainchain
7	Qe	76	SER	Mainchain
7	Qe	98	SER	Mainchain
7	Qf	135	GLY	Mainchain
7	Qf	250	THR	Mainchain
7	Qf	278	VAL	Mainchain
7	Qf	346	GLU	Mainchain
7	Qf	407	SER	Mainchain
7	Qf	487	LYS	Mainchain
7	Qf	508	VAL	Peptide
7	Qf	530	ASP	Mainchain
7	Qf	533	LEU	Mainchain
7	Qf	534	ARG	Mainchain
7	Qf	536	LYS	Mainchain
7	Qf	537	ALA	Mainchain
7	Qf	575	LEU	Mainchain
7	Qf	601	ARG	Mainchain
7	Qf	602	GLY	Peptide
7	Qf	616	LYS	Mainchain
7	Qf	633	ASP	Mainchain
7	Qf	635	GLN	Mainchain
7	Qf	76	SER	Mainchain
7	Qf	98	SER	Mainchain
7	Qg	135	GLY	Mainchain
7	Qg	250	THR	Mainchain
7	Qg	278	VAL	Mainchain
7	Qg	346	GLU	Mainchain
7	Qg	407	SER	Mainchain
7	Qg	487	LYS	Mainchain
7	Qg	508	VAL	Peptide
7	Qg	530	ASP	Mainchain
7	Qg	533	LEU	Mainchain
7	Qg	534	ARG	Mainchain
7	Qg	536	LYS	Mainchain
7	Qg	537	ALA	Mainchain
7	Qg	575	LEU	Mainchain
7	Qg	582	VAL	Mainchain
7	Qg	601	ARG	Mainchain
7	Qg	602	GLY	Peptide
7	Qg	616	LYS	Mainchain

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Mol	Chain	Res	Type	Group
7	Qg	633	ASP	Mainchain
7	Qg	635	GLN	Mainchain
7	Qg	76	SER	Mainchain
7	Qg	98	SER	Mainchain
7	Qh	135	GLY	Mainchain
7	Qh	250	THR	Mainchain
7	Qh	278	VAL	Mainchain
7	Qh	346	GLU	Mainchain
7	Qh	407	SER	Mainchain
7	Qh	508	VAL	Peptide
7	Qh	530	ASP	Mainchain
7	Qh	533	LEU	Mainchain
7	Qh	534	ARG	Mainchain
7	Qh	536	LYS	Mainchain
7	Qh	537	ALA	Mainchain
7	Qh	540	LYS	Mainchain
7	Qh	575	LEU	Mainchain
7	Qh	601	ARG	Mainchain
7	Qh	602	GLY	Peptide
7	Qh	616	LYS	Mainchain
7	Qh	633	ASP	Mainchain
7	Qh	635	GLN	Mainchain
7	Qh	76	SER	Mainchain
7	Qh	98	SER	Mainchain
7	Qi	135	GLY	Mainchain
7	Qi	250	THR	Mainchain
7	Qi	278	VAL	Mainchain
7	Qi	346	GLU	Mainchain
7	Qi	407	SER	Mainchain
7	Qi	487	LYS	Mainchain
7	Qi	498	ILE	Mainchain
7	Qi	508	VAL	Peptide
7	Qi	530	ASP	Mainchain
7	Qi	533	LEU	Mainchain
7	Qi	534	ARG	Mainchain
7	Qi	536	LYS	Mainchain
7	Qi	537	ALA	Mainchain
7	Qi	540	LYS	Mainchain
7	Qi	575	LEU	Mainchain
7	Qi	601	ARG	Mainchain
7	Qi	602	GLY	Peptide
7	Qi	616	LYS	Mainchain

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Mol	Chain	Res	Type	Group
7	Qi	633	ASP	Mainchain
7	Qi	635	GLN	Mainchain
7	Qi	76	SER	Mainchain
7	Qi	98	SER	Mainchain
7	Qj	135	GLY	Mainchain
7	Qj	250	THR	Mainchain
7	Qj	278	VAL	Mainchain
7	Qj	346	GLU	Mainchain
7	Qj	407	SER	Mainchain
7	Qj	487	LYS	Mainchain
7	Qj	498	ILE	Mainchain
7	Qj	508	VAL	Peptide
7	Qj	510	ASP	Mainchain
7	Qj	530	ASP	Mainchain
7	Qj	533	LEU	Mainchain
7	Qj	534	ARG	Mainchain
7	Qj	536	LYS	Mainchain
7	Qj	537	ALA	Mainchain
7	Qj	540	LYS	Mainchain
7	Qj	575	LEU	Mainchain
7	Qj	601	ARG	Mainchain
7	Qj	602	GLY	Peptide
7	Qj	616	LYS	Mainchain
7	Qj	633	ASP	Mainchain
7	Qj	635	GLN	Mainchain
7	Qj	76	SER	Mainchain
7	Qj	98	SER	Mainchain
7	Qk	135	GLY	Mainchain
7	Qk	250	THR	Mainchain
7	Qk	278	VAL	Mainchain
7	Qk	346	GLU	Mainchain
7	Qk	407	SER	Mainchain
7	Qk	487	LYS	Mainchain
7	Qk	508	VAL	Peptide
7	Qk	530	ASP	Mainchain
7	Qk	533	LEU	Mainchain
7	Qk	534	ARG	Mainchain
7	Qk	536	LYS	Mainchain
7	Qk	537	ALA	Mainchain
7	Qk	575	LEU	Mainchain
7	Qk	601	ARG	Mainchain
7	Qk	602	GLY	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
7	Qk	616	LYS	Mainchain
7	Qk	633	ASP	Mainchain
7	Qk	635	GLN	Mainchain
7	Qk	76	SER	Mainchain
7	Qk	98	SER	Mainchain
7	Ql	135	GLY	Mainchain
7	Ql	250	THR	Mainchain
7	Ql	278	VAL	Mainchain
7	Ql	346	GLU	Mainchain
7	Ql	407	SER	Mainchain
7	Ql	487	LYS	Mainchain
7	Ql	508	VAL	Peptide
7	Ql	530	ASP	Mainchain
7	Ql	533	LEU	Mainchain
7	Ql	534	ARG	Mainchain
7	Ql	536	LYS	Mainchain
7	Ql	537	ALA	Mainchain
7	Ql	540	LYS	Mainchain
7	Ql	575	LEU	Mainchain
7	Ql	601	ARG	Mainchain
7	Ql	602	GLY	Peptide
7	Ql	616	LYS	Mainchain
7	Ql	633	ASP	Mainchain
7	Ql	635	GLN	Mainchain
7	Ql	76	SER	Mainchain
7	Ql	98	SER	Mainchain
9	Ta	306	THR	Peptide
9	Ta	319	HIS	Mainchain
9	Ta	344	ASP	Peptide
9	Ta	345	PRO	Mainchain,Peptide
9	Ta	352	HIS	Mainchain
9	Tb	306	THR	Peptide
9	Tb	319	HIS	Mainchain
9	Tb	344	ASP	Peptide
9	Tb	345	PRO	Mainchain,Peptide
9	Tb	352	HIS	Mainchain
9	Tc	301	ASP	Mainchain
9	Tc	306	THR	Peptide
9	Tc	319	HIS	Mainchain
9	Tc	344	ASP	Peptide
9	Tc	345	PRO	Mainchain,Peptide
9	Tc	352	HIS	Mainchain

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Mol	Chain	Res	Type	Group
9	Td	306	THR	Peptide
9	Td	319	HIS	Mainchain
9	Td	344	ASP	Peptide
9	Td	345	PRO	Mainchain,Peptide
9	Td	352	HIS	Mainchain
9	Te	306	THR	Peptide
9	Te	319	HIS	Mainchain
9	Te	344	ASP	Peptide
9	Te	345	PRO	Mainchain,Peptide
9	Te	352	HIS	Mainchain
9	Tf	306	THR	Peptide
9	Tf	319	HIS	Mainchain
9	Tf	344	ASP	Peptide
9	Tf	345	PRO	Mainchain,Peptide
9	Tf	352	HIS	Mainchain
9	Tg	306	THR	Peptide
9	Tg	319	HIS	Mainchain
9	Tg	344	ASP	Peptide
9	Tg	345	PRO	Mainchain,Peptide
9	Tg	352	HIS	Mainchain
9	Th	306	THR	Peptide
9	Th	319	HIS	Mainchain
9	Th	344	ASP	Peptide
9	Th	345	PRO	Mainchain,Peptide
9	Th	352	HIS	Mainchain
9	Ti	127	PHE	Peptide
9	Ti	306	THR	Peptide
9	Ti	319	HIS	Mainchain
9	Ti	344	ASP	Peptide
9	Ti	345	PRO	Mainchain,Peptide
9	Ti	352	HIS	Mainchain
9	Tj	301	ASP	Mainchain
9	Tj	306	THR	Peptide
9	Tj	319	HIS	Mainchain
9	Tj	344	ASP	Peptide
9	Tj	345	PRO	Mainchain,Peptide
9	Tj	352	HIS	Mainchain
9	Tk	306	THR	Peptide
9	Tk	319	HIS	Mainchain
9	Tk	344	ASP	Peptide
9	Tk	345	PRO	Mainchain,Peptide
9	Tk	352	HIS	Mainchain

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Mol	Chain	Res	Type	Group
9	Tl	306	THR	Peptide
9	Tl	319	HIS	Mainchain
9	Tl	344	ASP	Peptide
9	Tl	345	PRO	Mainchain,Peptide
9	Tl	352	HIS	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:A1:26:ASP:N	1:A1:26:ASP:CA	1.76	1.46
1:A9:26:ASP:N	1:A9:26:ASP:CA	1.76	1.46
1:A7:26:ASP:N	1:A7:26:ASP:CA	1.76	1.45
1:A8:26:ASP:N	1:A8:26:ASP:CA	1.76	1.43
1:A3:115:GLY:O	1:A7:25:GLN:CA	1.83	1.27
1:A1:115:GLY:O	1:A5:25:GLN:CA	1.83	1.26
1:A2:115:GLY:O	1:A6:25:GLN:CA	1.83	1.26
1:A5:115:GLY:O	1:A9:25:GLN:CA	1.83	1.25
1:A4:115:GLY:O	1:A8:25:GLN:CA	1.83	1.25
1:A4:25:GLN:C	1:A4:26:ASP:CA	2.43	0.87
1:A6:25:GLN:C	1:A6:26:ASP:CA	2.43	0.87
1:A2:25:GLN:C	1:A2:26:ASP:CA	2.43	0.87
1:A3:25:GLN:C	1:A3:26:ASP:CA	2.43	0.87
1:A8:25:GLN:C	1:A8:26:ASP:CA	2.43	0.87
1:A7:25:GLN:C	1:A7:26:ASP:CA	2.43	0.86
1:A9:25:GLN:C	1:A9:26:ASP:CA	2.43	0.86
1:A1:25:GLN:C	1:A1:26:ASP:CA	2.43	0.86
1:A5:25:GLN:C	1:A5:26:ASP:CA	2.43	0.85
1:A9:25:GLN:O	1:A9:26:ASP:CA	2.49	0.61
1:A1:25:GLN:O	1:A1:26:ASP:CA	2.49	0.60
1:A3:25:GLN:O	1:A3:26:ASP:CA	2.49	0.60
1:A4:25:GLN:O	1:A4:26:ASP:CA	2.49	0.60
1:A6:25:GLN:O	1:A6:26:ASP:CA	2.49	0.60
1:A7:25:GLN:O	1:A7:26:ASP:CA	2.50	0.60
1:A2:25:GLN:O	1:A2:26:ASP:CA	2.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A8:25:GLN:O	1:A8:26:ASP:CA	2.49	0.59
1:A5:25:GLN:O	1:A5:26:ASP:CA	2.49	0.59
1:A8:66:VAL:O	1:A8:67:ALA:C	2.45	0.55
1:A5:66:VAL:O	1:A5:67:ALA:C	2.45	0.55
1:A4:66:VAL:O	1:A4:67:ALA:C	2.45	0.55
1:A7:66:VAL:O	1:A7:67:ALA:C	2.45	0.54
1:A2:66:VAL:O	1:A2:67:ALA:C	2.46	0.54
1:A6:66:VAL:O	1:A6:67:ALA:C	2.45	0.54
1:A3:66:VAL:O	1:A3:67:ALA:C	2.45	0.53
1:A1:66:VAL:O	1:A1:67:ALA:C	2.45	0.53
1:A9:66:VAL:O	1:A9:67:ALA:C	2.45	0.53
1:A3:41:GLU:C	1:A3:43:GLN:H	2.20	0.45
1:A1:41:GLU:C	1:A1:43:GLN:H	2.20	0.45
1:A6:41:GLU:C	1:A6:43:GLN:H	2.20	0.45
1:A2:41:GLU:C	1:A2:43:GLN:H	2.20	0.45
1:A4:26:ASP:N	1:A4:26:ASP:C	2.63	0.44
1:A4:41:GLU:C	1:A4:43:GLN:H	2.20	0.44
1:A5:41:GLU:C	1:A5:43:GLN:H	2.20	0.44
1:A9:41:GLU:C	1:A9:43:GLN:H	2.20	0.44
1:A2:77:TYR:O	1:A2:93:LEU:N	2.36	0.44
1:A7:41:GLU:C	1:A7:43:GLN:H	2.20	0.44
1:A1:26:ASP:N	1:A1:26:ASP:C	2.63	0.43
1:A4:77:TYR:O	1:A4:93:LEU:N	2.37	0.43
1:A6:66:VAL:O	1:A6:68:SER:N	2.51	0.43
1:A9:26:ASP:N	1:A9:26:ASP:C	2.63	0.43
1:A9:77:TYR:O	1:A9:93:LEU:N	2.36	0.43
1:A8:41:GLU:C	1:A8:43:GLN:H	2.20	0.43
1:A5:66:VAL:O	1:A5:68:SER:N	2.52	0.42
1:A3:66:VAL:O	1:A3:68:SER:N	2.52	0.42
1:A9:67:ALA:O	1:A9:69:SER:N	2.52	0.42
1:A7:66:VAL:O	1:A7:68:SER:N	2.53	0.42
1:A1:66:VAL:O	1:A1:68:SER:N	2.52	0.42
1:A5:67:ALA:O	1:A5:69:SER:N	2.53	0.42
1:A8:66:VAL:O	1:A8:68:SER:N	2.52	0.42
1:A9:66:VAL:O	1:A9:68:SER:N	2.52	0.42
1:A7:77:TYR:O	1:A7:93:LEU:N	2.37	0.42
1:A3:77:TYR:O	1:A3:93:LEU:N	2.36	0.42
1:A4:66:VAL:O	1:A4:68:SER:N	2.52	0.42
1:A3:26:ASP:N	1:A3:26:ASP:C	2.63	0.41
1:A7:67:ALA:O	1:A7:69:SER:N	2.53	0.41
1:A2:67:ALA:O	1:A2:69:SER:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A6:67:ALA:O	1:A6:69:SER:N	2.53	0.41
1:A8:67:ALA:O	1:A8:69:SER:N	2.53	0.41
1:A1:67:ALA:O	1:A1:69:SER:N	2.53	0.41
1:A2:66:VAL:O	1:A2:68:SER:N	2.53	0.41
1:A4:67:ALA:O	1:A4:69:SER:N	2.53	0.41
1:A1:77:TYR:O	1:A1:93:LEU:N	2.36	0.41
1:A7:26:ASP:N	1:A7:26:ASP:C	2.63	0.41
1:A3:67:ALA:O	1:A3:69:SER:N	2.53	0.40
1:A5:77:TYR:O	1:A5:93:LEU:N	2.37	0.40
1:A4:92:MET:O	1:A4:93:LEU:O	2.40	0.40
1:A7:92:MET:O	1:A7:93:LEU:O	2.40	0.40

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
1	Ac	98	ASN
1	Ad	93	LEU
1	Ad	98	ASN
1	Ae	93	LEU
1	Ae	98	ASN
1	Af	93	LEU
1	Af	98	ASN
1	Ag	93	LEU
1	Ag	98	ASN
1	Ah	93	LEU
1	Ah	98	ASN
1	Ai	93	LEU
1	Ai	98	ASN
1	Aj	93	LEU
1	Aj	98	ASN
1	Ak	93	LEU
1	Ak	98	ASN

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Mol	Chain	Res	Type
1	Al	93	LEU
1	Al	98	ASN
1	Am	93	LEU
1	Am	98	ASN
1	An	93	LEU
1	An	98	ASN
1	Ao	93	LEU
1	Ao	98	ASN
1	Ap	93	LEU
1	Ap	98	ASN
1	Aq	93	LEU
1	Aq	98	ASN
1	Ar	93	LEU
1	Ar	98	ASN
1	As	93	LEU
1	As	98	ASN
1	At	93	LEU
1	At	98	ASN
1	Au	93	LEU
1	Au	98	ASN
1	Av	93	LEU
1	Av	98	ASN
1	Aw	93	LEU
1	Aw	98	ASN
1	Ax	93	LEU
1	Ax	98	ASN
1	Ay	93	LEU
1	Ay	98	ASN
1	Az	93	LEU
1	Az	98	ASN
1	A1	93	LEU
1	A1	98	ASN
1	A2	93	LEU
1	A2	98	ASN
1	A3	93	LEU
1	A3	98	ASN
1	A4	93	LEU
1	A4	98	ASN
1	A5	93	LEU
1	A5	98	ASN
1	A6	93	LEU
1	A6	98	ASN

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Mol	Chain	Res	Type
1	A7	93	LEU
1	A7	98	ASN
1	A8	93	LEU
1	A8	98	ASN
1	A9	93	LEU
1	A9	98	ASN
2	Ba	77	VAL
2	Ba	95	PRO
2	Ba	202	PRO
2	Ba	223	PRO
2	Ba	379	PHE
2	Ba	494	ASN
2	Ba	501	ARG
2	Ba	529	GLN
2	Bb	77	VAL
2	Bb	95	PRO
2	Bb	178	PRO
2	Bb	202	PRO
2	Bb	223	PRO
2	Bb	379	PHE
2	Bb	494	ASN
2	Bb	501	ARG
2	Bb	529	GLN
2	Bc	77	VAL
2	Bc	95	PRO
2	Bc	178	PRO
2	Bc	202	PRO
2	Bc	223	PRO
2	Bc	379	PHE
2	Bc	494	ASN
2	Bc	501	ARG
2	Bc	529	GLN
2	Bd	77	VAL
2	Bd	95	PRO
2	Bd	178	PRO
2	Bd	202	PRO
2	Bd	223	PRO
2	Bd	379	PHE
2	Bd	494	ASN
2	Bd	501	ARG
2	Bd	529	GLN
2	Be	77	VAL

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Mol	Chain	Res	Type
2	Be	95	PRO
2	Be	178	PRO
2	Be	202	PRO
2	Be	223	PRO
2	Be	379	PHE
2	Be	494	ASN
2	Be	501	ARG
2	Be	529	GLN
2	Bf	77	VAL
2	Bf	95	PRO
2	Bf	178	PRO
2	Bf	202	PRO
2	Bf	223	PRO
2	Bf	351	PRO
2	Bf	379	PHE
2	Bf	494	ASN
2	Bf	501	ARG
2	Bf	529	GLN
3	Ca	219	LEU
3	Ca	257	GLN
3	Cb	257	GLN
4	Na	9	PRO
4	Na	38	TYR
4	Na	83	GLU
4	Na	101	ARG
4	Na	103	MET
4	Na	151	THR
4	Na	177	ALA
4	Na	179	ILE
4	Na	210	PRO
4	Na	211	ILE
6	Ma	278	ILE
4	Nb	9	PRO
4	Nb	38	TYR
4	Nb	83	GLU
4	Nb	101	ARG
4	Nb	103	MET
4	Nb	151	THR
4	Nb	177	ALA
4	Nb	179	ILE
4	Nb	210	PRO
4	Nb	211	ILE

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Mol	Chain	Res	Type
6	Mb	278	ILE
4	Nc	9	PRO
4	Nc	38	TYR
4	Nc	83	GLU
4	Nc	101	ARG
4	Nc	103	MET
4	Nc	151	THR
4	Nc	177	ALA
4	Nc	179	ILE
4	Nc	210	PRO
4	Nc	211	ILE
6	Mc	278	ILE
4	Nd	9	PRO
4	Nd	38	TYR
4	Nd	83	GLU
4	Nd	101	ARG
4	Nd	103	MET
4	Nd	151	THR
4	Nd	177	ALA
4	Nd	179	ILE
4	Nd	210	PRO
4	Nd	211	ILE
6	Md	278	ILE
4	Ne	9	PRO
4	Ne	38	TYR
4	Ne	83	GLU
4	Ne	101	ARG
4	Ne	103	MET
4	Ne	151	THR
4	Ne	177	ALA
4	Ne	179	ILE
4	Ne	210	PRO
4	Ne	211	ILE
6	Me	278	ILE
4	Nf	9	PRO
4	Nf	38	TYR
4	Nf	83	GLU
4	Nf	101	ARG
4	Nf	103	MET
4	Nf	151	THR
4	Nf	177	ALA
4	Nf	179	ILE

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Mol	Chain	Res	Type
4	Nf	210	PRO
4	Nf	211	ILE
6	Mf	278	ILE
4	Ng	9	PRO
4	Ng	38	TYR
4	Ng	83	GLU
4	Ng	101	ARG
4	Ng	103	MET
4	Ng	151	THR
4	Ng	177	ALA
4	Ng	179	ILE
4	Ng	210	PRO
4	Ng	211	ILE
6	Mg	278	ILE
4	Nh	9	PRO
4	Nh	38	TYR
4	Nh	83	GLU
4	Nh	101	ARG
4	Nh	103	MET
4	Nh	151	THR
4	Nh	177	ALA
4	Nh	179	ILE
4	Nh	210	PRO
4	Nh	211	ILE
6	Mh	278	ILE
4	Ni	9	PRO
4	Ni	38	TYR
4	Ni	83	GLU
4	Ni	101	ARG
4	Ni	103	MET
4	Ni	151	THR
4	Ni	177	ALA
4	Ni	179	ILE
4	Ni	210	PRO
4	Ni	211	ILE
6	Mi	278	ILE
4	Nj	9	PRO
4	Nj	38	TYR
4	Nj	83	GLU
4	Nj	101	ARG
4	Nj	103	MET
4	Nj	151	THR

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Mol	Chain	Res	Type
4	Nj	177	ALA
4	Nj	179	ILE
4	Nj	210	PRO
4	Nj	211	ILE
6	Mj	278	ILE
4	Nk	9	PRO
4	Nk	38	TYR
4	Nk	83	GLU
4	Nk	101	ARG
4	Nk	103	MET
4	Nk	151	THR
4	Nk	177	ALA
4	Nk	179	ILE
4	Nk	210	PRO
4	Nk	211	ILE
6	Mk	278	ILE
4	Nl	9	PRO
4	Nl	38	TYR
4	Nl	83	GLU
4	Nl	101	ARG
4	Nl	103	MET
4	Nl	151	THR
4	Nl	177	ALA
4	Nl	179	ILE
4	Nl	210	PRO
4	Nl	211	ILE
6	Ml	278	ILE
7	Qa	225	ILE
7	Qa	260	LEU
7	Qa	271	LYS
7	Qa	409	PRO
7	Qa	603	SER
8	Pa	10	ALA
8	Pa	11	PRO
8	Pa	14	PRO
8	Pa	24	VAL
8	Pa	25	PRO
8	Pa	26	VAL
8	Pa	28	ALA
8	Pa	29	ALA
8	Pa	32	GLU
8	Pa	39	PRO

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Mol	Chain	Res	Type
8	Pa	47	PRO
8	Pa	52	ASP
7	Qb	225	ILE
7	Qb	260	LEU
7	Qb	271	LYS
7	Qb	409	PRO
7	Qb	603	SER
8	Pb	10	ALA
8	Pb	11	PRO
8	Pb	17	LYS
8	Pb	24	VAL
8	Pb	25	PRO
8	Pb	26	VAL
8	Pb	28	ALA
8	Pb	29	ALA
8	Pb	32	GLU
8	Pb	39	PRO
8	Pb	47	PRO
8	Pb	48	VAL
8	Pb	52	ASP
7	Qc	225	ILE
7	Qc	260	LEU
7	Qc	271	LYS
7	Qc	409	PRO
7	Qc	603	SER
8	Pc	11	PRO
8	Pc	24	VAL
8	Pc	25	PRO
8	Pc	26	VAL
8	Pc	28	ALA
8	Pc	29	ALA
8	Pc	32	GLU
8	Pc	39	PRO
8	Pc	48	VAL
8	Pc	53	PRO
7	Qd	225	ILE
7	Qd	260	LEU
7	Qd	271	LYS
7	Qd	409	PRO
7	Qd	603	SER
8	Pd	11	PRO
8	Pd	24	VAL

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Mol	Chain	Res	Type
8	Pd	25	PRO
8	Pd	26	VAL
8	Pd	28	ALA
8	Pd	29	ALA
8	Pd	32	GLU
8	Pd	39	PRO
8	Pd	47	PRO
8	Pd	52	ASP
8	Pd	55	ARG
7	Qe	225	ILE
7	Qe	260	LEU
7	Qe	271	LYS
7	Qe	409	PRO
7	Qe	603	SER
8	Pe	11	PRO
8	Pe	24	VAL
8	Pe	26	VAL
8	Pe	28	ALA
8	Pe	29	ALA
8	Pe	32	GLU
8	Pe	39	PRO
8	Pe	47	PRO
8	Pe	52	ASP
7	Qf	225	ILE
7	Qf	260	LEU
7	Qf	271	LYS
7	Qf	409	PRO
7	Qf	603	SER
8	Pf	11	PRO
8	Pf	24	VAL
8	Pf	25	PRO
8	Pf	26	VAL
8	Pf	28	ALA
8	Pf	29	ALA
8	Pf	32	GLU
8	Pf	39	PRO
8	Pf	47	PRO
8	Pf	52	ASP
7	Qg	225	ILE
7	Qg	260	LEU
7	Qg	271	LYS
7	Qg	409	PRO

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Mol	Chain	Res	Type
7	Qg	513	SER
7	Qg	603	SER
8	Pg	11	PRO
8	Pg	24	VAL
8	Pg	25	PRO
8	Pg	26	VAL
8	Pg	28	ALA
8	Pg	29	ALA
8	Pg	39	PRO
8	Pg	47	PRO
7	Qh	225	ILE
7	Qh	260	LEU
7	Qh	271	LYS
7	Qh	409	PRO
7	Qh	603	SER
8	Ph	9	PRO
8	Ph	10	ALA
8	Ph	11	PRO
8	Ph	24	VAL
8	Ph	25	PRO
8	Ph	26	VAL
8	Ph	28	ALA
8	Ph	29	ALA
8	Ph	32	GLU
8	Ph	39	PRO
8	Ph	47	PRO
8	Ph	52	ASP
7	Qi	225	ILE
7	Qi	260	LEU
7	Qi	271	LYS
7	Qi	409	PRO
7	Qi	603	SER
8	Pi	11	PRO
8	Pi	24	VAL
8	Pi	25	PRO
8	Pi	26	VAL
8	Pi	28	ALA
8	Pi	29	ALA
8	Pi	32	GLU
8	Pi	39	PRO
8	Pi	47	PRO
8	Pi	52	ASP

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Mol	Chain	Res	Type
7	Qj	225	ILE
7	Qj	260	LEU
7	Qj	271	LYS
7	Qj	409	PRO
7	Qj	603	SER
8	Pj	11	PRO
8	Pj	24	VAL
8	Pj	25	PRO
8	Pj	26	VAL
8	Pj	28	ALA
8	Pj	29	ALA
8	Pj	39	PRO
8	Pj	47	PRO
8	Pj	52	ASP
7	Qk	225	ILE
7	Qk	260	LEU
7	Qk	271	LYS
7	Qk	409	PRO
7	Qk	603	SER
8	Pk	11	PRO
8	Pk	16	ALA
8	Pk	24	VAL
8	Pk	26	VAL
8	Pk	28	ALA
8	Pk	29	ALA
8	Pk	39	PRO
8	Pk	47	PRO
8	Pk	52	ASP
7	Ql	225	ILE
7	Ql	260	LEU
7	Ql	271	LYS
7	Ql	409	PRO
7	Ql	603	SER
8	Pl	11	PRO
8	Pl	24	VAL
8	Pl	26	VAL
8	Pl	29	ALA
8	Pl	39	PRO
8	Pl	47	PRO
8	Pl	52	ASP
9	Ta	76	ALA
9	Ta	77	PRO

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Mol	Chain	Res	Type
9	Ta	313	THR
9	Tb	76	ALA
9	Tb	77	PRO
9	Tb	313	THR
9	Tc	76	ALA
9	Tc	77	PRO
9	Tc	313	THR
9	Td	76	ALA
9	Td	77	PRO
9	Td	313	THR
9	Te	76	ALA
9	Te	77	PRO
9	Te	313	THR
9	Tf	76	ALA
9	Tf	77	PRO
9	Tf	313	THR
9	Tg	76	ALA
9	Tg	77	PRO
9	Tg	313	THR
9	Th	76	ALA
9	Th	77	PRO
9	Th	313	THR
9	Ti	76	ALA
9	Ti	77	PRO
9	Ti	313	THR
9	Tj	76	ALA
9	Tj	77	PRO
9	Tj	313	THR
9	Tk	76	ALA
9	Tk	77	PRO
9	Tk	313	THR
9	Tl	76	ALA
9	Tl	77	PRO
9	Tl	313	THR
1	Aa	99	ASN
1	Ab	99	ASN
1	Ac	99	ASN
1	Ad	99	ASN
1	Ae	99	ASN
1	Af	99	ASN
1	Ag	99	ASN
1	Ah	99	ASN

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Mol	Chain	Res	Type
1	Ai	99	ASN
1	Aj	99	ASN
1	Ak	99	ASN
1	Al	99	ASN
1	Am	99	ASN
1	An	99	ASN
1	An	136	ALA
1	Ao	99	ASN
1	Ap	99	ASN
1	Aq	99	ASN
1	Ar	99	ASN
1	As	99	ASN
1	At	99	ASN
1	Au	99	ASN
1	Av	99	ASN
1	Aw	99	ASN
1	Ax	99	ASN
1	Ay	99	ASN
1	Az	99	ASN
1	A1	99	ASN
1	A2	99	ASN
1	A3	99	ASN
1	A4	99	ASN
1	A5	99	ASN
1	A6	99	ASN
1	A7	99	ASN
1	A8	99	ASN
1	A9	99	ASN
2	Ba	150	VAL
2	Ba	178	PRO
2	Ba	240	SER
2	Ba	309	ALA
2	Ba	351	PRO
2	Ba	360	ASN
2	Ba	502	VAL
2	Bb	150	VAL
2	Bb	240	SER
2	Bb	258	MET
2	Bb	259	GLY
2	Bb	309	ALA
2	Bb	351	PRO
2	Bb	360	ASN

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Mol	Chain	Res	Type
2	Bb	502	VAL
2	Bb	532	ILE
2	Bc	150	VAL
2	Bc	240	SER
2	Bc	309	ALA
2	Bc	351	PRO
2	Bc	360	ASN
2	Bc	502	VAL
2	Bd	150	VAL
2	Bd	240	SER
2	Bd	258	MET
2	Bd	259	GLY
2	Bd	309	ALA
2	Bd	351	PRO
2	Bd	360	ASN
2	Bd	502	VAL
2	Bd	527	LEU
2	Bd	532	ILE
2	Be	150	VAL
2	Be	240	SER
2	Be	309	ALA
2	Be	351	PRO
2	Be	360	ASN
2	Be	502	VAL
2	Be	527	LEU
2	Bf	150	VAL
2	Bf	240	SER
2	Bf	258	MET
2	Bf	259	GLY
2	Bf	287	SER
2	Bf	309	ALA
2	Bf	360	ASN
2	Bf	502	VAL
2	Bf	527	LEU
2	Bf	532	ILE
3	Ca	237	PHE
3	Cb	219	LEU
3	Cb	237	PHE
4	Na	39	LEU
4	Na	102	MET
5	Oa	82	SER
4	Nb	102	MET

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Mol	Chain	Res	Type
5	Ob	82	SER
4	Nc	102	MET
5	Oc	82	SER
4	Nd	102	MET
5	Od	82	SER
4	Ne	39	LEU
4	Ne	102	MET
5	Oe	82	SER
4	Nf	102	MET
5	Of	82	SER
6	Mf	320	ALA
4	Ng	102	MET
5	Og	82	SER
6	Mg	320	ALA
4	Nh	39	LEU
4	Nh	102	MET
5	Oh	82	SER
4	Ni	102	MET
5	Oi	82	SER
6	Mi	320	ALA
4	Nj	39	LEU
4	Nj	102	MET
5	Oj	82	SER
6	Mj	320	ALA
4	Nk	39	LEU
4	Nk	102	MET
5	Ok	82	SER
4	Nl	39	LEU
4	Nl	102	MET
5	Ol	82	SER
6	Ml	320	ALA
7	Qa	91	PRO
7	Qa	135	GLY
7	Qa	261	ARG
7	Qa	435	THR
7	Qa	509	ALA
7	Qa	513	SER
8	Pa	9	PRO
8	Pa	13	PRO
8	Pa	63	PRO
8	Pa	71	ALA
7	Qb	91	PRO

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Mol	Chain	Res	Type
7	Qb	135	GLY
7	Qb	261	ARG
7	Qb	435	THR
7	Qb	509	ALA
7	Qb	513	SER
8	Pb	13	PRO
8	Pb	63	PRO
8	Pb	71	ALA
7	Qc	91	PRO
7	Qc	135	GLY
7	Qc	261	ARG
7	Qc	435	THR
7	Qc	509	ALA
7	Qc	513	SER
8	Pc	51	ARG
8	Pc	63	PRO
8	Pc	71	ALA
7	Qd	91	PRO
7	Qd	135	GLY
7	Qd	261	ARG
7	Qd	435	THR
7	Qd	509	ALA
7	Qd	513	SER
8	Pd	48	VAL
8	Pd	63	PRO
8	Pd	71	ALA
7	Qe	91	PRO
7	Qe	135	GLY
7	Qe	261	ARG
7	Qe	435	THR
7	Qe	509	ALA
7	Qe	513	SER
8	Pe	25	PRO
8	Pe	63	PRO
8	Pe	71	ALA
7	Qf	91	PRO
7	Qf	135	GLY
7	Qf	261	ARG
7	Qf	435	THR
7	Qf	509	ALA
7	Qf	513	SER
8	Pf	63	PRO

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Mol	Chain	Res	Type
8	Pf	71	ALA
7	Qg	91	PRO
7	Qg	135	GLY
7	Qg	261	ARG
7	Qg	435	THR
7	Qg	509	ALA
8	Pg	52	ASP
8	Pg	63	PRO
8	Pg	71	ALA
7	Qh	91	PRO
7	Qh	135	GLY
7	Qh	261	ARG
7	Qh	435	THR
7	Qh	509	ALA
7	Qh	513	SER
8	Ph	63	PRO
8	Ph	71	ALA
7	Qi	91	PRO
7	Qi	135	GLY
7	Qi	261	ARG
7	Qi	435	THR
7	Qi	509	ALA
7	Qi	513	SER
8	Pi	63	PRO
8	Pi	71	ALA
7	Qj	91	PRO
7	Qj	135	GLY
7	Qj	261	ARG
7	Qj	435	THR
7	Qj	509	ALA
7	Qj	513	SER
8	Pj	63	PRO
8	Pj	71	ALA
7	Qk	91	PRO
7	Qk	135	GLY
7	Qk	261	ARG
7	Qk	435	THR
7	Qk	509	ALA
7	Qk	513	SER
8	Pk	25	PRO
8	Pk	63	PRO
8	Pk	71	ALA

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Mol	Chain	Res	Type
7	Ql	91	PRO
7	Ql	135	GLY
7	Ql	261	ARG
7	Ql	435	THR
7	Ql	509	ALA
7	Ql	513	SER
8	Pl	13	PRO
8	Pl	63	PRO
8	Pl	71	ALA
9	Ta	71	ARG
9	Ta	116	PRO
9	Ta	118	TRP
9	Ta	358	SER
9	Tb	71	ARG
9	Tb	116	PRO
9	Tb	118	TRP
9	Tb	358	SER
9	Tc	71	ARG
9	Tc	116	PRO
9	Tc	118	TRP
9	Tc	358	SER
9	Td	71	ARG
9	Td	116	PRO
9	Td	118	TRP
9	Td	358	SER
9	Te	71	ARG
9	Te	116	PRO
9	Te	118	TRP
9	Te	358	SER
9	Tf	71	ARG
9	Tf	116	PRO
9	Tf	118	TRP
9	Tf	358	SER
9	Tg	71	ARG
9	Tg	116	PRO
9	Tg	118	TRP
9	Tg	358	SER
9	Th	71	ARG
9	Th	116	PRO
9	Th	118	TRP
9	Th	358	SER
9	Ti	71	ARG

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Mol	Chain	Res	Type
9	Ti	116	PRO
9	Ti	118	TRP
9	Ti	358	SER
9	Tj	71	ARG
9	Tj	116	PRO
9	Tj	118	TRP
9	Tj	358	SER
9	Tk	71	ARG
9	Tk	116	PRO
9	Tk	118	TRP
9	Tk	358	SER
9	Tl	71	ARG
9	Tl	116	PRO
9	Tl	118	TRP
9	Tl	358	SER
1	Aa	67	ALA
1	Aa	68	SER
1	Aa	114	ASN
1	Aa	124	PRO
1	Ab	67	ALA
1	Ab	68	SER
1	Ab	114	ASN
1	Ab	124	PRO
1	Ac	67	ALA
1	Ac	68	SER
1	Ac	114	ASN
1	Ac	124	PRO
1	Ad	67	ALA
1	Ad	68	SER
1	Ad	114	ASN
1	Ad	124	PRO
1	Ae	67	ALA
1	Ae	68	SER
1	Ae	114	ASN
1	Ae	124	PRO
1	Af	67	ALA
1	Af	68	SER
1	Af	114	ASN
1	Af	124	PRO
1	Ag	67	ALA
1	Ag	68	SER
1	Ag	114	ASN

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Mol	Chain	Res	Type
1	Ag	124	PRO
1	Ah	67	ALA
1	Ah	68	SER
1	Ah	114	ASN
1	Ah	124	PRO
1	Ai	67	ALA
1	Ai	68	SER
1	Ai	114	ASN
1	Ai	124	PRO
1	Aj	67	ALA
1	Aj	68	SER
1	Aj	114	ASN
1	Aj	124	PRO
1	Ak	67	ALA
1	Ak	68	SER
1	Ak	114	ASN
1	Ak	124	PRO
1	Al	67	ALA
1	Al	68	SER
1	Al	114	ASN
1	Al	124	PRO
1	Am	67	ALA
1	Am	68	SER
1	Am	114	ASN
1	Am	124	PRO
1	An	67	ALA
1	An	68	SER
1	An	114	ASN
1	An	124	PRO
1	Ao	67	ALA
1	Ao	68	SER
1	Ao	114	ASN
1	Ao	124	PRO
1	Ap	67	ALA
1	Ap	68	SER
1	Ap	114	ASN
1	Ap	124	PRO
1	Aq	67	ALA
1	Aq	68	SER
1	Aq	114	ASN
1	Aq	124	PRO
1	Ar	67	ALA

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Mol	Chain	Res	Type
1	Ar	68	SER
1	Ar	124	PRO
1	As	67	ALA
1	As	68	SER
1	As	114	ASN
1	As	124	PRO
1	At	67	ALA
1	At	68	SER
1	At	114	ASN
1	At	124	PRO
1	Au	67	ALA
1	Au	68	SER
1	Au	114	ASN
1	Au	124	PRO
1	Av	67	ALA
1	Av	68	SER
1	Av	124	PRO
1	Aw	67	ALA
1	Aw	68	SER
1	Aw	114	ASN
1	Aw	124	PRO
1	Ax	67	ALA
1	Ax	68	SER
1	Ax	114	ASN
1	Ax	124	PRO
1	Ay	67	ALA
1	Ay	68	SER
1	Ay	114	ASN
1	Ay	124	PRO
1	Az	67	ALA
1	Az	68	SER
1	Az	114	ASN
1	Az	124	PRO
1	A1	67	ALA
1	A1	68	SER
1	A1	114	ASN
1	A1	124	PRO
1	A2	67	ALA
1	A2	68	SER
1	A2	114	ASN
1	A2	124	PRO
1	A3	67	ALA

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Mol	Chain	Res	Type
1	A3	68	SER
1	A3	114	ASN
1	A3	124	PRO
1	A4	67	ALA
1	A4	68	SER
1	A4	124	PRO
1	A5	67	ALA
1	A5	68	SER
1	A5	114	ASN
1	A5	124	PRO
1	A6	67	ALA
1	A6	68	SER
1	A6	114	ASN
1	A6	124	PRO
1	A7	67	ALA
1	A7	68	SER
1	A7	114	ASN
1	A7	124	PRO
1	A8	67	ALA
1	A8	68	SER
1	A8	124	PRO
1	A9	67	ALA
1	A9	68	SER
1	A9	114	ASN
1	A9	124	PRO
2	Ba	498	TYR
2	Ba	527	LEU
2	Bb	287	SER
2	Bb	498	TYR
2	Bb	527	LEU
2	Bc	498	TYR
2	Bc	527	LEU
2	Bd	287	SER
2	Bd	498	TYR
2	Be	498	TYR
2	Bf	498	TYR
3	Ca	222	PRO
3	Cb	222	PRO
6	Ma	129	PRO
6	Ma	267	ASN
6	Ma	320	ALA
4	Nb	39	LEU

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Mol	Chain	Res	Type
6	Mb	129	PRO
6	Mb	320	ALA
4	Nc	39	LEU
6	Mc	129	PRO
6	Mc	267	ASN
6	Mc	320	ALA
4	Nd	39	LEU
6	Md	88	LEU
6	Md	129	PRO
6	Md	267	ASN
6	Md	320	ALA
6	Me	129	PRO
6	Me	320	ALA
4	Nf	39	LEU
6	Mf	129	PRO
6	Mf	267	ASN
4	Ng	39	LEU
6	Mg	129	PRO
6	Mg	267	ASN
6	Mh	129	PRO
6	Mh	267	ASN
6	Mh	320	ALA
4	Ni	39	LEU
6	Mi	129	PRO
6	Mi	267	ASN
6	Mj	129	PRO
6	Mj	267	ASN
6	Mk	129	PRO
6	Mk	267	ASN
6	Mk	320	ALA
6	Ml	129	PRO
6	Ml	267	ASN
8	Pa	75	PRO
8	Pb	14	PRO
8	Pb	16	ALA
8	Pb	50	LYS
8	Pb	75	PRO
8	Pc	75	PRO
8	Pd	45	TYR
8	Pd	75	PRO
8	Pe	75	PRO
8	Pf	75	PRO

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Mol	Chain	Res	Type
8	Pg	75	PRO
8	Ph	75	PRO
8	Pi	75	PRO
8	Pj	75	PRO
8	Pk	75	PRO
8	Pl	14	PRO
8	Pl	16	ALA
8	Pl	75	PRO
9	Td	389	SER
9	Th	389	SER
9	Tk	389	SER
1	Aa	80	GLU
1	Ab	80	GLU
1	Ac	80	GLU
1	Ad	80	GLU
1	Ae	80	GLU
1	Af	80	GLU
1	Ag	80	GLU
1	Ah	80	GLU
1	Aj	80	GLU
1	Ak	80	GLU
1	Al	80	GLU
1	An	80	GLU
1	Ao	80	GLU
1	Ap	80	GLU
1	Aq	80	GLU
1	Ar	80	GLU
1	Ar	114	ASN
1	As	80	GLU
1	Au	80	GLU
1	Av	114	ASN
1	Aw	80	GLU
1	Ax	80	GLU
1	A1	80	GLU
1	A2	80	GLU
1	A4	80	GLU
1	A4	114	ASN
1	A5	80	GLU
1	A6	80	GLU
1	A7	80	GLU
1	A8	80	GLU
1	A8	114	ASN

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Mol	Chain	Res	Type
1	A9	80	GLU
2	Ba	275	PHE
2	Ba	382	GLN
2	Bb	275	PHE
2	Bb	382	GLN
2	Bc	275	PHE
2	Bd	275	PHE
2	Bd	382	GLN
2	Be	275	PHE
2	Bf	275	PHE
2	Bf	382	GLN
5	Oa	72	ARG
5	Ob	72	ARG
5	Ob	170	LEU
6	Mb	79	PRO
6	Mb	267	ASN
5	Oc	72	ARG
5	Od	72	ARG
5	Od	170	LEU
6	Md	79	PRO
5	Oe	72	ARG
5	Oe	170	LEU
6	Me	267	ASN
5	Of	72	ARG
5	Of	170	LEU
5	Og	72	ARG
5	Oh	72	ARG
5	Oi	72	ARG
5	Oi	170	LEU
5	Oj	72	ARG
5	Oj	170	LEU
6	Mj	79	PRO
5	Ok	72	ARG
4	Nl	75	ILE
5	Ol	72	ARG
5	Ol	170	LEU
7	Qa	407	SER
8	Pa	15	PRO
8	Pa	38	ALA
8	Pa	121	GLY
7	Qb	407	SER
7	Qc	407	SER

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Mol	Chain	Res	Type
8	Pc	38	ALA
8	Pc	50	LYS
7	Qd	407	SER
8	Pd	38	ALA
8	Pd	50	LYS
7	Qe	407	SER
8	Pe	16	ALA
8	Pe	38	ALA
7	Qf	407	SER
8	Pf	38	ALA
7	Qg	407	SER
7	Qh	407	SER
8	Ph	53	PRO
7	Qi	407	SER
7	Qj	407	SER
8	Pj	38	ALA
7	Qk	407	SER
8	Pk	38	ALA
7	Ql	407	SER
8	Pl	10	ALA
8	Pl	38	ALA
9	Ta	73	ARG
9	Ta	389	SER
9	Tb	73	ARG
9	Tb	389	SER
9	Tc	73	ARG
9	Tc	389	SER
9	Td	73	ARG
9	Te	73	ARG
9	Te	389	SER
9	Tf	73	ARG
9	Tf	389	SER
9	Tg	73	ARG
9	Tg	389	SER
9	Th	73	ARG
9	Ti	73	ARG
9	Tj	73	ARG
9	Tj	389	SER
9	Tk	73	ARG
9	Tl	73	ARG
9	Tl	389	SER
1	Aa	138	ASP

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Mol	Chain	Res	Type
1	Ab	138	ASP
1	Ac	138	ASP
1	Ad	138	ASP
1	Ae	138	ASP
1	Af	138	ASP
1	Ag	138	ASP
1	Ah	138	ASP
1	Ai	80	GLU
1	Ai	138	ASP
1	Aj	138	ASP
1	Ak	138	ASP
1	Al	138	ASP
1	Am	80	GLU
1	Am	138	ASP
1	An	135	ASP
1	Ao	138	ASP
1	Ap	138	ASP
1	Aq	138	ASP
1	Ar	138	ASP
1	As	138	ASP
1	At	80	GLU
1	At	138	ASP
1	Au	138	ASP
1	Av	80	GLU
1	Av	138	ASP
1	Aw	138	ASP
1	Ax	138	ASP
1	Ay	80	GLU
1	Ay	138	ASP
1	Az	80	GLU
1	Az	138	ASP
1	A1	138	ASP
1	A2	138	ASP
1	A3	80	GLU
1	A3	138	ASP
1	A4	138	ASP
1	A5	138	ASP
1	A6	138	ASP
1	A7	138	ASP
1	A8	138	ASP
1	A9	138	ASP
2	Ba	249	PRO

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Mol	Chain	Res	Type
2	Ba	258	MET
2	Bb	249	PRO
2	Bc	249	PRO
2	Bc	258	MET
2	Bc	382	GLN
2	Bd	249	PRO
2	Bd	453	LEU
2	Be	249	PRO
2	Be	258	MET
2	Be	382	GLN
2	Be	454	CYS
2	Bf	249	PRO
2	Bf	453	LEU
3	Ca	215	PHE
4	Na	8	LEU
4	Na	75	ILE
5	Oa	170	LEU
6	Ma	242	ASN
4	Nb	8	LEU
4	Nb	75	ILE
6	Mb	242	ASN
4	Nc	8	LEU
4	Nc	75	ILE
5	Oc	170	LEU
6	Mc	242	ASN
4	Nd	8	LEU
4	Nd	75	ILE
6	Md	242	ASN
4	Ne	8	LEU
4	Ne	75	ILE
6	Me	242	ASN
4	Nf	8	LEU
4	Nf	75	ILE
6	Mf	79	PRO
6	Mf	242	ASN
4	Ng	8	LEU
4	Ng	75	ILE
5	Og	170	LEU
6	Mg	242	ASN
4	Nh	8	LEU
4	Nh	75	ILE
5	Oh	170	LEU

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Mol	Chain	Res	Type
6	Mh	79	PRO
6	Mh	242	ASN
4	Ni	8	LEU
4	Ni	75	ILE
6	Mi	242	ASN
4	Nj	8	LEU
4	Nj	75	ILE
6	Mj	242	ASN
4	Nk	8	LEU
4	Nk	75	ILE
5	Ok	170	LEU
4	Nl	8	LEU
6	Ml	242	ASN
8	Pb	53	PRO
8	Pb	121	GLY
8	Pc	10	ALA
8	Pc	121	GLY
8	Pd	10	ALA
8	Pd	121	GLY
8	Pe	10	ALA
8	Pe	121	GLY
8	Pf	10	ALA
8	Pf	121	GLY
8	Pg	10	ALA
8	Pg	121	GLY
8	Ph	121	GLY
8	Pi	10	ALA
8	Pi	121	GLY
8	Pj	10	ALA
8	Pj	121	GLY
8	Pk	10	ALA
8	Pk	121	GLY
8	Pl	28	ALA
8	Pl	121	GLY
9	Ti	389	SER
9	Tj	92	LEU
9	Tk	92	LEU
2	Ba	454	CYS
2	Bb	453	LEU
2	Bb	454	CYS
2	Bc	454	CYS
2	Bd	454	CYS

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Mol	Chain	Res	Type
2	Bf	94	GLY
2	Bf	454	CYS
3	Ca	192	VAL
3	Cb	192	VAL
6	Md	49	SER
6	Mk	242	ASN
8	Pa	154	PRO
8	Pb	154	PRO
8	Pc	154	PRO
8	Pe	154	PRO
8	Pf	154	PRO
8	Pg	154	PRO
8	Pi	17	LYS
8	Pi	154	PRO
8	Pj	154	PRO
8	Pk	154	PRO
8	Pl	154	PRO
9	Ta	92	LEU
9	Ta	95	ARG
9	Tb	92	LEU
9	Tb	95	ARG
9	Tc	92	LEU
9	Tc	95	ARG
9	Td	92	LEU
9	Tg	95	ARG
9	Th	92	LEU
9	Ti	92	LEU
9	Ti	95	ARG
9	Tk	95	ARG
9	Tl	92	LEU
9	Tl	95	ARG
9	Tl	310	PRO
2	Ba	94	GLY
2	Bb	94	GLY
2	Bc	94	GLY
2	Bd	94	GLY
2	Be	94	GLY
3	Cb	387	GLU
6	Mg	128	MET
8	Pb	12	ALA
8	Pd	154	PRO
8	Ph	154	PRO

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Mol	Chain	Res	Type
8	Pl	15	PRO
9	Ta	310	PRO
9	Tb	310	PRO
9	Tc	310	PRO
9	Td	310	PRO
9	Te	310	PRO
9	Tf	310	PRO
9	Th	310	PRO
9	Ti	310	PRO
9	Tj	310	PRO
2	Bb	310	ILE
2	Bc	310	ILE
2	Be	310	ILE
2	Bf	310	ILE
3	Ca	387	GLU
6	Ma	128	MET
6	Mb	128	MET
6	Me	128	MET
6	Mh	128	MET
6	Mi	128	MET
6	Mj	128	MET
8	Pc	64	VAL
8	Pd	64	VAL
8	Pf	64	VAL
8	Pg	64	VAL
8	Ph	64	VAL
8	Pi	64	VAL
8	Pj	64	VAL
8	Pk	64	VAL
8	Pl	17	LYS
8	Pl	64	VAL
9	Tg	310	PRO
9	Tk	310	PRO
2	Ba	272	PRO
2	Ba	310	ILE
2	Bd	310	ILE
2	Be	272	PRO
6	Mc	128	MET
6	Md	128	MET
6	Mf	128	MET
6	Mk	128	MET
6	Ml	128	MET

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Mol	Chain	Res	Type
7	Qa	363	GLY
8	Pa	64	VAL
7	Qb	363	GLY
8	Pb	64	VAL
7	Qc	363	GLY
8	Pc	47	PRO
7	Qd	363	GLY
7	Qe	363	GLY
8	Pe	64	VAL
7	Qf	363	GLY
7	Qg	363	GLY
7	Qh	363	GLY
8	Ph	13	PRO
7	Qi	363	GLY
7	Qj	363	GLY
7	Qk	363	GLY
7	Ql	363	GLY
9	Ta	354	VAL
9	Tb	354	VAL
9	Tc	354	VAL
9	Td	354	VAL
9	Te	354	VAL
9	Tf	354	VAL
9	Tg	354	VAL
9	Th	354	VAL
9	Ti	354	VAL
9	Tj	354	VAL
9	Tk	354	VAL
9	Tl	354	VAL
2	Bc	272	PRO
4	Ne	99	PRO
8	Ph	12	ALA
8	Ph	15	PRO
8	Pl	25	PRO
4	Nb	99	PRO
4	Nf	99	PRO
4	Ni	99	PRO
6	Mj	220	PRO

5.3.2 Protein sidechains ⓘ

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	-	-
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	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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

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Mol	Chain	Number of breaks
8	Pa	1
8	Pe	1
8	Pf	1
8	Pg	1
8	Ph	1
8	Pj	1
8	Pl	1

All 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
1	Pa	63:PRO	C	64:VAL	N	1.65
1	Pe	63:PRO	C	64:VAL	N	1.65
1	Pf	63:PRO	C	64:VAL	N	1.65
1	Pg	63:PRO	C	64:VAL	N	1.65
1	Ph	63:PRO	C	64:VAL	N	1.65
1	Pj	63:PRO	C	64:VAL	N	1.65
1	Pl	63:PRO	C	64:VAL	N	1.65

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.