wwPDB EM Validation Summary Report

Nov 13, 2024 – 10:21 AM EST

PDB ID	:	3JC9
EMDB ID	:	EMD-3260
Title	:	Architectural model of the type IVa pilus machine in a non-piliated state
Authors	:	Chang, Y.-W.; Rettberg, L.A.; Jensen, G.J.
Deposited on	:	2015-11-24
Resolution	:	Not provided

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

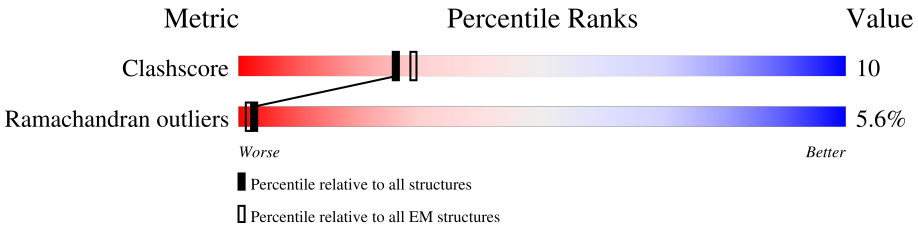
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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	210492	15764
Ramachandran outliers	207382	16835

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	Aa	158	93% 7%
1	Ab	158	93% 7%
1	Ac	158	93% 7%
1	Ad	158	93% 7%
1	Ae	158	93% 7%
2	Ca	417	71% 5% • 24%
2	Cb	417	71% 5% 24%
3	Na	225	91% 7% • •
3	Nb	225	91% 7% • •
3	Nc	225	91% 7% • •

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Mol	Chain	Length	Quality of chain
3	Nd	225	91% 7%
3	Ne	225	91% 7%
3	Nf	225	91% 7%
3	Ng	225	91% 7%
3	Nh	225	91% 7%
3	Ni	225	91% 7%
3	Nj	225	91% 7%
3	Nk	225	91% 7%
3	Nl	225	91% 7%
4	Oa	205	87% 8%
4	Ob	205	86% 5% 8%
4	Oc	205	86% 5% 8%
4	Od	205	87% 8%
4	Oe	205	86% 5% 8%
4	Of	205	86% 5% 8%
4	Og	205	86% 5% 8%
4	Oh	205	87% 8%
4	Oi	205	86% 5% 8%
4	Oj	205	86% 5% 8%
4	Ok	205	86% 5% 8%
4	Ol	205	86% 6% 8%
5	Ma	395	86% 10%
5	Mb	395	86% 10%
5	Mc	395	86% 10%
5	Md	395	86% 10%

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Mol	Chain	Length	Quality of chain
5	Me	395	86% • 10%
5	Mf	395	86% • 10%
5	Mg	395	86% • 10%
5	Mh	395	86% • 10%
5	Mi	395	86% • 10%
5	Mj	395	86% • 10%
5	Mk	395	86% • 10%
5	Ml	395	86% • 10%
6	Qa	901	43% • 54%
6	Qb	901	43% • 54%
6	Qc	901	43% • 54%
6	Qd	901	43% • 54%
6	Qe	901	42% • 54%
6	Qf	901	42% • 54%
6	Qg	901	42% • 54%
6	Qh	901	42% • 54%
6	Qi	901	42% • 54%
6	Qj	901	43% • 54%
6	Qk	901	42% • 54%
6	Ql	901	42% • 54%
7	Pa	172	72% 13% 5% 10%
7	Pb	172	73% 13% • 10%
7	Pc	172	73% 13% • 10%
7	Pd	172	73% 12% 5% 10%
7	Pe	172	73% 13% • 10%

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Mol	Chain	Length	Quality of chain
7	Pf	172	73% 13% • 10%
7	Pg	172	73% 12% 6% 10%
7	Ph	172	73% 12% 5% 10%
7	Pi	172	73% 12% 5% 10%
7	Pj	172	73% 12% 6% 10%
7	Pk	172	72% 13% 5% 10%
7	Pl	172	73% 14% • 10%
8	Ta	411	36% • 60%
8	Tb	411	36% • 60%
8	Tc	411	36% • 60%
8	Td	411	36% • 60%
8	Te	411	36% • 60%
8	Tf	411	36% • 60%
8	Tg	411	36% • 60%
8	Th	411	36% • 60%
8	Ti	411	36% • 60%
8	Tj	411	36% • 60%
8	Tk	411	36% • 60%
8	Tl	411	36% • 60%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 78216 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PilA.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	Aa	158	Total 632	C 316	N 158	O 158	0	0
1	Ab	158	Total 632	C 316	N 158	O 158	0	0
1	Ac	158	Total 632	C 316	N 158	O 158	0	0
1	Ad	158	Total 632	C 316	N 158	O 158	0	0
1	Ae	158	Total 632	C 316	N 158	O 158	0	0

- Molecule 2 is a protein called PilC.

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

- Molecule 3 is a protein called PilN.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	Na	223	Total 892	C 446	N 223	O 223	0	0
3	Nb	223	Total 892	C 446	N 223	O 223	0	0
3	Nc	223	Total 892	C 446	N 223	O 223	0	0
3	Nd	223	Total 892	C 446	N 223	O 223	0	0
3	Ne	223	Total 892	C 446	N 223	O 223	0	0
3	Nf	223	Total 892	C 446	N 223	O 223	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	Ng	223	Total 892	C 446	N 223	O 223	0	0
3	Nh	223	Total 892	C 446	N 223	O 223	0	0
3	Ni	223	Total 892	C 446	N 223	O 223	0	0
3	Nj	223	Total 892	C 446	N 223	O 223	0	0
3	Nk	223	Total 892	C 446	N 223	O 223	0	0
3	Nl	223	Total 892	C 446	N 223	O 223	0	0

- Molecule 4 is a protein called PilO.

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

- Molecule 5 is a protein called PilM.

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

- Molecule 6 is a protein called PilQ.

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

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

- Molecule 7 is a protein called PilP.

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

- Molecule 8 is a protein called TsaP.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	Ta	163	Total 652	C 326	N 163	O 163	0	0

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

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	Ma	1	Total 1	Mg 1	0
9	Mb	1	Total 1	Mg 1	0
9	Mc	1	Total 1	Mg 1	0
9	Md	1	Total 1	Mg 1	0
9	Me	1	Total 1	Mg 1	0
9	Mf	1	Total 1	Mg 1	0
9	Mg	1	Total 1	Mg 1	0
9	Mh	1	Total 1	Mg 1	0

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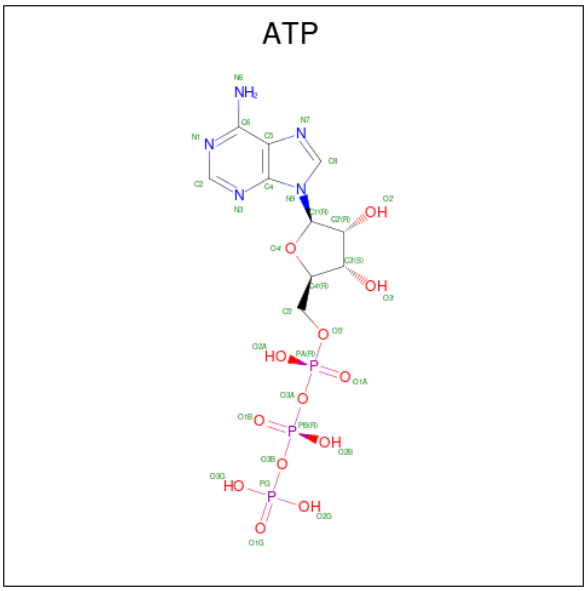
Mol	Chain	Residues	Atoms	AltConf
9	Mi	1	Total Mg 1 1	0
9	Mj	1	Total Mg 1 1	0
9	Mk	1	Total Mg 1 1	0
9	Ml	1	Total Mg 1 1	0

- Molecule 10 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms	AltConf
10	Ma	1	Total C N O P 31 10 5 13 3	0
10	Mb	1	Total C N O P 31 10 5 13 3	0
10	Mc	1	Total C N O P 31 10 5 13 3	0
10	Md	1	Total C N O P 31 10 5 13 3	0
10	Me	1	Total C N O P 31 10 5 13 3	0
10	Mf	1	Total C N O P 31 10 5 13 3	0
10	Mg	1	Total C N O P 31 10 5 13 3	0

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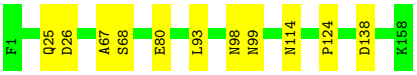
Mol	Chain	Residues	Atoms					AltConf
10	Mh	1	Total	C	N	O	P	0
			31	10	5	13	3	
10	Mi	1	Total	C	N	O	P	0
			31	10	5	13	3	
10	Mj	1	Total	C	N	O	P	0
			31	10	5	13	3	
10	Mk	1	Total	C	N	O	P	0
			31	10	5	13	3	
10	Ml	1	Total	C	N	O	P	0
			31	10	5	13	3	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

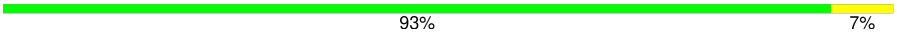
- Molecule 1: PilA

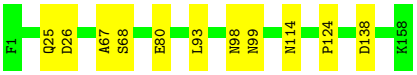
Chain Aa:



- Molecule 1: PilA

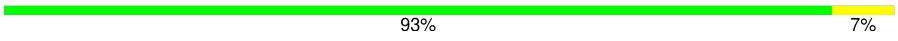
Chain Ab:

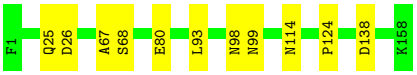




- Molecule 1: PilA

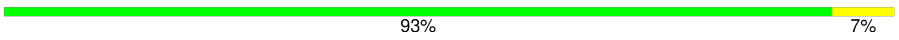
Chain Ac:

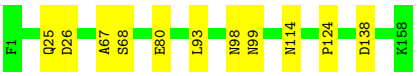




- Molecule 1: PilA

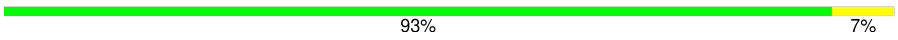
Chain Ad:

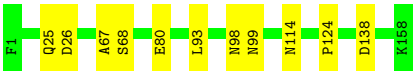




- Molecule 1: PilA

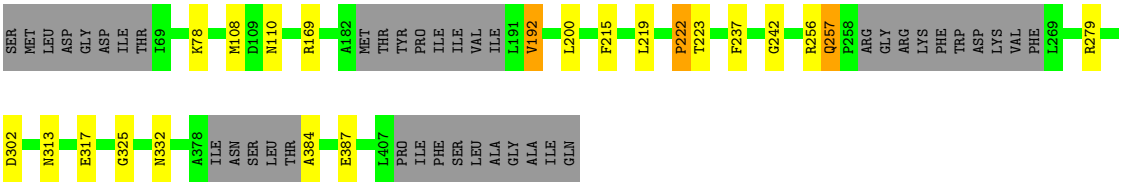
Chain Ae:





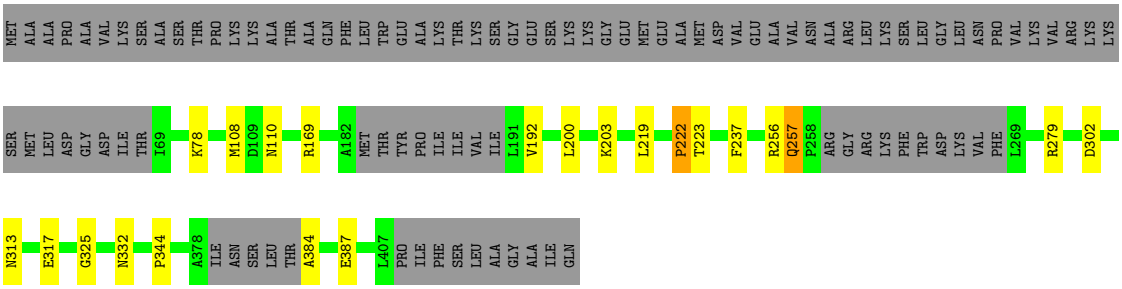
- Molecule 2: PilC

Chain Ca:



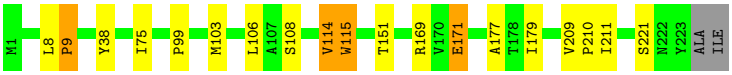
• Molecule 2: PilC

Chain Cb:



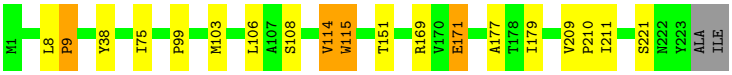
• Molecule 3: PilN

Chain Na:



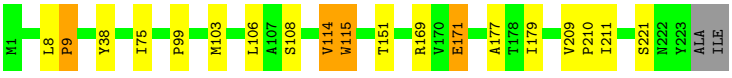
• Molecule 3: PilN

Chain Nb:



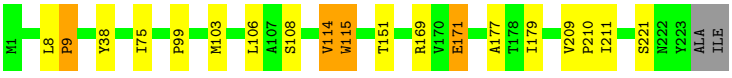
• Molecule 3: PilN

Chain Nc:



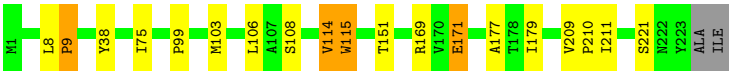
• Molecule 3: PilN

Chain Nd:



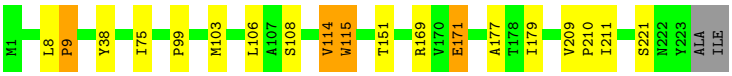
• Molecule 3: PilN

Chain Ne:



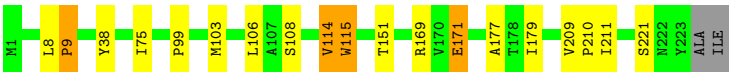
• Molecule 3: PilN

Chain Nf:



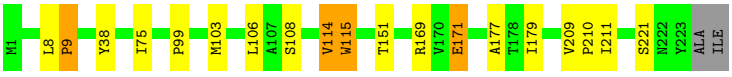
• Molecule 3: PilN

Chain Ng:



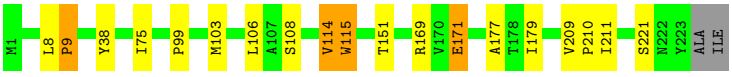
• Molecule 3: PilN

Chain Nh:



• Molecule 3: PilN

Chain Ni:

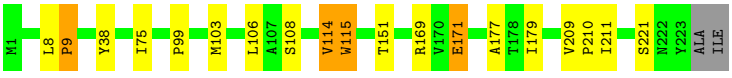


• Molecule 3: PilN

Chain Nj:

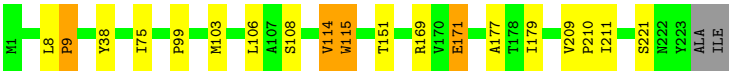
• Molecule 3: PilN

Chain Nk:



• Molecule 3: PilN

Chain Nl:

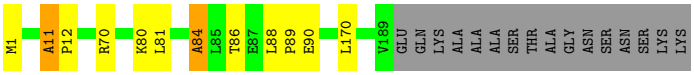


• Molecule 4: PilO

Chain Oa:

• Molecule 4: PilO

Chain Ob:

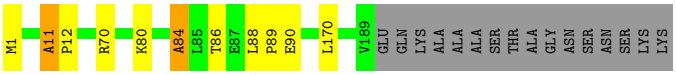


• Molecule 4: PilO

Chain Oc:

• Molecule 4: PilO

Chain Od:

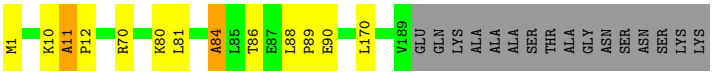


• Molecule 4: PilO

Chain Oe:

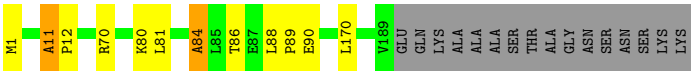
• Molecule 4: PilO

Chain Of:



• Molecule 4: PilO

Chain Og:

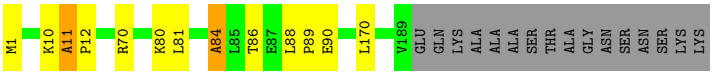


• Molecule 4: PilO

Chain Oh:

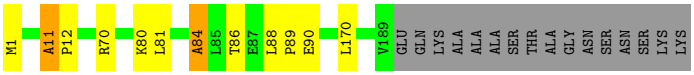
• Molecule 4: PilO

Chain Oi:



• Molecule 4: PilO

Chain Oj:

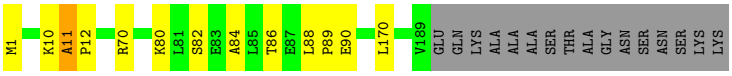


• Molecule 4: PilO

Chain Ok:

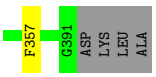
• Molecule 4: PilO

Chain Ol:



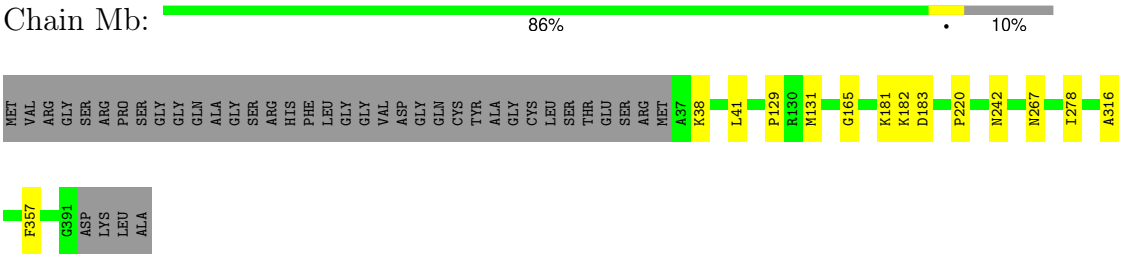
• Molecule 5: PilM

Chain Ma:



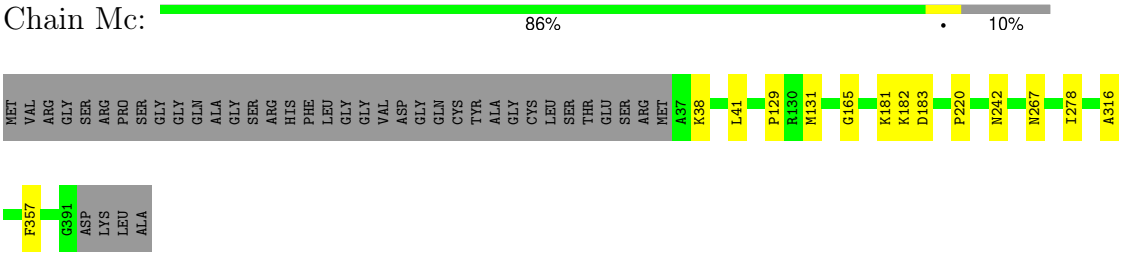
• Molecule 5: PilM

Chain Mb:



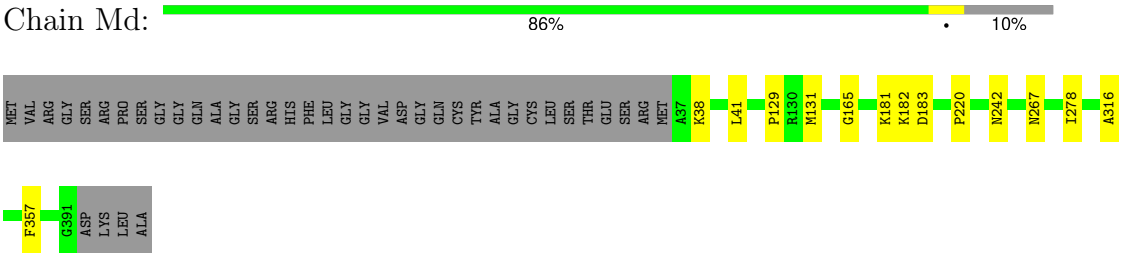
• Molecule 5: PilM

Chain Mc:



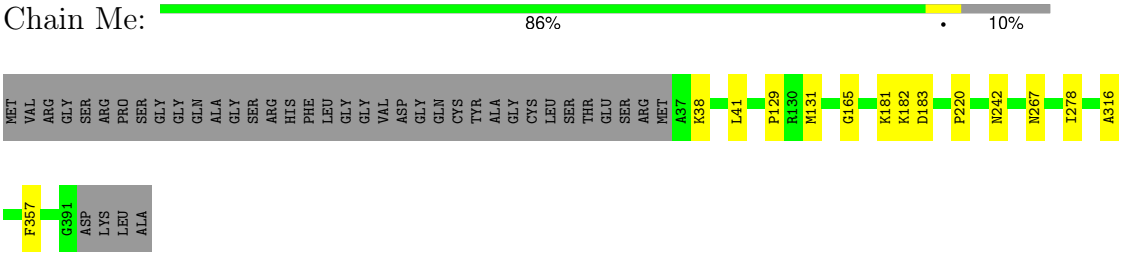
• Molecule 5: PilM

Chain Md:



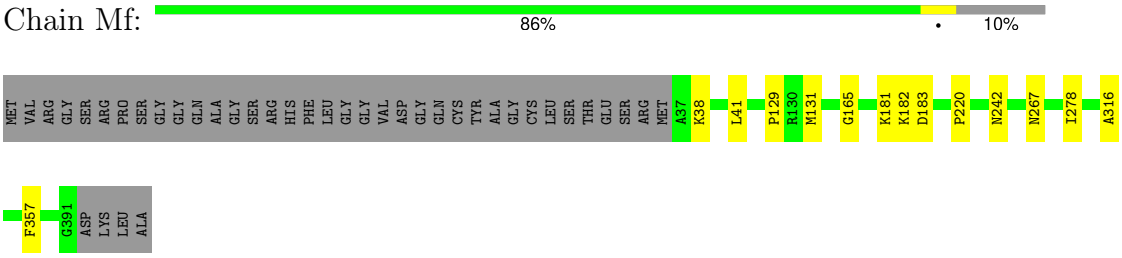
• Molecule 5: PilM

Chain Me:



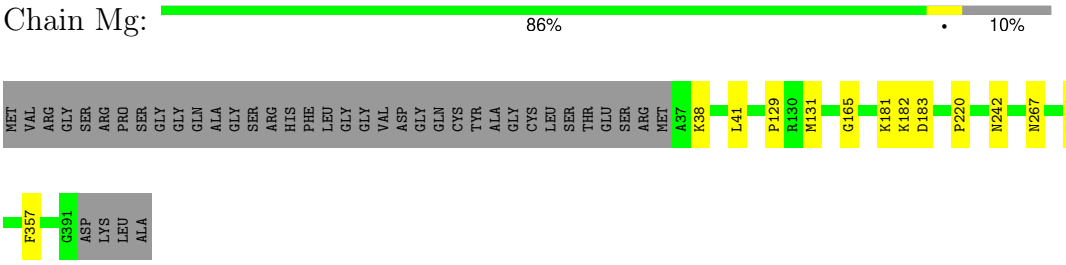
• Molecule 5: PilM

Chain Mf:



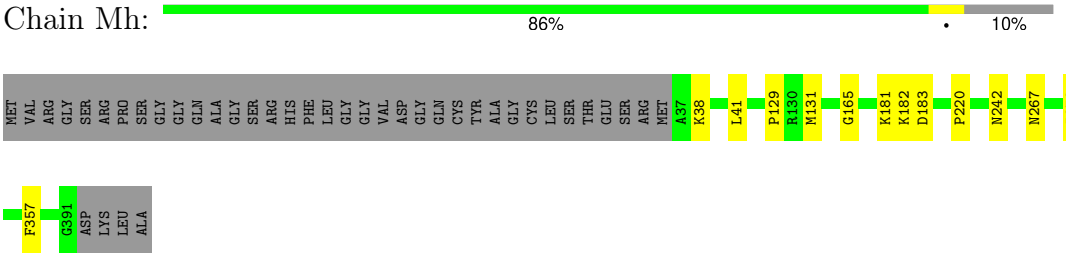
• Molecule 5: PilM

Chain Mg:



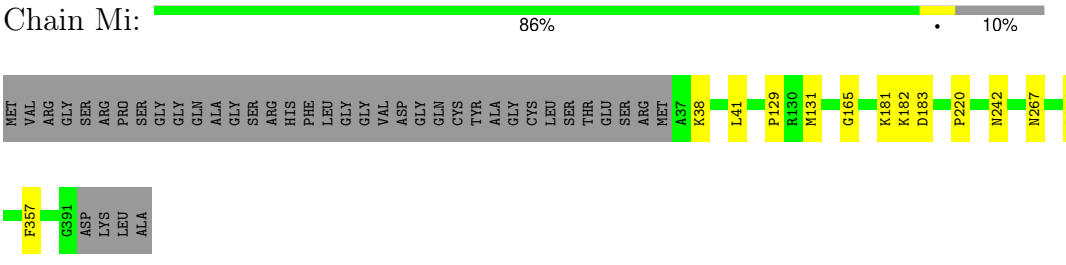
• Molecule 5: PilM

Chain Mh:



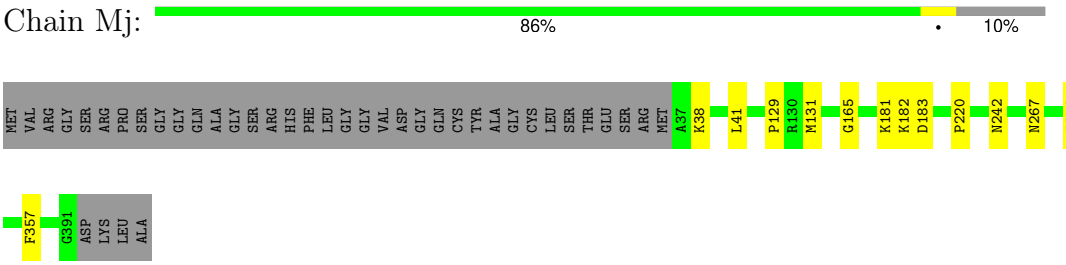
• Molecule 5: PilM

Chain Mi:



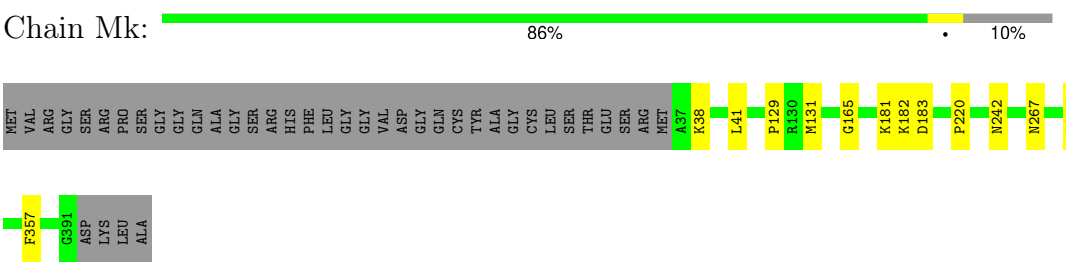
• Molecule 5: PilM

Chain Mj:



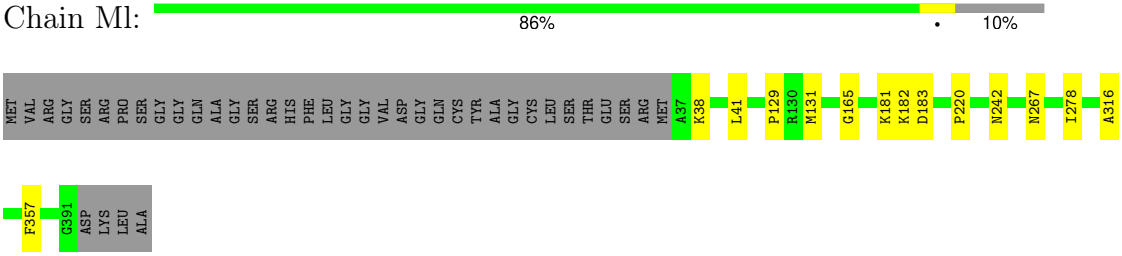
• Molecule 5: PilM

Chain Mk:



• Molecule 5: PilM

Chain Ml:

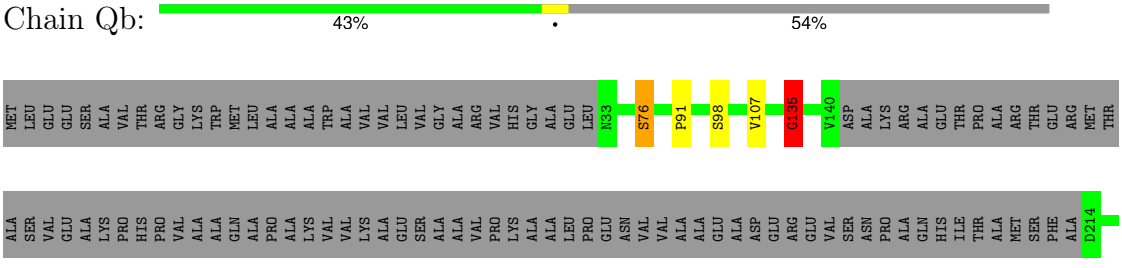


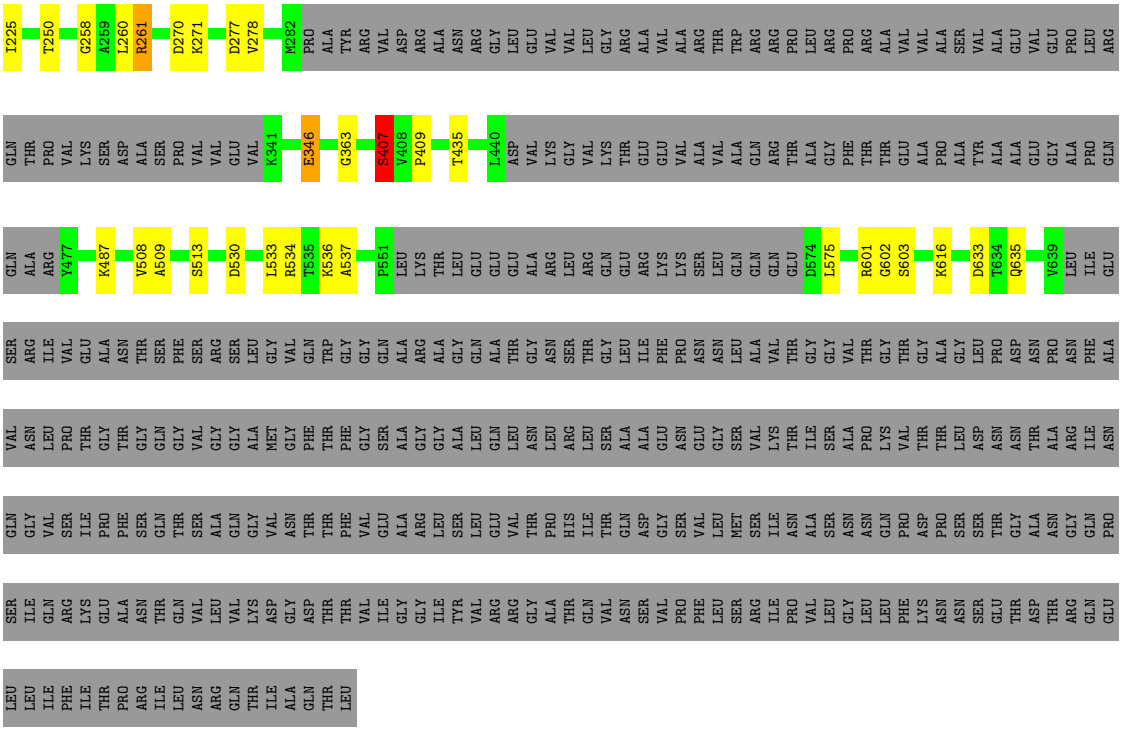
- Molecule 6: PilQ

Chain Qa:

- Molecule 6: PilQ

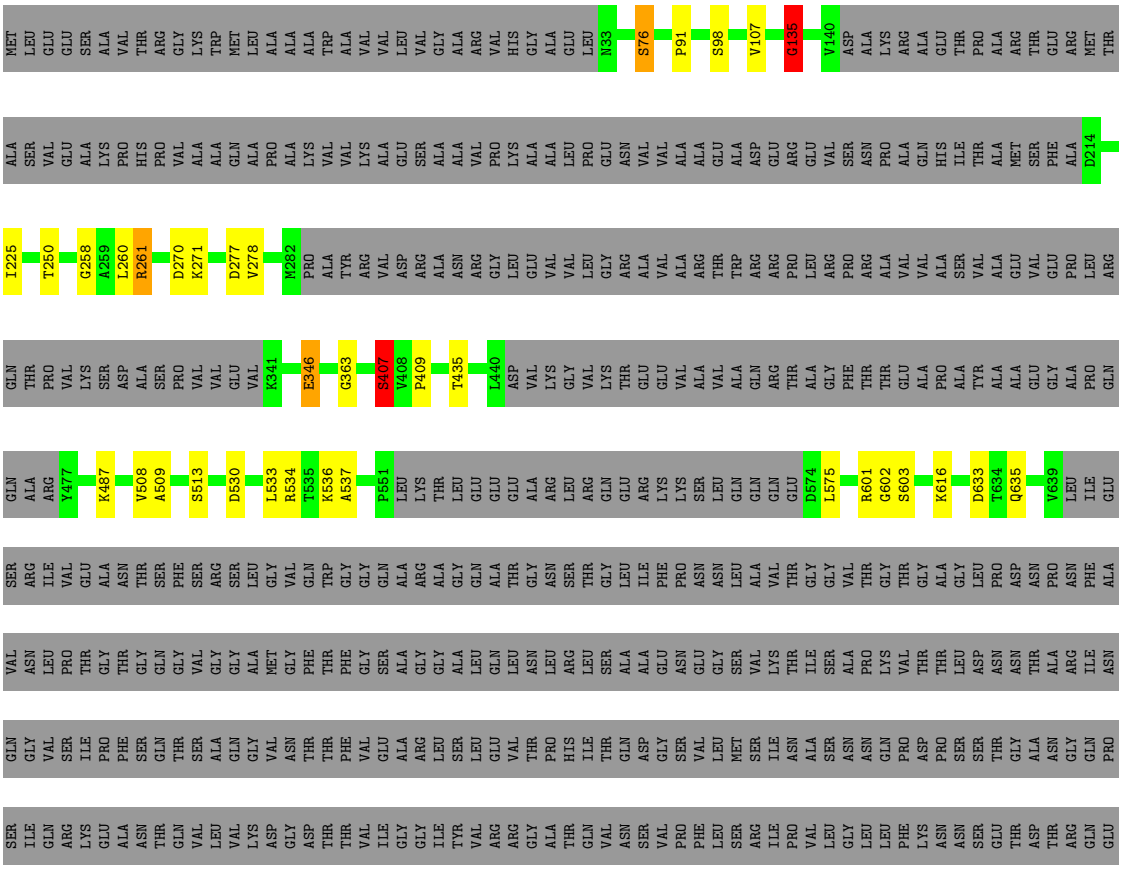
Chain Qb:





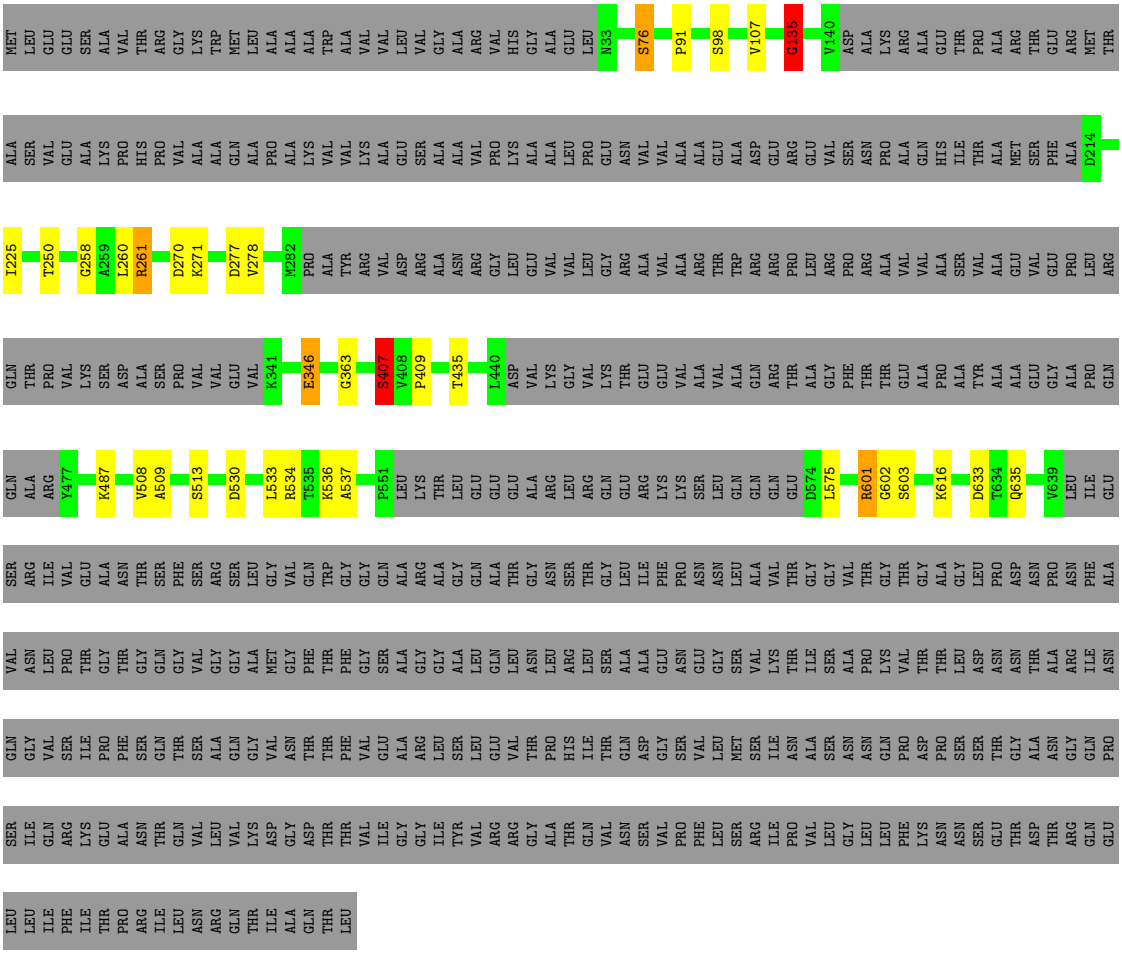
• Molecule 6: PilQ

Chain Qc:



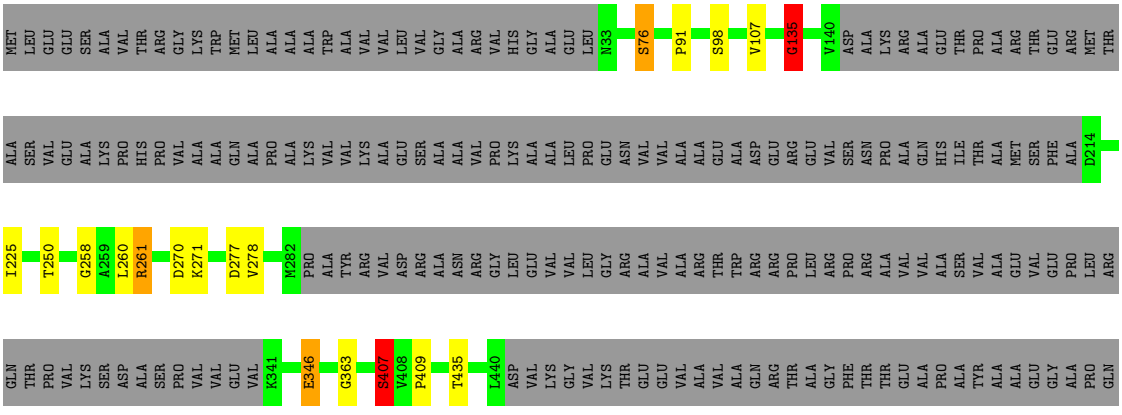
• Molecule 6: PilQ

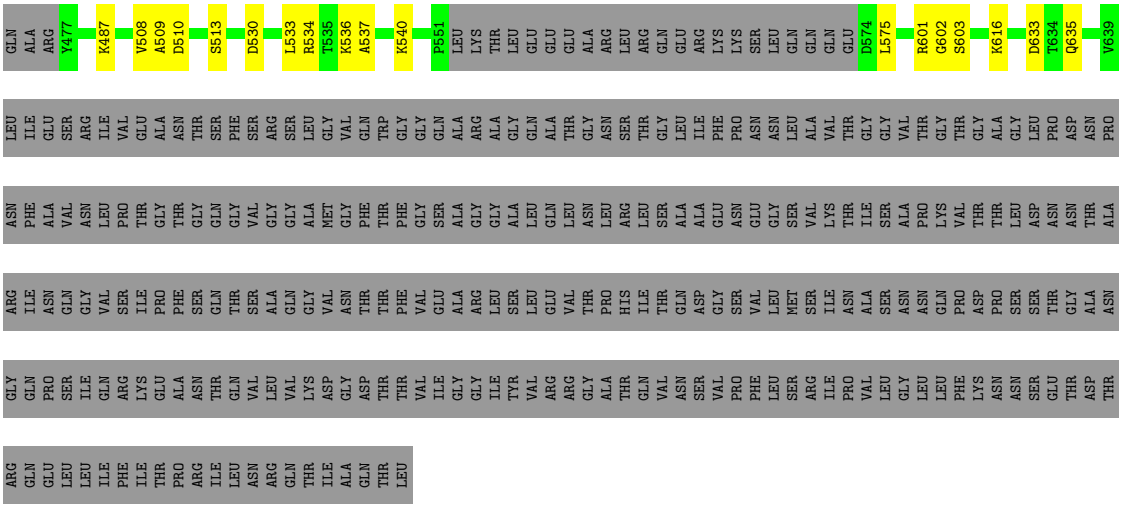
Chain Qd:



• Molecule 6: PilQ

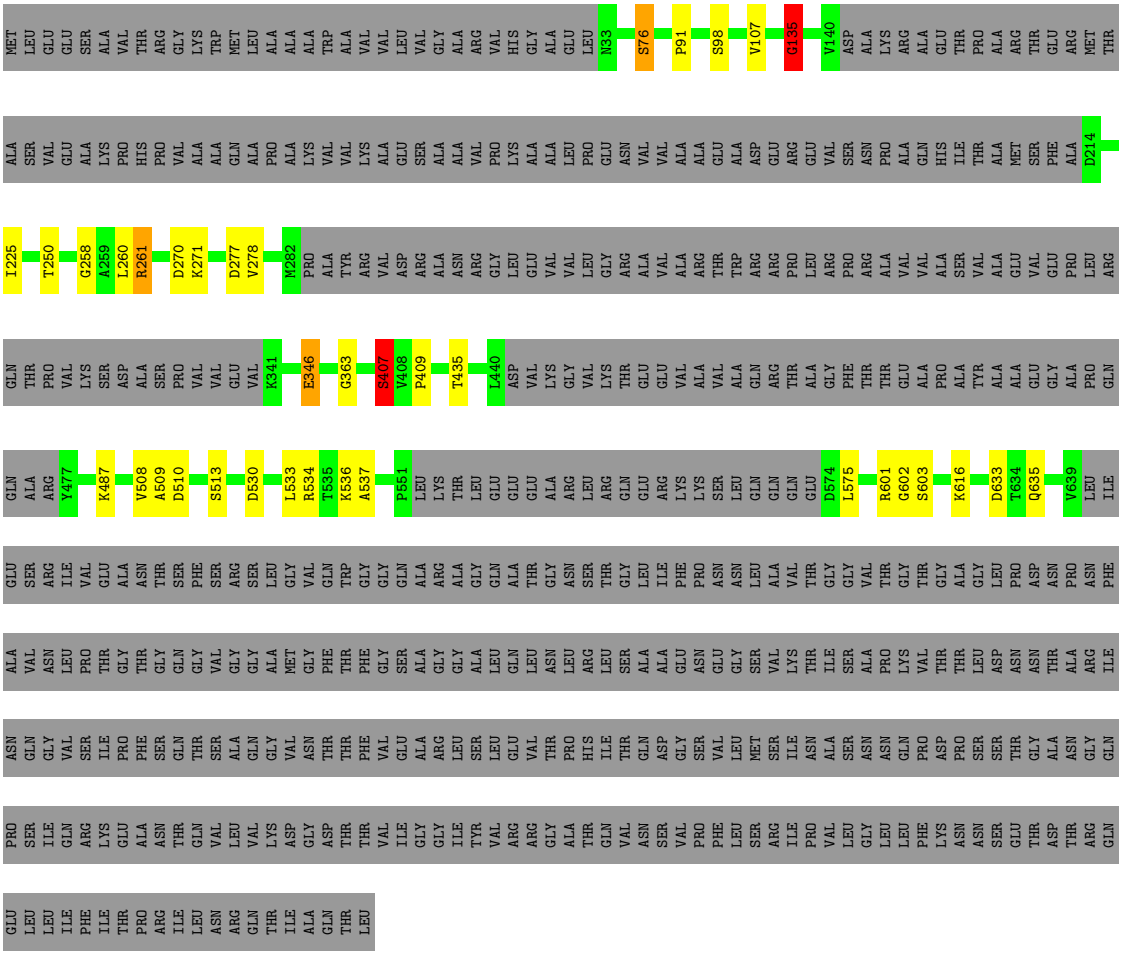
Chain Qe:





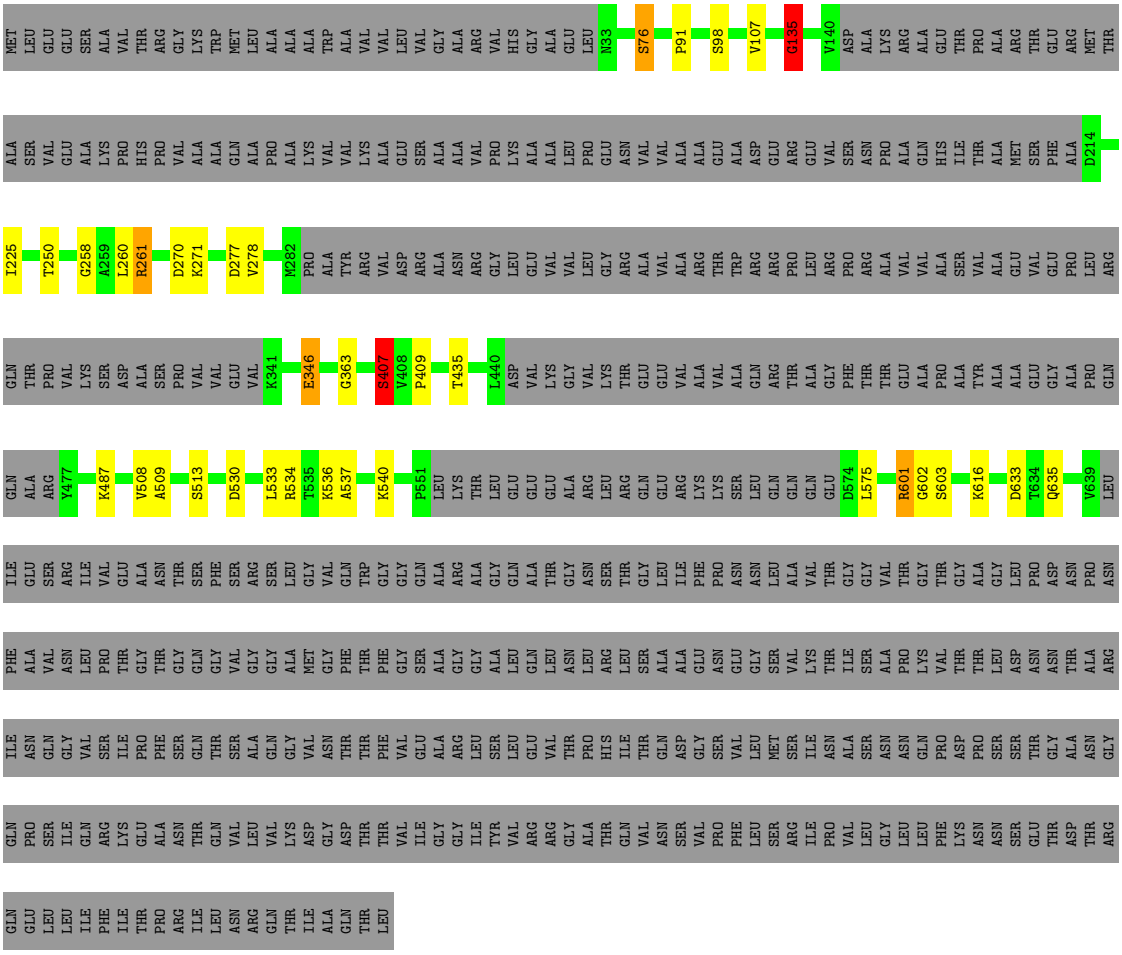
• Molecule 6: PilQ

Chain Qf:



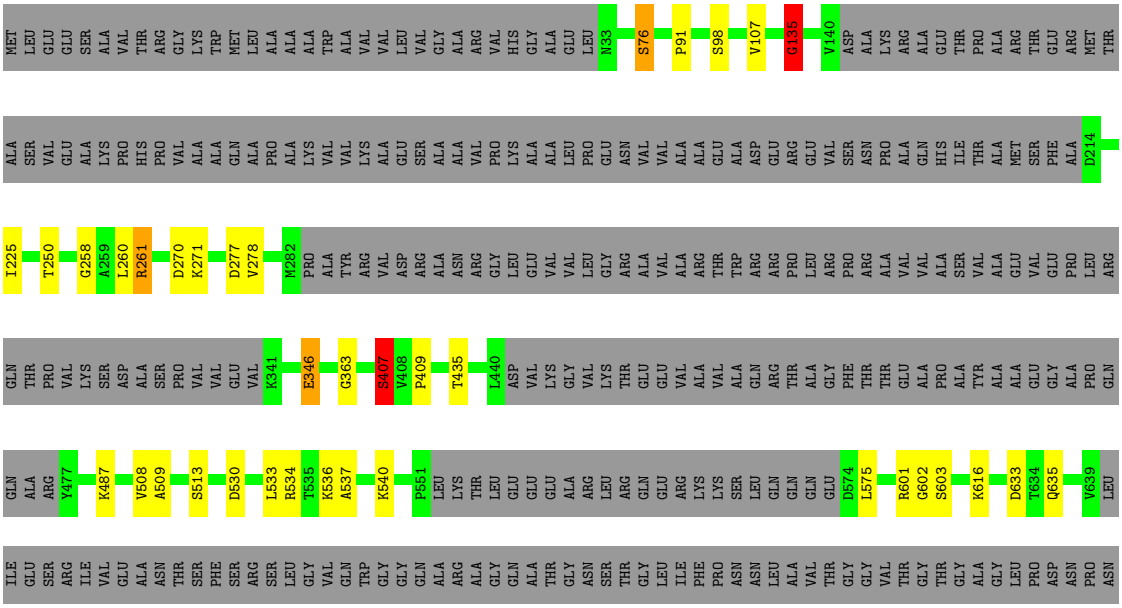
• Molecule 6: PilQ

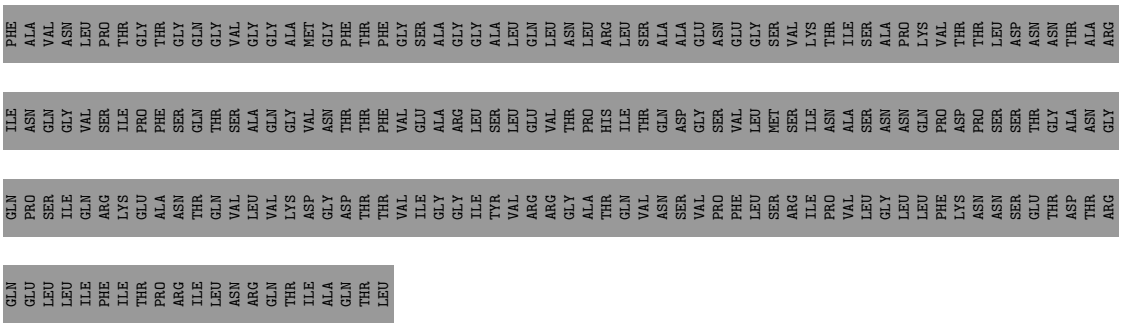
Chain Qg:



- Molecule 6: PilQ

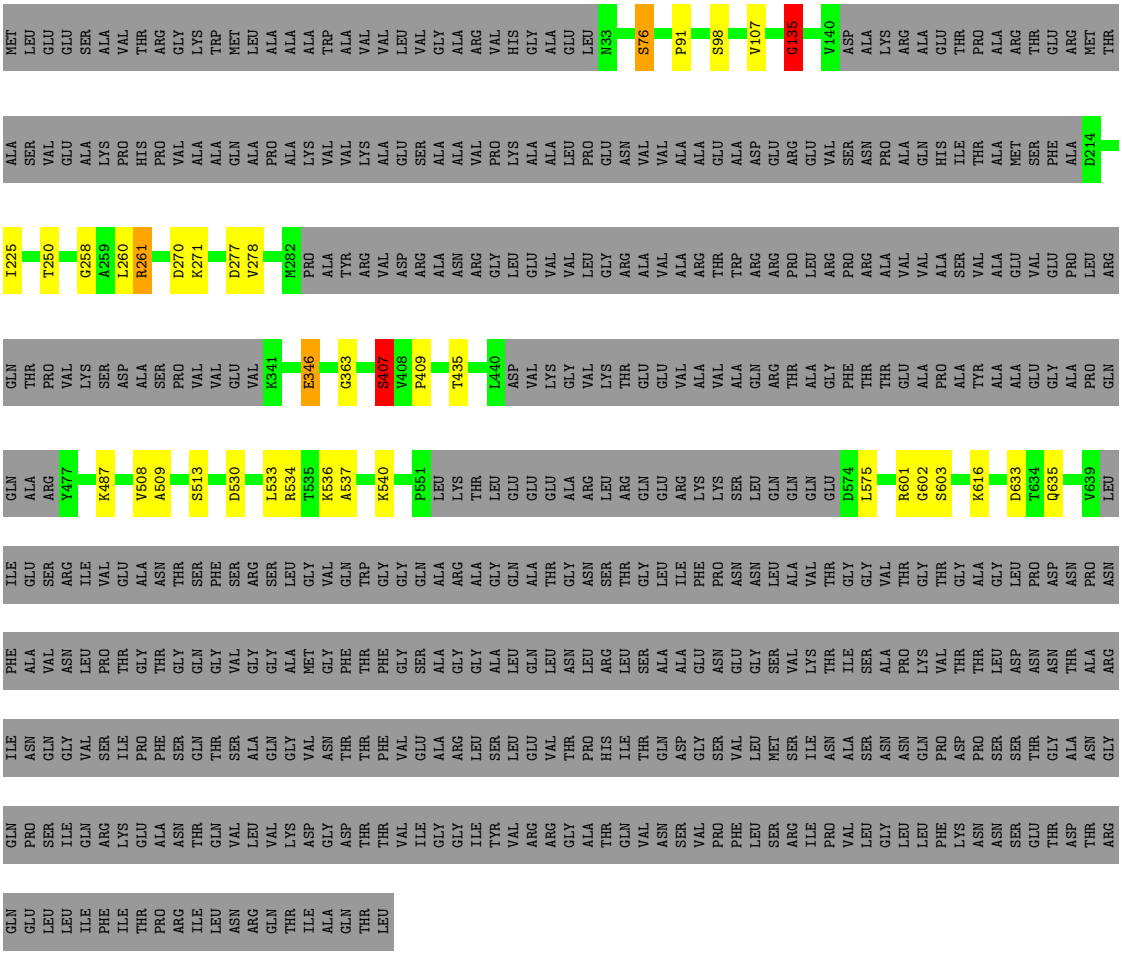
Chain Qh:





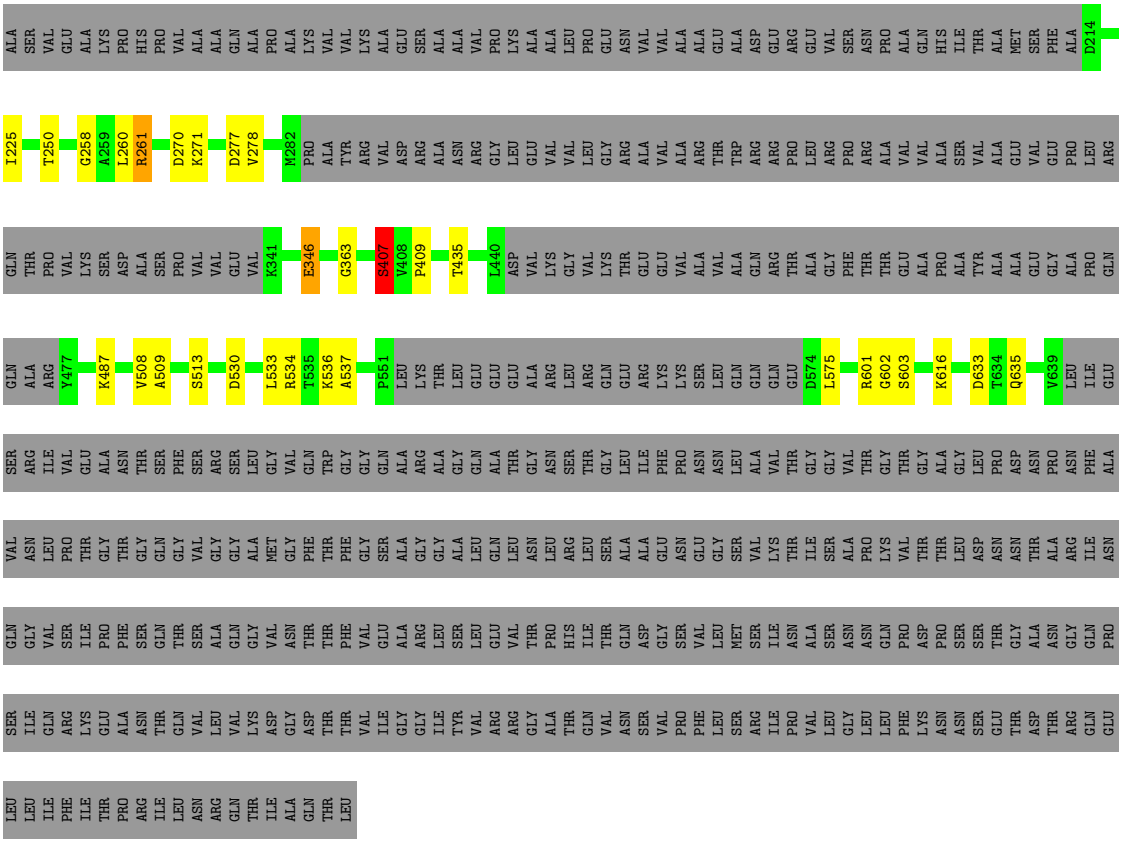
• Molecule 6: PilQ

Chain Qi:



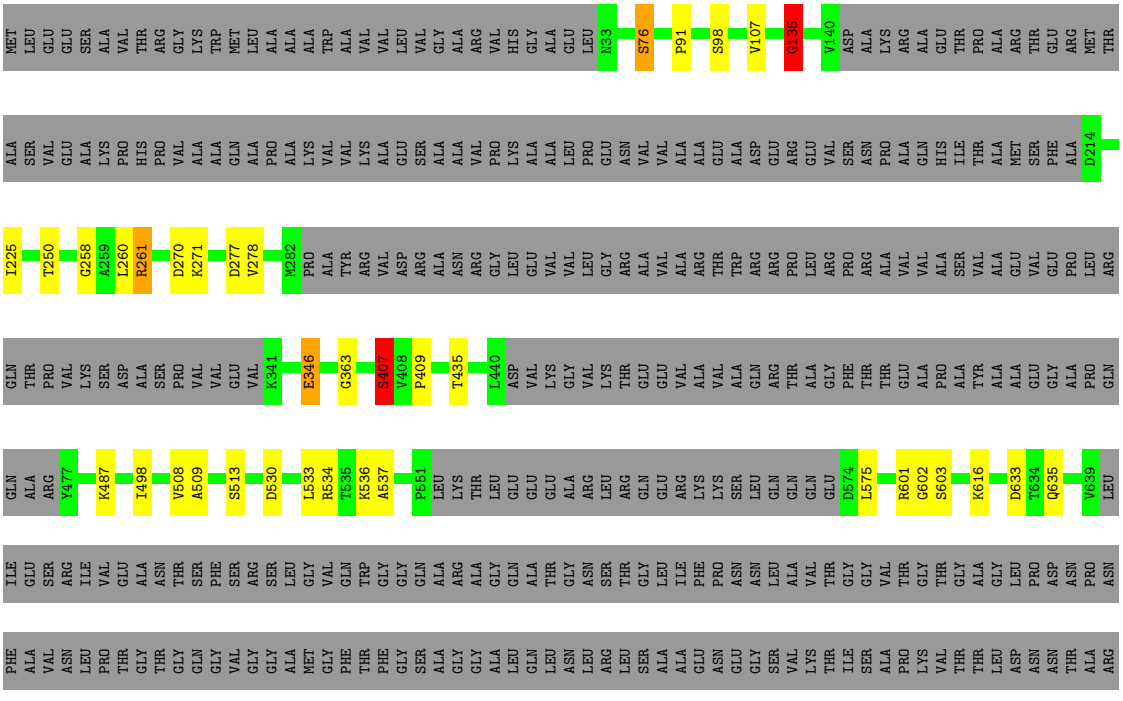
• Molecule 6: PilQ

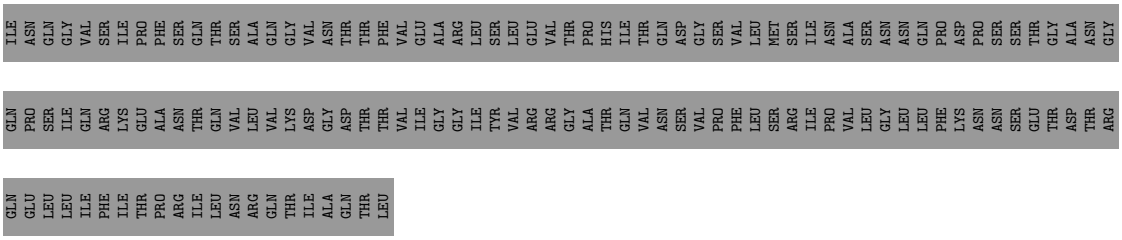
Chain Qj:



- Molecule 6: PilQ

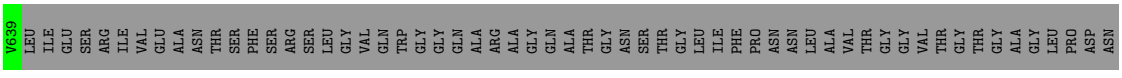
Chain Qk:





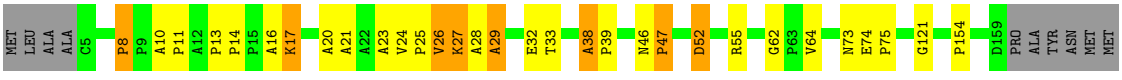
• Molecule 6: PilQ

Chain Ql:



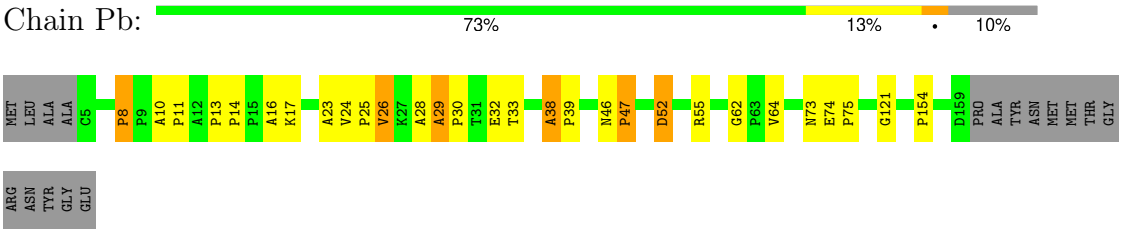
• Molecule 7: PilP

Chain Pa:



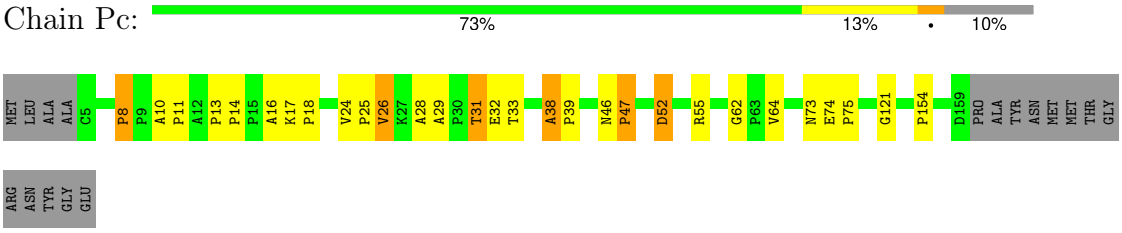
• Molecule 7: PilP

Chain Pb:



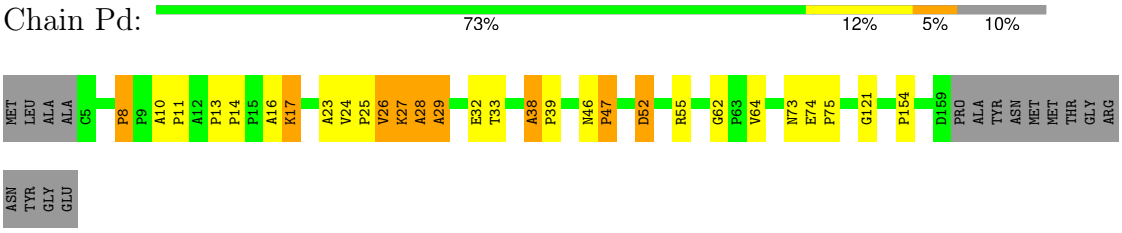
• Molecule 7: PilP

Chain Pc:



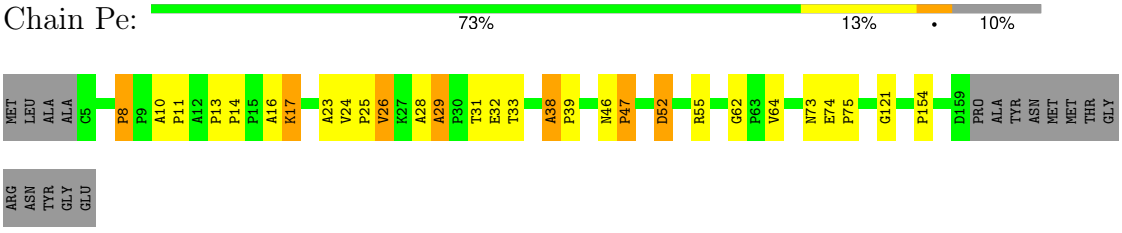
• Molecule 7: PilP

Chain Pd:



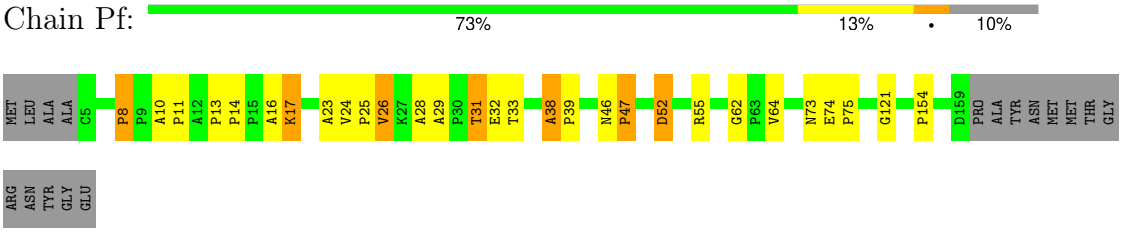
• Molecule 7: PilP

Chain Pe:



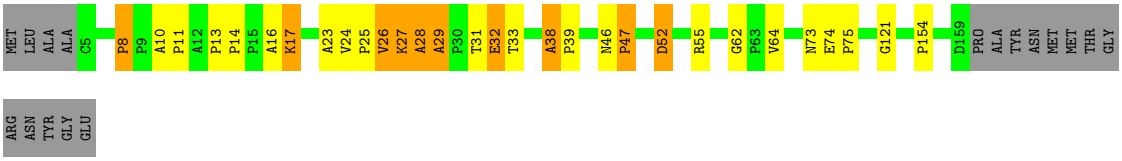
• Molecule 7: PilP

Chain Pf:



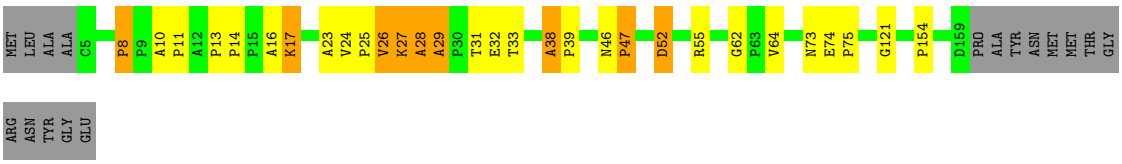
• Molecule 7: PilP

Chain Pg:



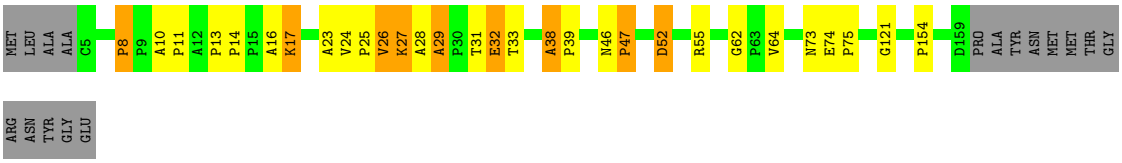
• Molecule 7: PilP

Chain Ph:



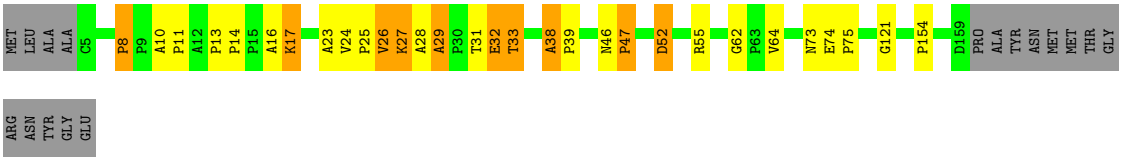
• Molecule 7: PilP

Chain Pi:



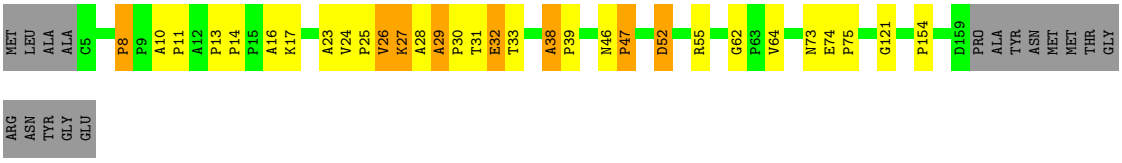
• Molecule 7: PilP

Chain Pj:



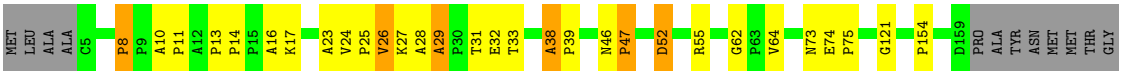
• Molecule 7: PilP

Chain Pk:



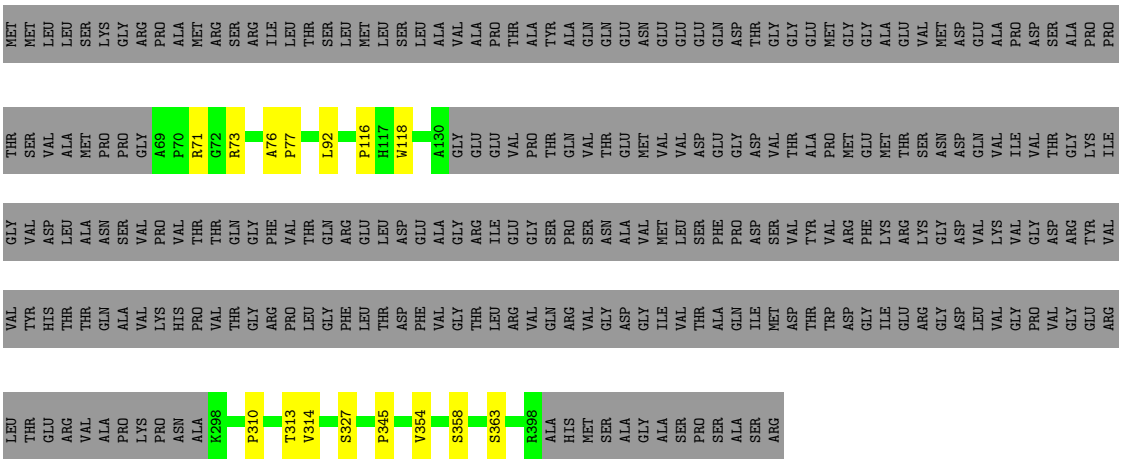
• Molecule 7: PilP

Chain Pl:



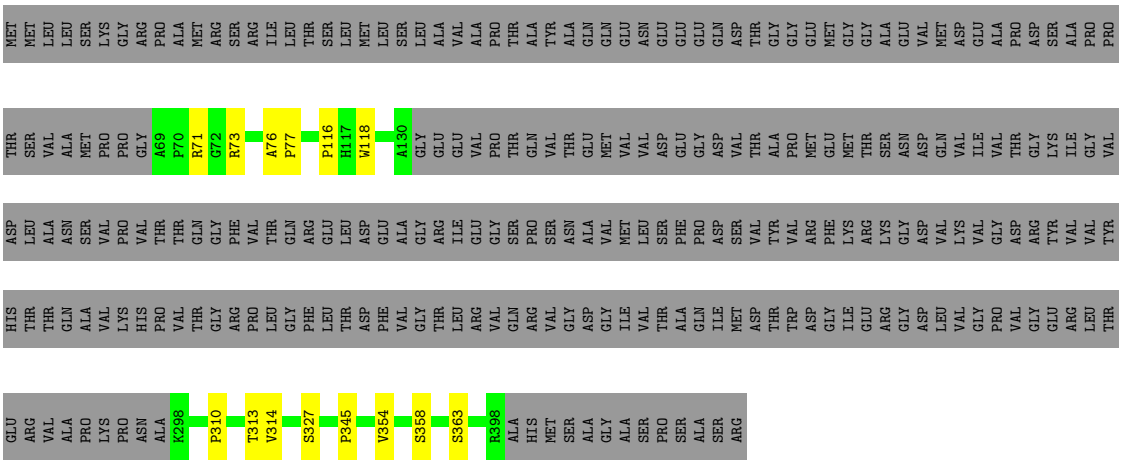
• Molecule 8: TsaP

Chain Ta:



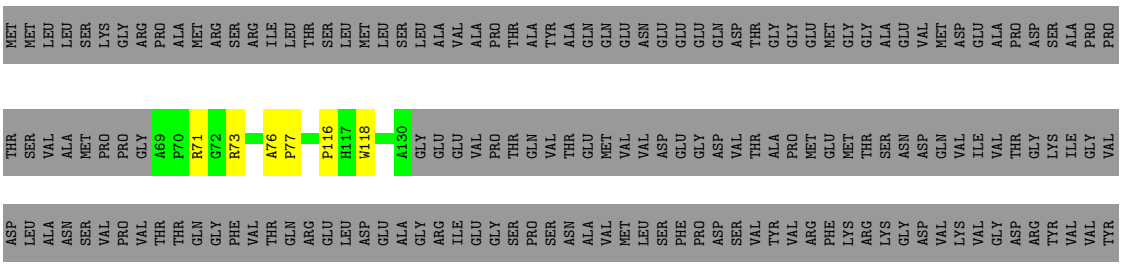
• Molecule 8: TsaP

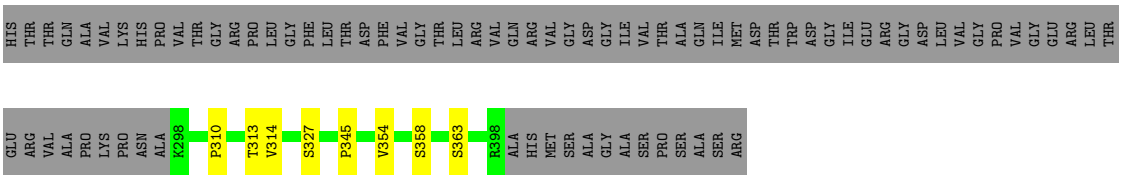
Chain Tb:



• Molecule 8: TsaP

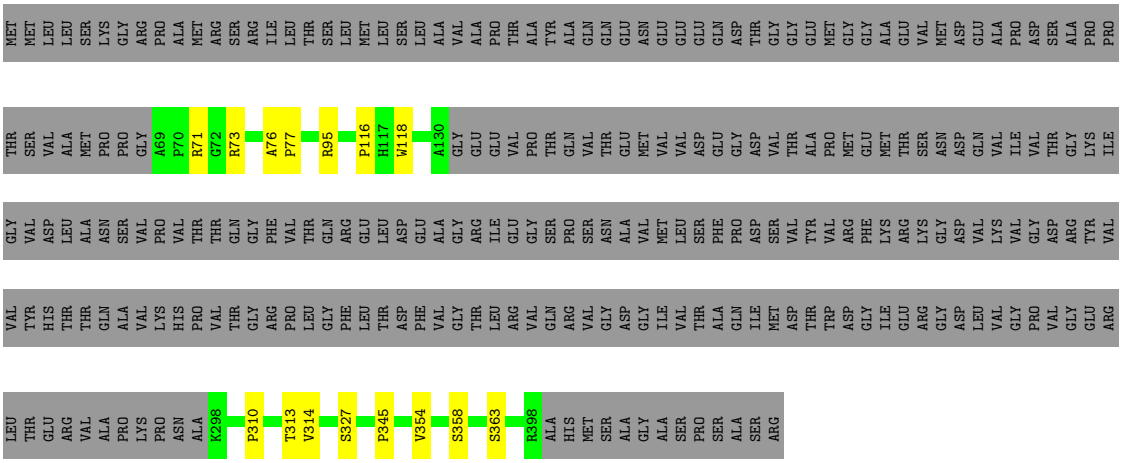
Chain Tc:





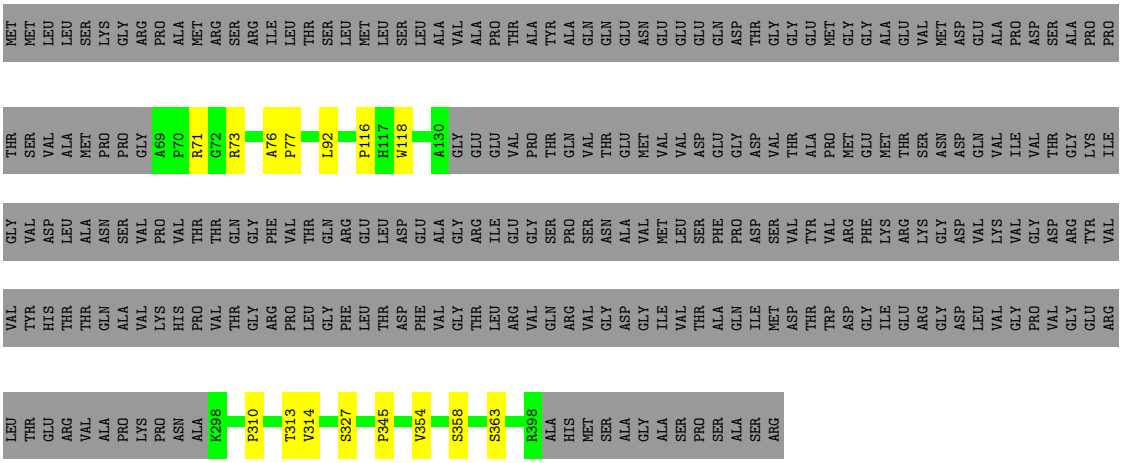
• Molecule 8: TsaP

Chain Td:



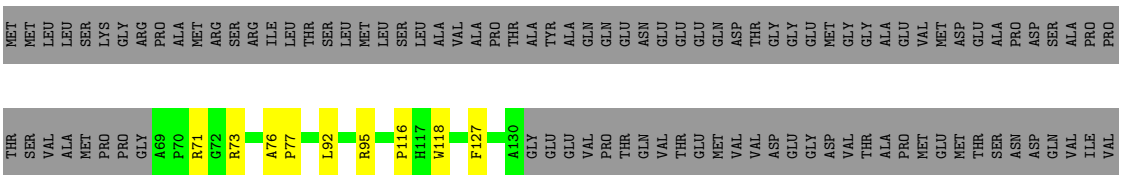
• Molecule 8: TsaP

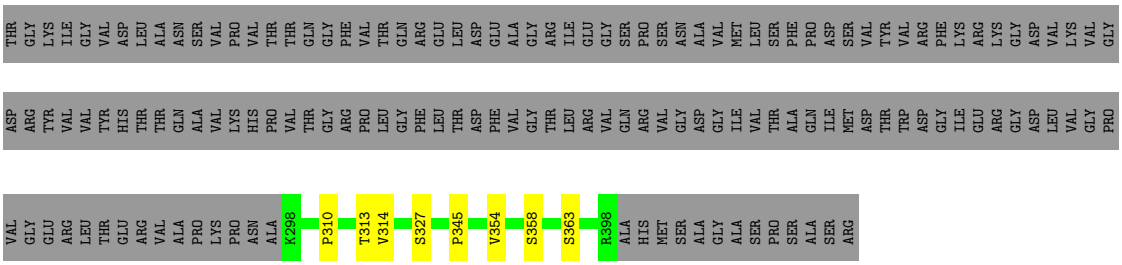
Chain Te:



• Molecule 8: TsaP

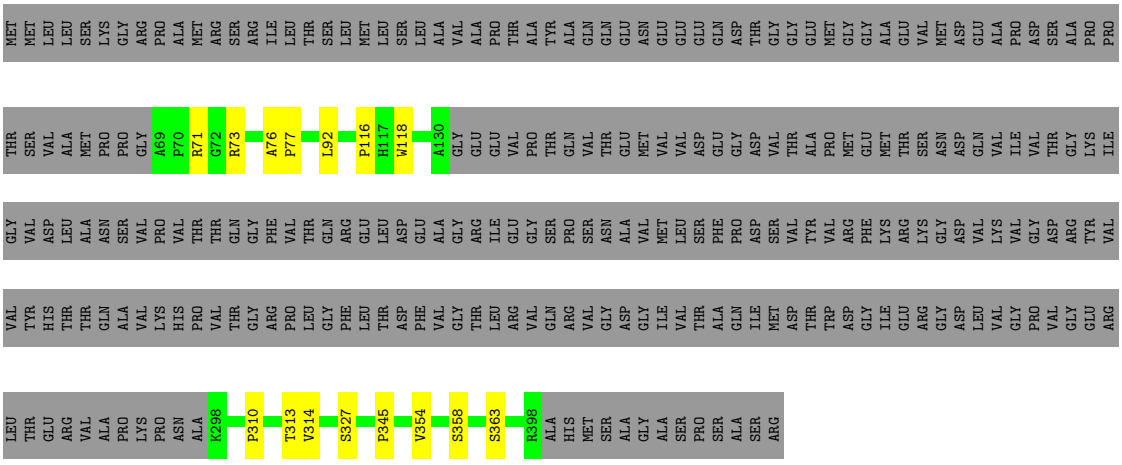
Chain Tf:





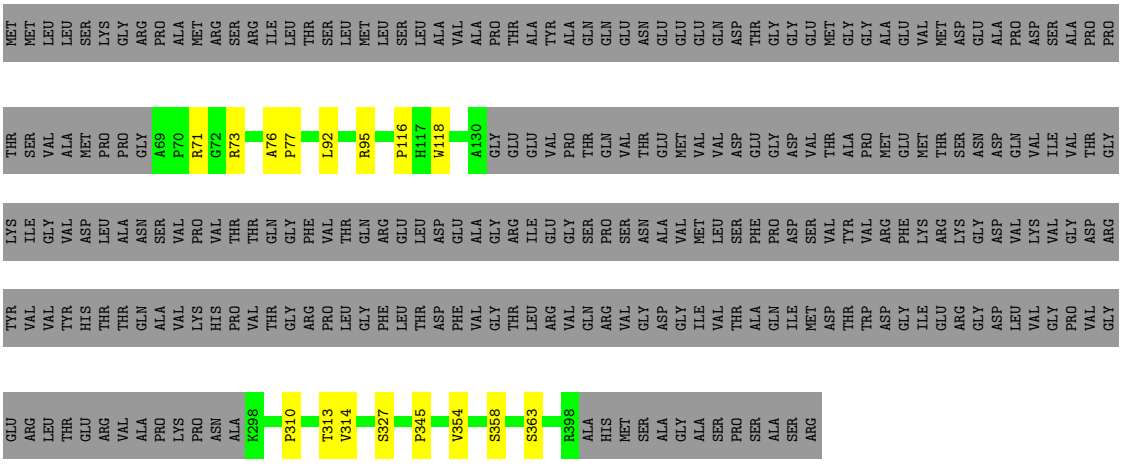
• Molecule 8: TsaP

Chain Tg:



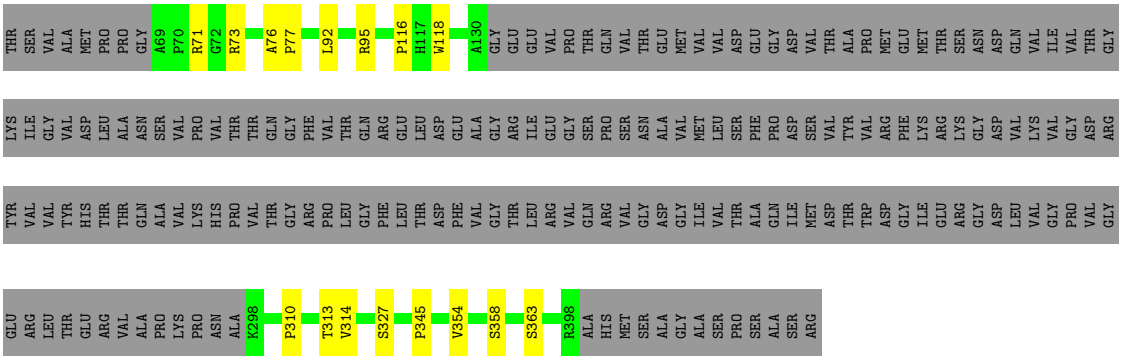
• Molecule 8: TsaP

Chain Th:



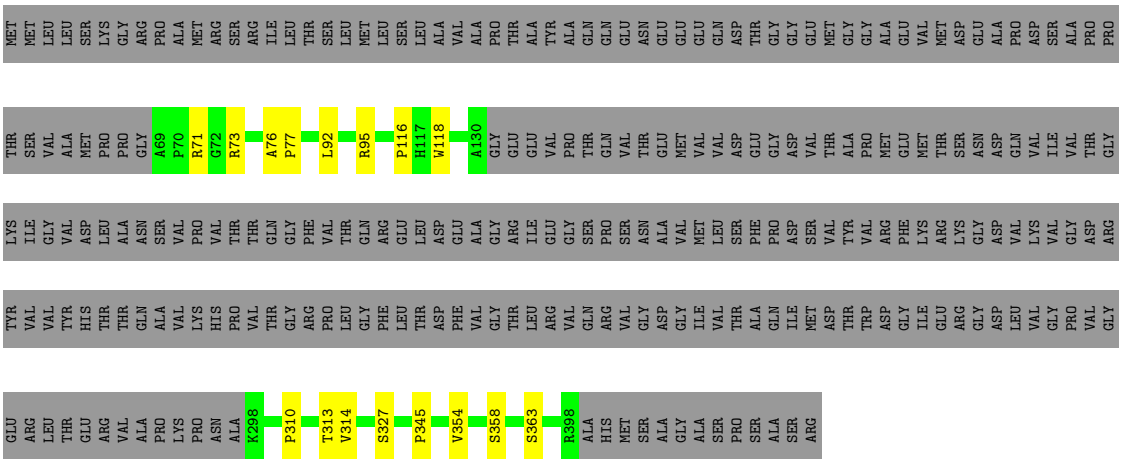
• Molecule 8: TsaP

Chain Ti:



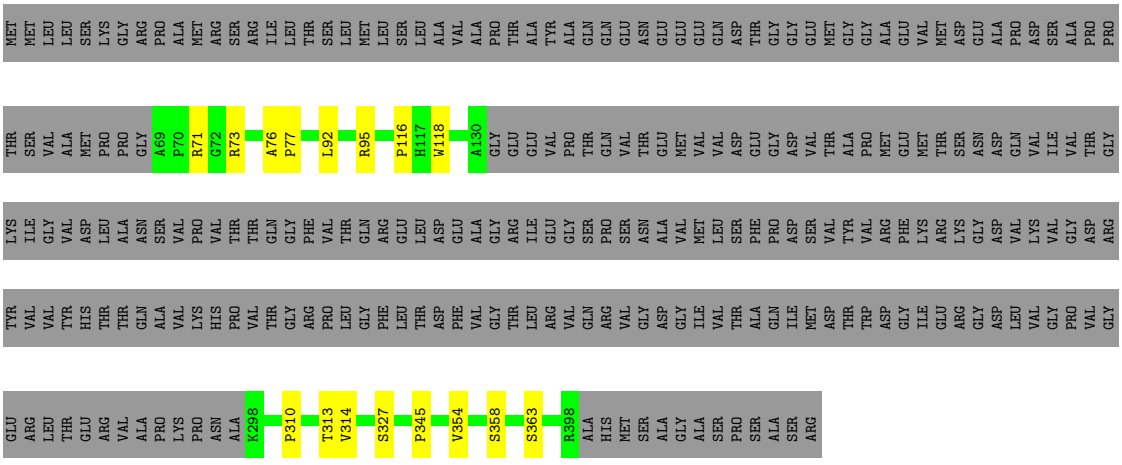
- Molecule 8: TsaP

Chain Tj:



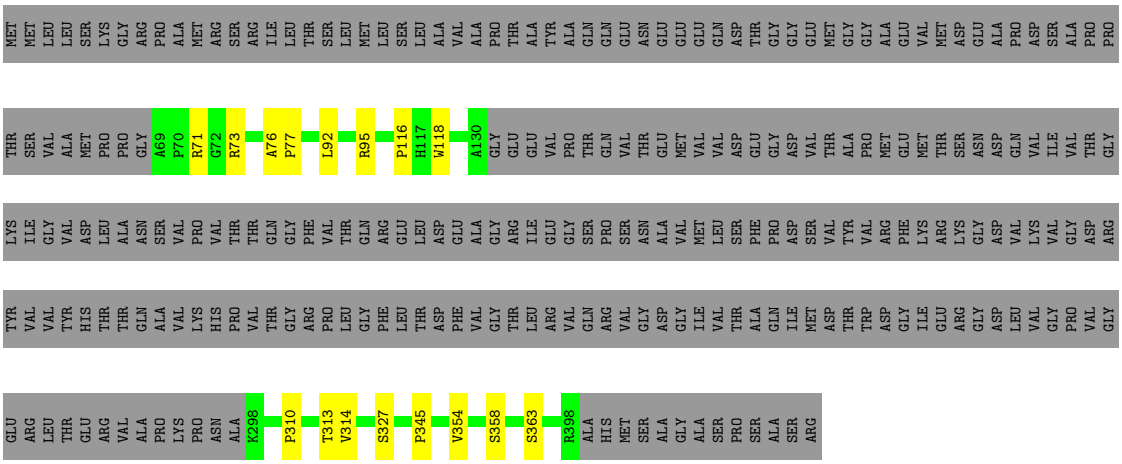
- Molecule 8: TsaP

Chain Tk:



- Molecule 8: TsaP

Chain Tl:


MET MET LEU LEU SER LYS GLY ARG PRO ALA MET ARG SER ARG ILE LEU THR SER LEU MET LEU SER LEU ALA VAL ALA PRO THR ALA TYR ALA GLN GLN GLU ASN GLU GLU GLU GLN ASP THR GLY GLY GLU MET GLY GLY ALA GLU VAL MET ASP GLU ALA PRO ASP SER ALA PRO PRO
THR SER VAL ALA MET PRO PRO GLY A69 P70 R71 G72 R73 A76 P77 L92 R95 P116 H117 W118 A130 GLY GLU GLU VAL PRO THR GLN VAL THR GLU MET VAL VAL ASP GLU GLY ASP VAL THR ALA PRO MET GLU MET THR SER ASN ASP GLN VAL ILE VAL THR GLY
LYS ILE GLY VAL ASP LEU ALA ASN SER VAL PRO VAL THR THR GLN GLY PHE VAL THR GLN ARG GLU LEU ASP GLU ALA GLY ARG ILE GLU GLY SER PRO SER ASN ALA VAL MET LEU SER PHE PRO ASP SER VAL TYR VAL ARG PHE LYS ARG LYS GLY ASP VAL LYS VAL GLY PRO ASP ARG
TYR VAL VAL TYR HIS THR THR GLN ALA VAL LYS HIS PRO VAL THR GLY ARG PRO LEU GLY PHE LEU THR ASP PHE VAL GLY THR LEU ARG VAL GLN ARG VAL GLY ASP GLY ILE VAL THR ALA GLN ILE MET ASP THR TRP ASP GLY ILE GLU ARG GLY ASP LEU VAL GLY PRO VAL GLY
GLU ARG LEU THR GLU ARG VAL ALA PRO LYS PRO ASN ALA K298 P310 T313 V314 S327 P345 V354 S358 S363 R398 ALA HIS MET SER ALA GLY ALA SER PRO SER ALA SER ARG

4 Experimental information (i)

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 ($e^-/Å^2$)	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 (i)

5.1 Standard geometry (i)

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

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	Aa	0.71	1/627 (0.2%)	0.72	1/782 (0.1%)
1	Ab	0.70	1/627 (0.2%)	0.72	1/782 (0.1%)
1	Ac	0.70	1/627 (0.2%)	0.72	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%)
2	Ca	0.62	0/1260	0.93	1/1568 (0.1%)
2	Cb	0.62	0/1260	0.92	1/1568 (0.1%)
3	Na	0.57	1/891 (0.1%)	0.74	2/1112 (0.2%)
3	Nb	0.56	1/891 (0.1%)	0.74	2/1112 (0.2%)
3	Nc	0.57	1/891 (0.1%)	0.74	2/1112 (0.2%)
3	Nd	0.56	1/891 (0.1%)	0.74	2/1112 (0.2%)
3	Ne	0.57	1/891 (0.1%)	0.75	2/1112 (0.2%)
3	Nf	0.56	1/891 (0.1%)	0.74	2/1112 (0.2%)
3	Ng	0.57	1/891 (0.1%)	0.75	2/1112 (0.2%)
3	Nh	0.56	1/891 (0.1%)	0.75	2/1112 (0.2%)
3	Ni	0.56	1/891 (0.1%)	0.75	2/1112 (0.2%)
3	Nj	0.57	1/891 (0.1%)	0.74	2/1112 (0.2%)
3	Nk	0.57	1/891 (0.1%)	0.74	2/1112 (0.2%)
3	Nl	0.57	1/891 (0.1%)	0.74	2/1112 (0.2%)
4	Oa	0.35	0/755	0.68	0/942
4	Ob	0.35	0/755	0.66	0/942
4	Oc	0.35	0/755	0.67	0/942
4	Od	0.35	0/755	0.68	0/942
4	Oe	0.35	0/755	0.68	0/942
4	Of	0.35	0/755	0.68	0/942
4	Og	0.36	0/755	0.68	0/942
4	Oh	0.35	0/755	0.68	0/942
4	Oi	0.35	0/755	0.68	0/942
4	Oj	0.35	0/755	0.68	0/942
4	Ok	0.35	0/755	0.66	0/942
4	Ol	0.37	0/755	0.67	1/942 (0.1%)
5	Ma	0.31	0/1419	0.61	0/1772

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
5	Mb	0.32	0/1419	0.61	0/1772
5	Mc	0.31	0/1419	0.61	0/1772
5	Md	0.31	0/1419	0.61	0/1772
5	Me	0.32	0/1419	0.61	0/1772
5	Mf	0.31	0/1419	0.62	0/1772
5	Mg	0.31	0/1419	0.61	0/1772
5	Mh	0.32	0/1419	0.61	0/1772
5	Mi	0.31	0/1419	0.61	0/1772
5	Mj	0.31	0/1419	0.61	0/1772
5	Mk	0.32	0/1419	0.61	0/1772
5	Ml	0.32	0/1419	0.61	0/1772
6	Qa	0.62	1/1667 (0.1%)	1.72	10/2075 (0.5%)
6	Qb	0.62	1/1667 (0.1%)	1.71	10/2075 (0.5%)
6	Qc	0.62	1/1667 (0.1%)	1.72	10/2075 (0.5%)
6	Qd	0.62	1/1667 (0.1%)	1.72	11/2075 (0.5%)
6	Qe	0.62	1/1667 (0.1%)	1.72	10/2075 (0.5%)
6	Qf	0.62	1/1667 (0.1%)	1.71	10/2075 (0.5%)
6	Qg	0.62	1/1667 (0.1%)	1.71	11/2075 (0.5%)
6	Qh	0.62	1/1667 (0.1%)	1.71	10/2075 (0.5%)
6	Qi	0.62	1/1667 (0.1%)	1.71	10/2075 (0.5%)
6	Qj	0.62	1/1667 (0.1%)	1.72	10/2075 (0.5%)
6	Qk	0.62	1/1667 (0.1%)	1.72	10/2075 (0.5%)
6	Ql	0.62	1/1667 (0.1%)	1.71	10/2075 (0.5%)
7	Pa	0.55	0/619	1.00	0/772
7	Pb	0.54	0/619	1.01	0/772
7	Pc	0.55	0/619	1.03	0/772
7	Pd	0.57	0/619	1.02	0/772
7	Pe	0.57	0/619	1.05	0/772
7	Pf	0.56	0/619	1.05	0/772
7	Pg	0.56	0/619	1.02	0/772
7	Ph	0.56	0/619	1.02	0/772
7	Pi	0.57	0/619	1.01	0/772
7	Pj	0.57	0/619	1.01	0/772
7	Pk	0.54	0/619	0.99	0/772
7	Pl	0.53	0/619	0.99	0/772
8	Ta	0.33	0/650	0.66	0/809
8	Tb	0.32	0/650	0.66	0/809
8	Tc	0.33	0/650	0.66	0/809
8	Td	0.32	0/650	0.66	0/809
8	Te	0.32	0/650	0.66	0/809
8	Tf	0.34	0/650	0.66	0/809
8	Tg	0.33	0/650	0.66	0/809
8	Th	0.32	0/650	0.66	0/809

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
8	Ti	0.32	0/650	0.65	0/809
8	Tj	0.32	0/650	0.66	0/809
8	Tk	0.32	0/650	0.66	0/809
8	Tl	0.33	0/650	0.65	0/809
All	All	0.50	29/77667 (0.0%)	1.08	154/96830 (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	Ca	0	18
2	Cb	0	18
3	Na	0	7
3	Nb	0	7
3	Nc	0	7
3	Nd	0	7
3	Ne	0	7
3	Nf	0	7
3	Ng	0	7
3	Nh	0	7
3	Ni	0	7
3	Nj	0	7
3	Nk	0	7
3	Nl	0	7
4	Oa	0	4
4	Ob	0	4
4	Oc	0	4
4	Od	0	4
4	Oe	0	4
4	Of	0	4
4	Og	0	4
4	Oh	0	4
4	Oi	0	4
4	Oj	0	4
4	Ok	0	5
4	Ol	0	3
5	Ma	0	2
5	Mb	0	2
5	Mc	0	2
5	Md	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	Me	0	2
5	Mf	0	2
5	Mg	0	2
5	Mh	0	2
5	Mi	0	2
5	Mj	0	2
5	Mk	0	2
5	Ml	0	2
6	Qa	0	20
6	Qb	0	20
6	Qc	0	20
6	Qd	0	20
6	Qe	0	22
6	Qf	0	21
6	Qg	0	21
6	Qh	0	21
6	Qi	0	21
6	Qj	0	20
6	Qk	0	21
6	Ql	0	22
7	Pa	0	22
7	Pb	0	21
7	Pc	0	19
7	Pd	0	21
7	Pe	0	23
7	Pf	0	21
7	Pg	0	23
7	Ph	0	23
7	Pi	0	23
7	Pj	0	23
7	Pk	0	22
7	Pl	0	19
8	Tf	0	1
All	All	0	702

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	15.14	1.76	1.46
1	Ab	26	ASP	N-CA	15.05	1.76	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Ac	26	ASP	N-CA	15.02	1.76	1.46

The worst 5 of 154 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	Qf	407	SER	O-C-N	-54.05	36.22	122.70
6	Qg	407	SER	O-C-N	-54.05	36.22	122.70
6	Qk	407	SER	O-C-N	-54.05	36.23	122.70
6	Qh	407	SER	O-C-N	-54.04	36.23	122.70
6	Qb	407	SER	O-C-N	-54.04	36.23	122.70

There are no chirality outliers.

5 of 702 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Ca	108	MET	Mainchain
2	Ca	169	ARG	Mainchain
2	Ca	192	VAL	Mainchain
2	Ca	200	LEU	Mainchain
2	Ca	78	LYS	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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
2	Ca	1264	0	354	0	0
2	Cb	1264	0	354	0	0
3	Na	892	0	248	0	0
3	Nb	892	0	248	0	0
3	Nc	892	0	248	0	0
3	Nd	892	0	248	0	0
3	Ne	892	0	248	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Nf	892	0	248	0	0
3	Ng	892	0	248	0	0
3	Nh	892	0	248	0	0
3	Ni	892	0	248	0	0
3	Nj	892	0	248	0	0
3	Nk	892	0	248	0	0
3	Nl	892	0	248	0	0
4	Oa	756	0	207	0	0
4	Ob	756	0	207	0	0
4	Oc	756	0	207	0	0
4	Od	756	0	207	0	0
4	Oe	756	0	207	0	0
4	Of	756	0	207	0	0
4	Og	756	0	207	0	0
4	Oh	756	0	207	0	0
4	Oi	756	0	207	0	0
4	Oj	756	0	206	0	0
4	Ok	756	0	207	0	0
4	Ol	756	0	207	0	0
5	Ma	1420	0	396	0	0
5	Mb	1420	0	396	0	0
5	Mc	1420	0	396	0	0
5	Md	1420	0	396	0	0
5	Me	1420	0	396	0	0
5	Mf	1420	0	396	0	0
5	Mg	1420	0	396	0	0
5	Mh	1420	0	396	0	0
5	Mi	1420	0	396	0	0
5	Mj	1420	0	396	0	0
5	Mk	1420	0	396	0	0
5	Ml	1420	0	396	0	0
6	Qa	1672	0	462	0	0
6	Qb	1672	0	462	0	0
6	Qc	1672	0	462	0	0
6	Qd	1672	0	462	0	0
6	Qe	1672	0	462	0	0
6	Qf	1672	0	462	0	0
6	Qg	1672	0	462	0	0
6	Qh	1672	0	462	0	0
6	Qi	1672	0	462	0	0
6	Qj	1672	0	462	0	0
6	Qk	1672	0	462	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Ql	1672	0	462	0	0
7	Pa	620	0	155	0	0
7	Pb	620	0	155	0	0
7	Pc	620	0	155	0	0
7	Pd	620	0	155	0	0
7	Pe	620	0	155	0	0
7	Pf	620	0	155	0	0
7	Pg	620	0	155	0	0
7	Ph	620	0	155	0	0
7	Pi	620	0	155	0	0
7	Pj	620	0	155	0	0
7	Pk	620	0	155	0	0
7	Pl	620	0	155	0	0
8	Ta	652	0	177	0	0
8	Tb	652	0	177	0	0
8	Tc	652	0	177	0	0
8	Td	652	0	177	0	0
8	Te	652	0	177	0	0
8	Tf	652	0	177	0	0
8	Tg	652	0	177	0	0
8	Th	652	0	177	0	0
8	Ti	652	0	177	0	0
8	Tj	652	0	177	0	0
8	Tk	652	0	177	0	0
8	Tl	652	0	177	0	0
9	Ma	1	0	0	0	0
9	Mb	1	0	0	0	0
9	Mc	1	0	0	0	0
9	Md	1	0	0	0	0
9	Me	1	0	0	0	0
9	Mf	1	0	0	0	0
9	Mg	1	0	0	0	0
9	Mh	1	0	0	0	0
9	Mi	1	0	0	0	0
9	Mj	1	0	0	0	0
9	Mk	1	0	0	0	0
9	Ml	1	0	0	0	0
10	Ma	31	0	12	0	0
10	Mb	31	0	12	0	0
10	Mc	31	0	12	0	0
10	Md	31	0	12	0	0
10	Me	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	Mf	31	0	12	0	0
10	Mg	31	0	12	0	0
10	Mh	31	0	12	0	0
10	Mi	31	0	12	0	0
10	Mj	31	0	12	0	0
10	Mk	31	0	12	0	0
10	Ml	31	0	12	0	0
All	All	78216	0	21461	0	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 10.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Aa	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ab	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ac	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ad	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ae	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
2	Ca	308/417 (74%)	292 (95%)	9 (3%)	7 (2%)	5	5
2	Cb	308/417 (74%)	292 (95%)	10 (3%)	6 (2%)	6	6
3	Na	221/225 (98%)	182 (82%)	25 (11%)	14 (6%)	1	1
3	Nb	221/225 (98%)	181 (82%)	26 (12%)	14 (6%)	1	1
3	Nc	221/225 (98%)	181 (82%)	26 (12%)	14 (6%)	1	1
3	Nd	221/225 (98%)	182 (82%)	25 (11%)	14 (6%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Ne	221/225 (98%)	182 (82%)	25 (11%)	14 (6%)	1	1
3	Nf	221/225 (98%)	181 (82%)	26 (12%)	14 (6%)	1	1
3	Ng	221/225 (98%)	182 (82%)	25 (11%)	14 (6%)	1	1
3	Nh	221/225 (98%)	181 (82%)	26 (12%)	14 (6%)	1	1
3	Ni	221/225 (98%)	181 (82%)	26 (12%)	14 (6%)	1	1
3	Nj	221/225 (98%)	181 (82%)	26 (12%)	14 (6%)	1	1
3	Nk	221/225 (98%)	181 (82%)	26 (12%)	14 (6%)	1	1
3	Nl	221/225 (98%)	181 (82%)	26 (12%)	14 (6%)	1	1
4	Oa	187/205 (91%)	164 (88%)	14 (8%)	9 (5%)	2	2
4	Ob	187/205 (91%)	164 (88%)	13 (7%)	10 (5%)	1	1
4	Oc	187/205 (91%)	164 (88%)	13 (7%)	10 (5%)	1	1
4	Od	187/205 (91%)	164 (88%)	14 (8%)	9 (5%)	2	2
4	Oe	187/205 (91%)	164 (88%)	12 (6%)	11 (6%)	1	1
4	Of	187/205 (91%)	164 (88%)	12 (6%)	11 (6%)	1	1
4	Og	187/205 (91%)	164 (88%)	13 (7%)	10 (5%)	1	1
4	Oh	187/205 (91%)	164 (88%)	14 (8%)	9 (5%)	2	2
4	Oi	187/205 (91%)	164 (88%)	12 (6%)	11 (6%)	1	1
4	Oj	187/205 (91%)	164 (88%)	13 (7%)	10 (5%)	1	1
4	Ok	187/205 (91%)	164 (88%)	12 (6%)	11 (6%)	1	1
4	Ol	187/205 (91%)	163 (87%)	14 (8%)	10 (5%)	1	1
5	Ma	353/395 (89%)	317 (90%)	24 (7%)	12 (3%)	3	3
5	Mb	353/395 (89%)	317 (90%)	24 (7%)	12 (3%)	3	3
5	Mc	353/395 (89%)	317 (90%)	24 (7%)	12 (3%)	3	3
5	Md	353/395 (89%)	318 (90%)	23 (6%)	12 (3%)	3	3
5	Me	353/395 (89%)	317 (90%)	24 (7%)	12 (3%)	3	3
5	Mf	353/395 (89%)	317 (90%)	24 (7%)	12 (3%)	3	3
5	Mg	353/395 (89%)	318 (90%)	23 (6%)	12 (3%)	3	3
5	Mh	353/395 (89%)	317 (90%)	24 (7%)	12 (3%)	3	3
5	Mi	353/395 (89%)	316 (90%)	25 (7%)	12 (3%)	3	3
5	Mj	353/395 (89%)	316 (90%)	25 (7%)	12 (3%)	3	3
5	Mk	353/395 (89%)	317 (90%)	24 (7%)	12 (3%)	3	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Ml	353/395 (89%)	318 (90%)	23 (6%)	12 (3%)	3	3
6	Qa	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
6	Qb	408/901 (45%)	359 (88%)	36 (9%)	13 (3%)	3	3
6	Qc	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
6	Qd	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
6	Qe	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
6	Qf	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
6	Qg	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
6	Qh	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
6	Qi	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
6	Qj	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
6	Qk	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
6	Ql	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
7	Pa	153/172 (89%)	113 (74%)	19 (12%)	21 (14%)	0	0
7	Pb	153/172 (89%)	112 (73%)	22 (14%)	19 (12%)	0	0
7	Pc	153/172 (89%)	113 (74%)	20 (13%)	20 (13%)	0	0
7	Pd	153/172 (89%)	113 (74%)	19 (12%)	21 (14%)	0	0
7	Pe	153/172 (89%)	114 (74%)	21 (14%)	18 (12%)	0	0
7	Pf	153/172 (89%)	114 (74%)	19 (12%)	20 (13%)	0	0
7	Pg	153/172 (89%)	114 (74%)	18 (12%)	21 (14%)	0	0
7	Ph	153/172 (89%)	113 (74%)	20 (13%)	20 (13%)	0	0
7	Pi	153/172 (89%)	113 (74%)	20 (13%)	20 (13%)	0	0
7	Pj	153/172 (89%)	113 (74%)	19 (12%)	21 (14%)	0	0
7	Pk	153/172 (89%)	113 (74%)	20 (13%)	20 (13%)	0	0
7	Pl	153/172 (89%)	115 (75%)	18 (12%)	20 (13%)	0	0
8	Ta	159/411 (39%)	110 (69%)	34 (21%)	15 (9%)	0	0
8	Tb	159/411 (39%)	109 (69%)	36 (23%)	14 (9%)	0	0
8	Tc	159/411 (39%)	110 (69%)	35 (22%)	14 (9%)	0	0
8	Td	159/411 (39%)	109 (69%)	35 (22%)	15 (9%)	0	0
8	Te	159/411 (39%)	110 (69%)	34 (21%)	15 (9%)	0	0
8	Tf	159/411 (39%)	110 (69%)	33 (21%)	16 (10%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	Tg	159/411 (39%)	110 (69%)	34 (21%)	15 (9%)	0	0
8	Th	159/411 (39%)	109 (69%)	34 (21%)	16 (10%)	0	0
8	Ti	159/411 (39%)	110 (69%)	33 (21%)	16 (10%)	0	0
8	Tj	159/411 (39%)	109 (69%)	34 (21%)	16 (10%)	0	0
8	Tk	159/411 (39%)	109 (69%)	34 (21%)	16 (10%)	0	0
8	Tl	159/411 (39%)	110 (69%)	33 (21%)	16 (10%)	0	0
All	All	19168/29332 (65%)	16216 (85%)	1880 (10%)	1072 (6%)	2	1

5 of 1072 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

5 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	Ab	1	1	3,3,13	0.97	0	1,2,16	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MEA	Ae	1	1	3,3,13	0.98	0	1,2,16	0.34	0
1	MEA	Ad	1	1	3,3,13	1.01	0	1,2,16	0.33	0
1	MEA	Ac	1	1	3,3,13	0.99	0	1,2,16	0.32	0
1	MEA	Aa	1	1	3,3,13	0.94	0	1,2,16	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MEA	Ab	1	1	-	0/0/1/10	-
1	MEA	Ae	1	1	-	0/0/1/10	-
1	MEA	Ad	1	1	-	0/0/1/10	-
1	MEA	Ac	1	1	-	0/0/1/10	-
1	MEA	Aa	1	1	-	0/0/1/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 for Mogul analysis.

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	$\#\|Z\|>2$
10	ATP	Mj	502	9	28,33,33	0.98	1 (3%)	34,52,52	1.24	3 (8%)
10	ATP	Mb	502	9	28,33,33	0.97	1 (3%)	34,52,52	1.21	3 (8%)
10	ATP	Ma	502	9	28,33,33	1.02	1 (3%)	34,52,52	1.21	3 (8%)
10	ATP	Mh	502	9	28,33,33	0.97	1 (3%)	34,52,52	1.14	2 (5%)
10	ATP	Mf	502	9	28,33,33	0.97	1 (3%)	34,52,52	1.18	2 (5%)
10	ATP	Me	502	9	28,33,33	0.95	1 (3%)	34,52,52	1.18	2 (5%)
10	ATP	Mi	502	9	28,33,33	0.98	1 (3%)	34,52,52	1.15	2 (5%)
10	ATP	Mg	502	9	28,33,33	0.95	1 (3%)	34,52,52	1.18	3 (8%)
10	ATP	Ml	502	9	28,33,33	0.98	1 (3%)	34,52,52	1.22	3 (8%)
10	ATP	Mc	502	9	28,33,33	0.99	1 (3%)	34,52,52	1.25	3 (8%)
10	ATP	Mk	502	9	28,33,33	0.94	1 (3%)	34,52,52	1.26	3 (8%)
10	ATP	Md	502	9	28,33,33	0.94	1 (3%)	34,52,52	1.15	2 (5%)

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
10	ATP	Mj	502	9	-	3/18/38/38	0/3/3/3
10	ATP	Mb	502	9	-	4/18/38/38	0/3/3/3
10	ATP	Ma	502	9	-	4/18/38/38	0/3/3/3
10	ATP	Mh	502	9	-	1/18/38/38	0/3/3/3
10	ATP	Mf	502	9	-	1/18/38/38	0/3/3/3
10	ATP	Me	502	9	-	1/18/38/38	0/3/3/3
10	ATP	Mi	502	9	-	2/18/38/38	0/3/3/3
10	ATP	Mg	502	9	-	1/18/38/38	0/3/3/3
10	ATP	Ml	502	9	-	4/18/38/38	0/3/3/3
10	ATP	Mc	502	9	-	2/18/38/38	0/3/3/3
10	ATP	Mk	502	9	-	4/18/38/38	0/3/3/3
10	ATP	Md	502	9	-	1/18/38/38	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Ma	502	ATP	PB-O3B	3.21	1.63	1.59
10	Ml	502	ATP	PB-O3B	3.09	1.62	1.59
10	Mf	502	ATP	PB-O3B	3.06	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Me	502	ATP	PB-O3B	2.90	1.62	1.59
10	Mi	502	ATP	PB-O3B	2.89	1.62	1.59

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	Mg	502	ATP	N3-C2-N1	-3.95	123.31	128.67
10	Mc	502	ATP	N3-C2-N1	-3.86	123.44	128.67
10	Me	502	ATP	N3-C2-N1	-3.85	123.44	128.67
10	Mf	502	ATP	N3-C2-N1	-3.85	123.44	128.67
10	Mk	502	ATP	N3-C2-N1	-3.77	123.55	128.67

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

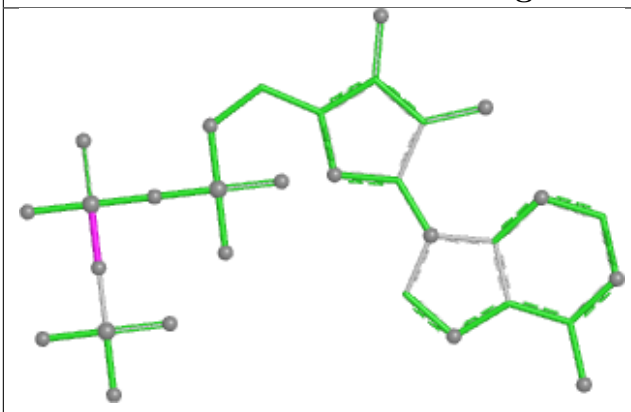
Mol	Chain	Res	Type	Atoms
10	Ma	502	ATP	PB-O3B-PG-O3G
10	Mb	502	ATP	PB-O3B-PG-O3G
10	Mi	502	ATP	PB-O3B-PG-O3G
10	Mj	502	ATP	PB-O3B-PG-O3G
10	Mk	502	ATP	PB-O3B-PG-O3G

There are no ring outliers.

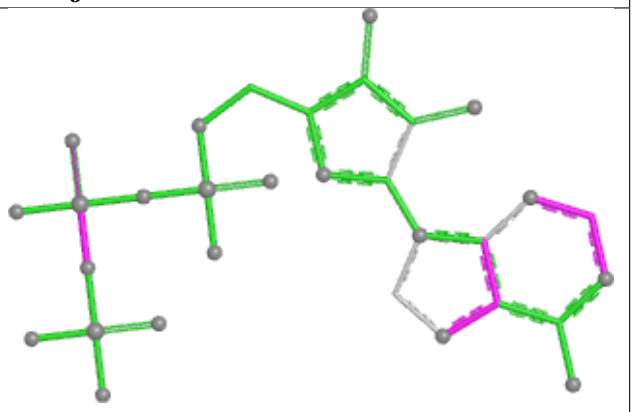
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

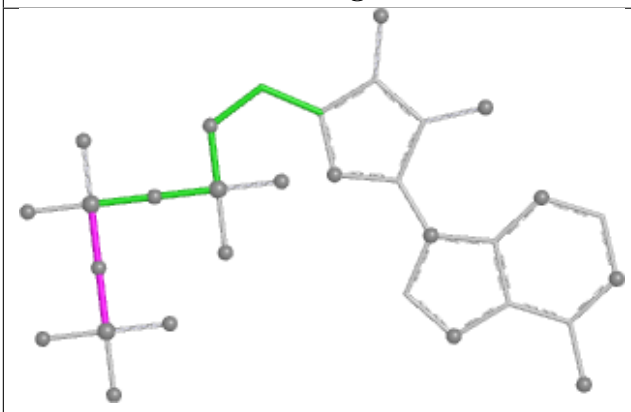
Ligand ATP Mj 502



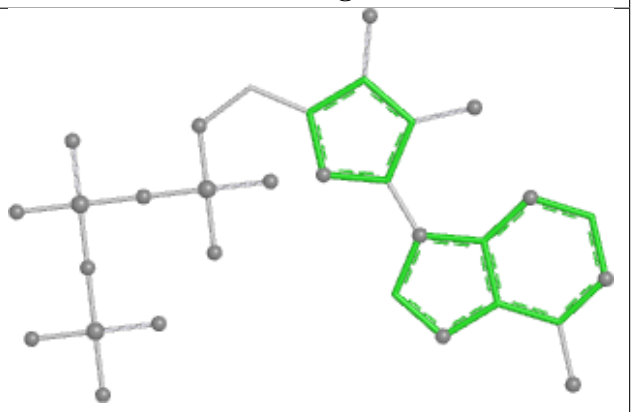
Bond lengths



Bond angles

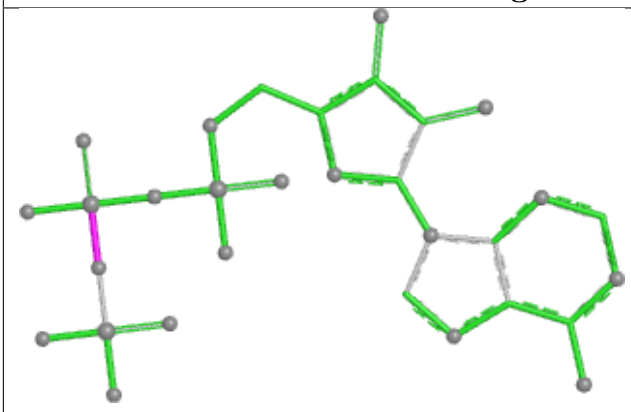


Torsions



Rings

Ligand ATP Mb 502



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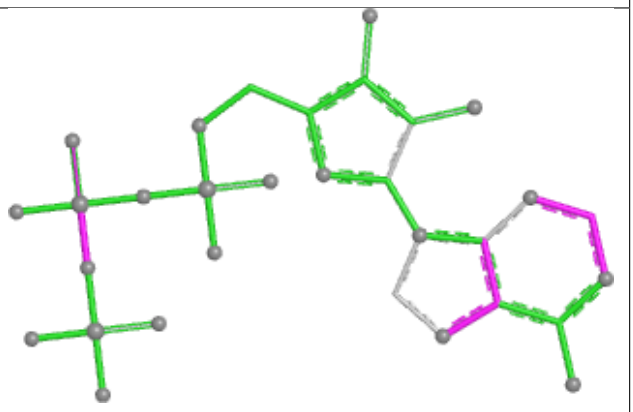

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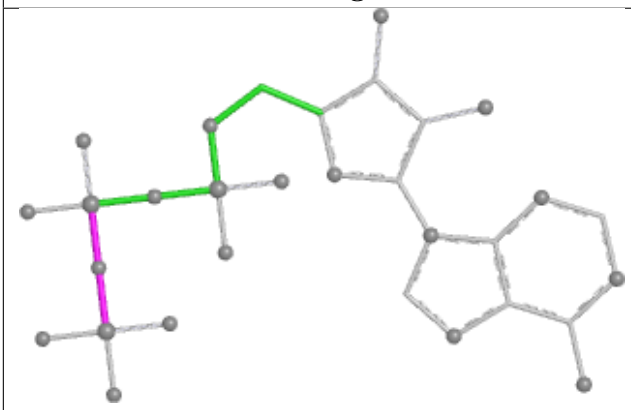

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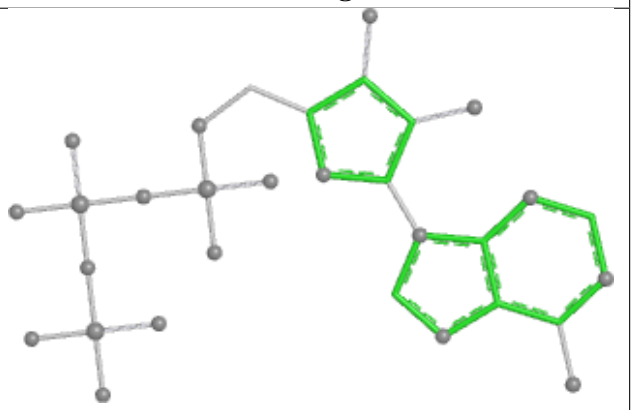
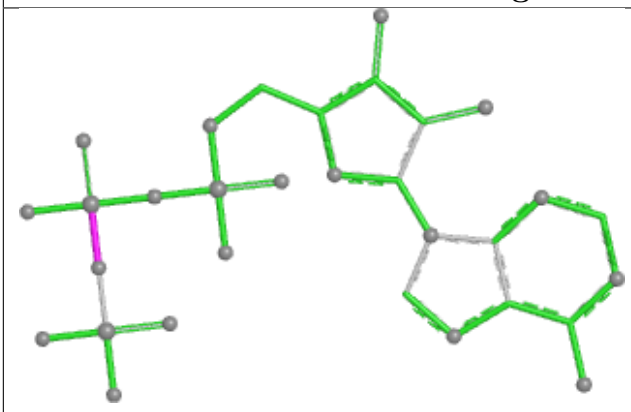


Rings

Ligand ATP Ma 502



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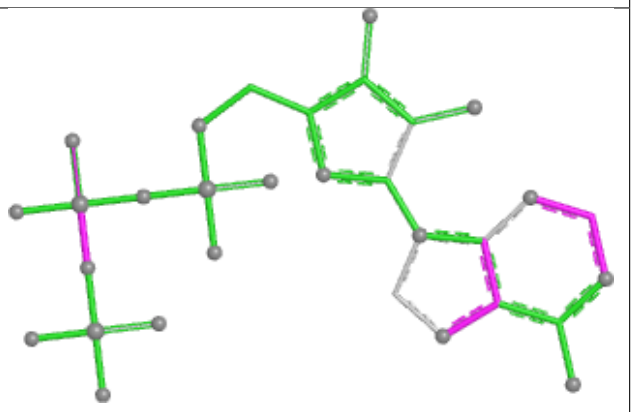
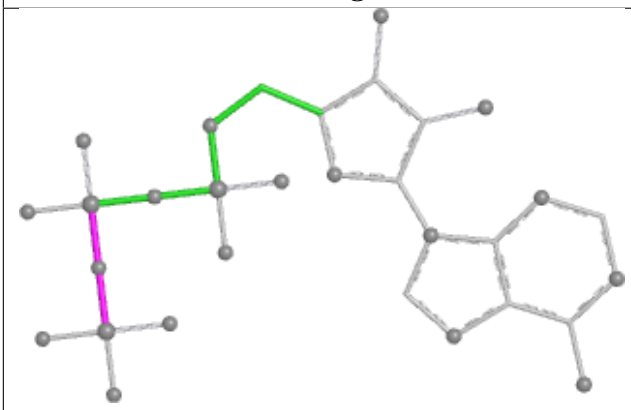
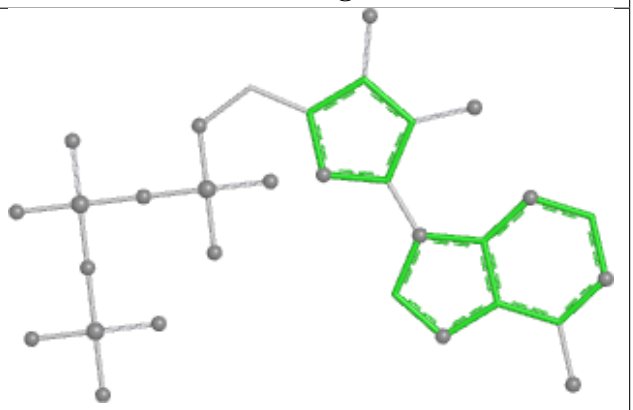


Bond angles

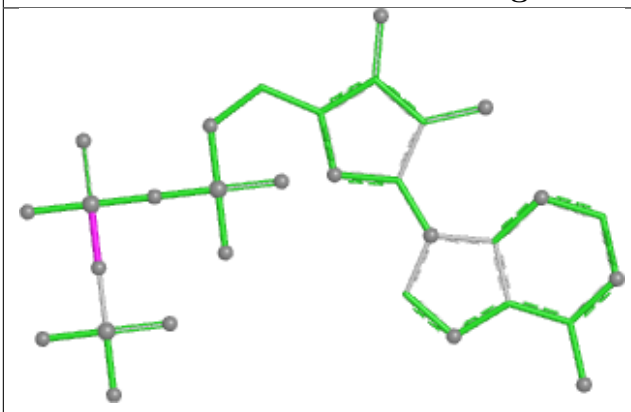


Torsions

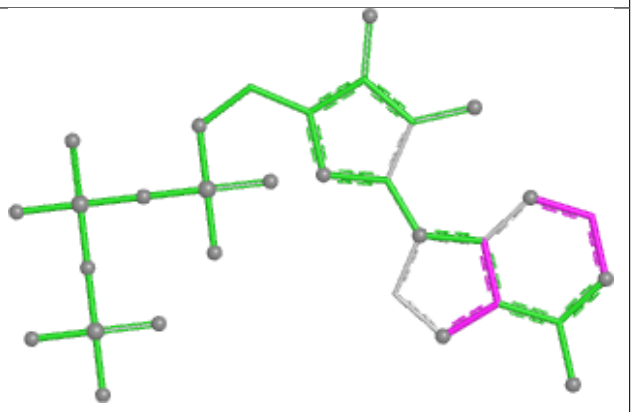


Rings

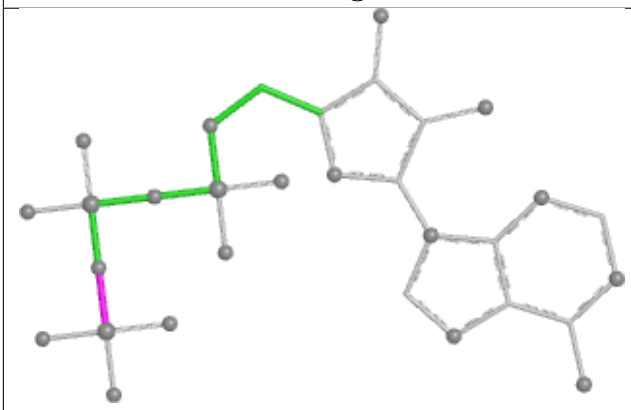
Ligand ATP Mh 502



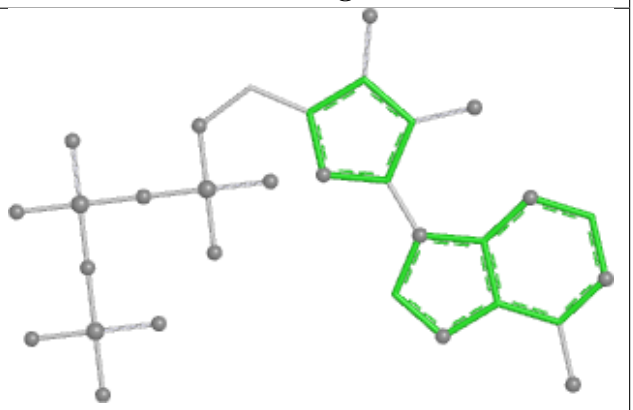
Bond lengths



Bond angles

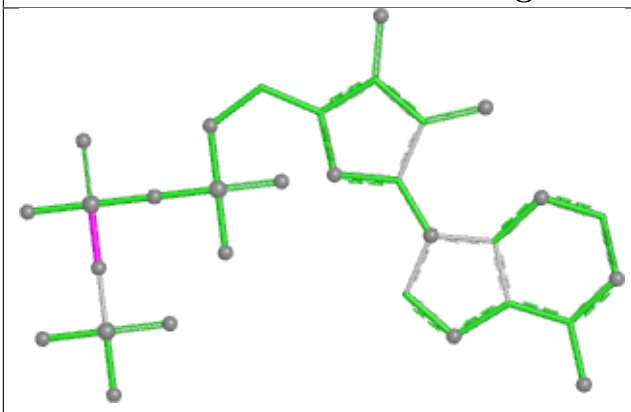


Torsions

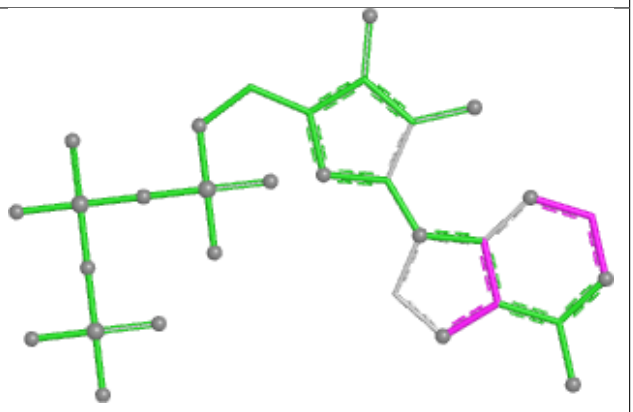


Rings

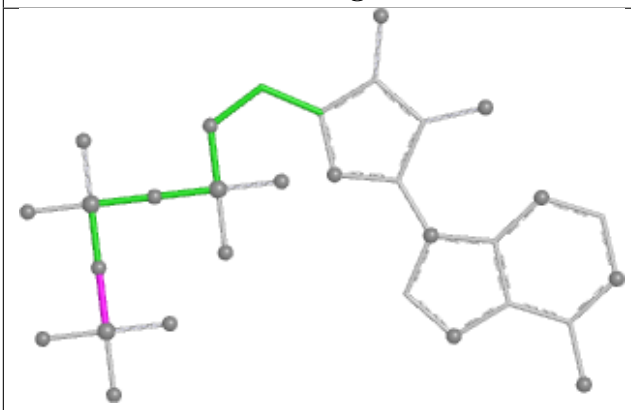
Ligand ATP Mf 502



Bond lengths



Bond angles



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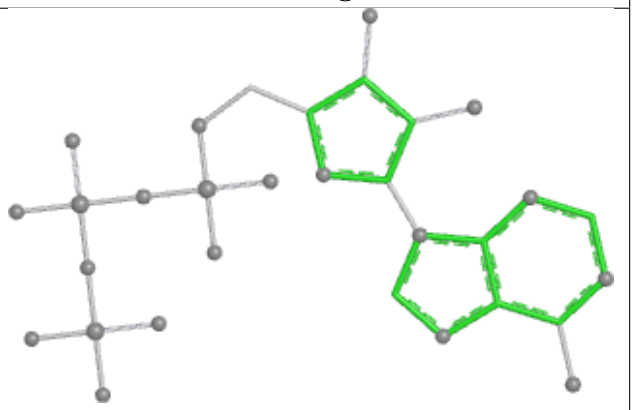
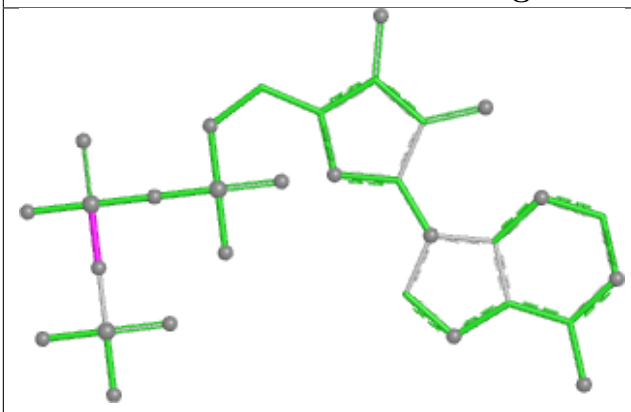


Rings

Ligand ATP Me 502



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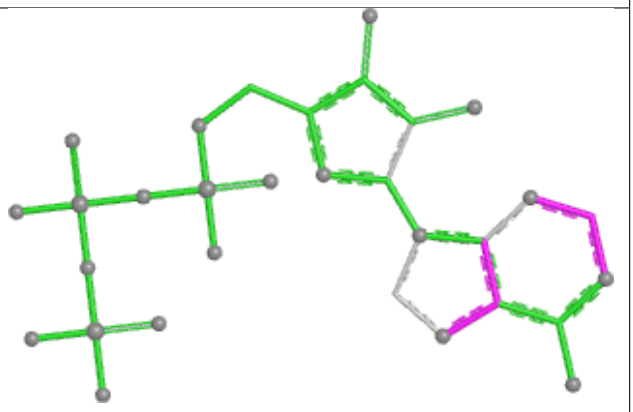

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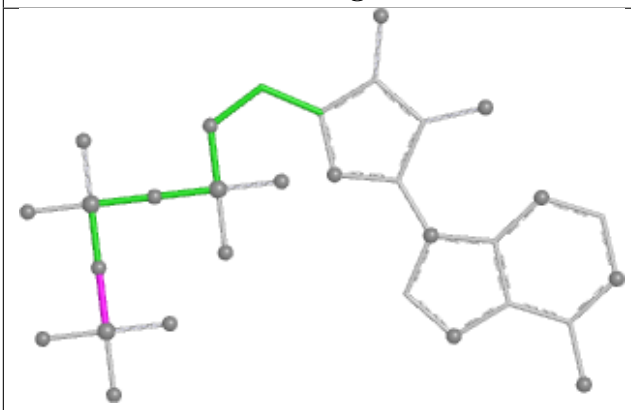
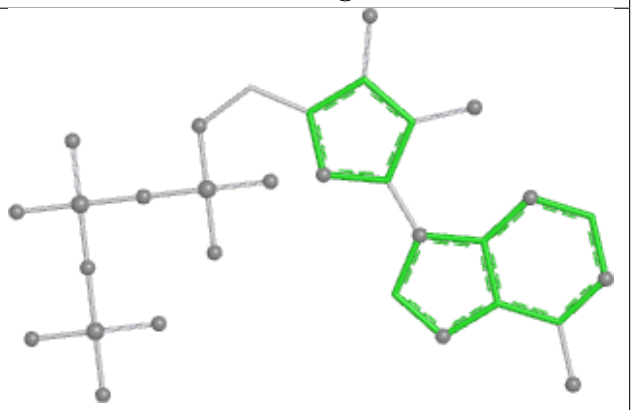
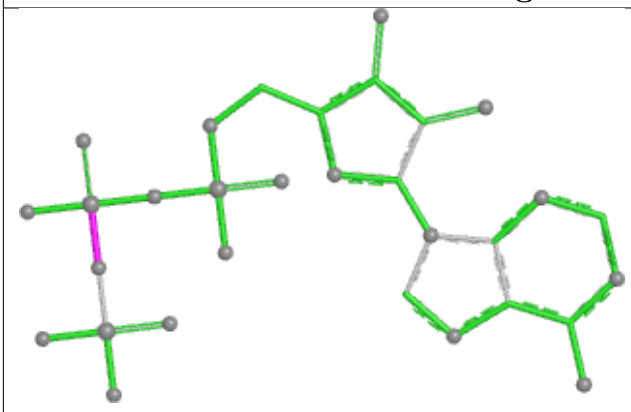


Torsions

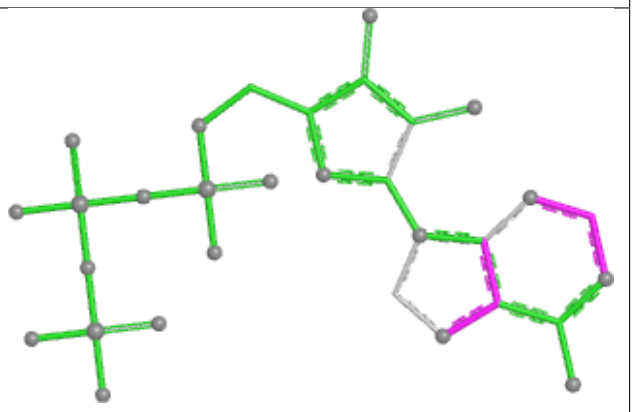


Rings

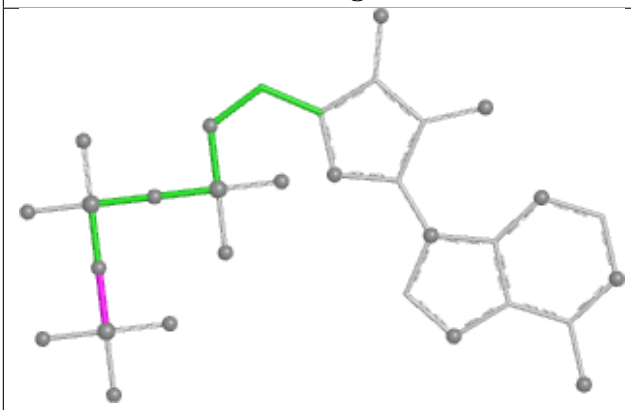
Ligand ATP Mi 502



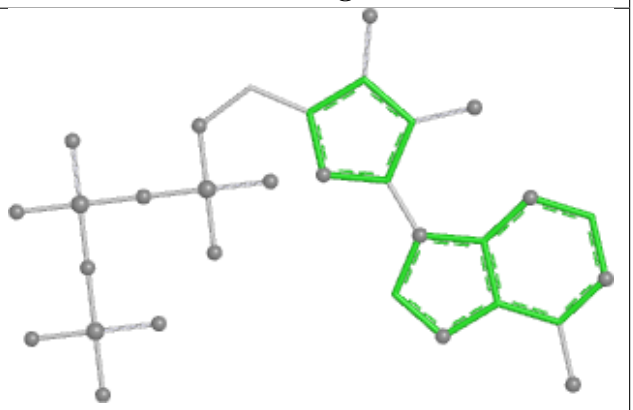
Bond lengths



Bond angles

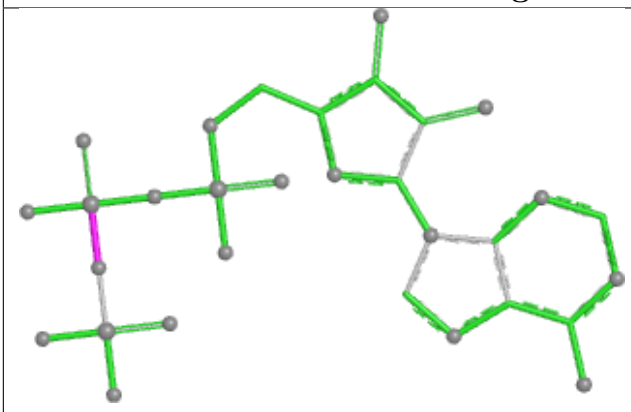


Torsions

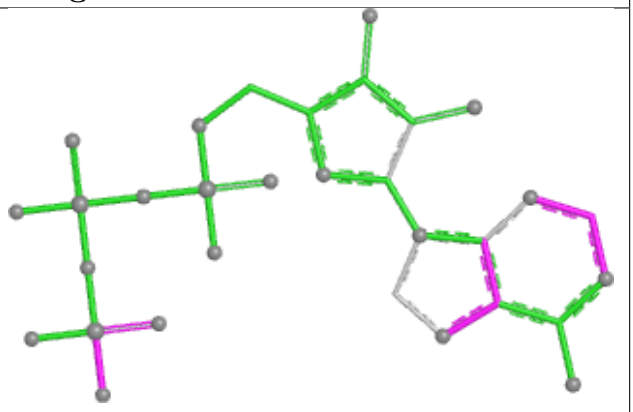


Rings

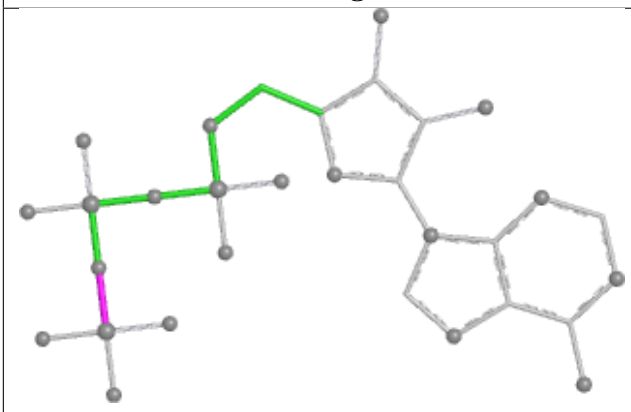
Ligand ATP Mg 502



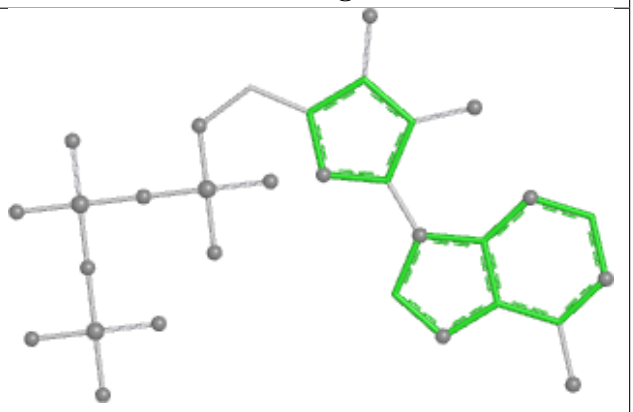
Bond lengths



Bond angles

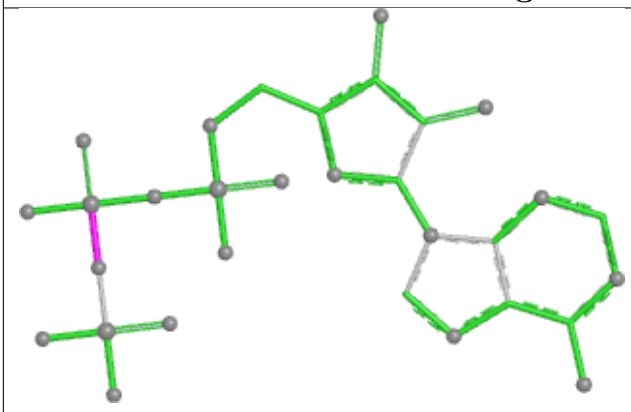


Torsions

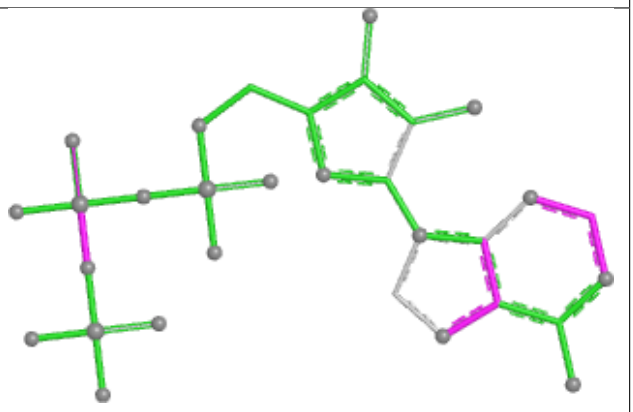


Rings

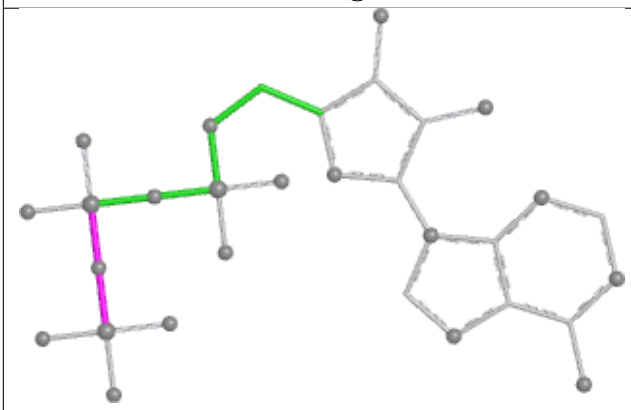
Ligand ATP Ml 502



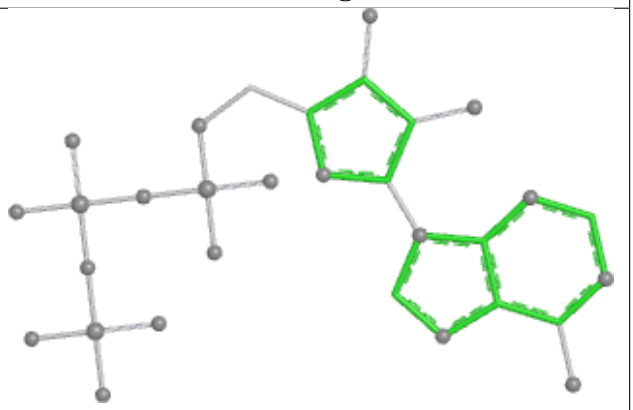
Bond lengths



Bond angles

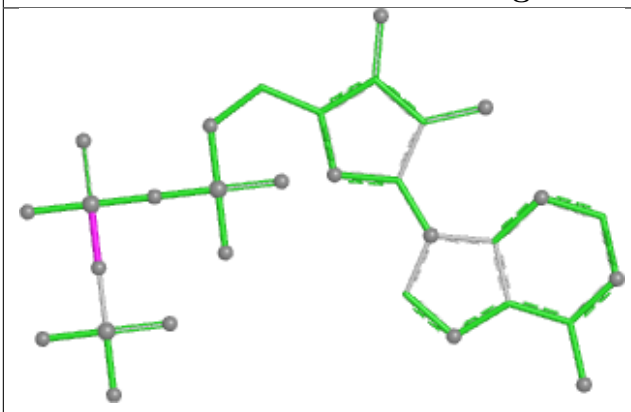


Torsions

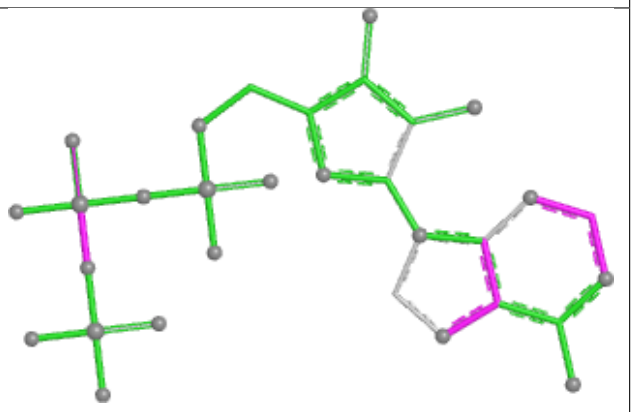


Rings

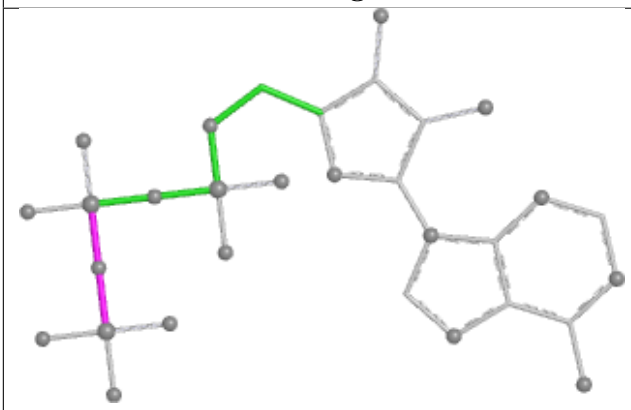
Ligand ATP Mc 502



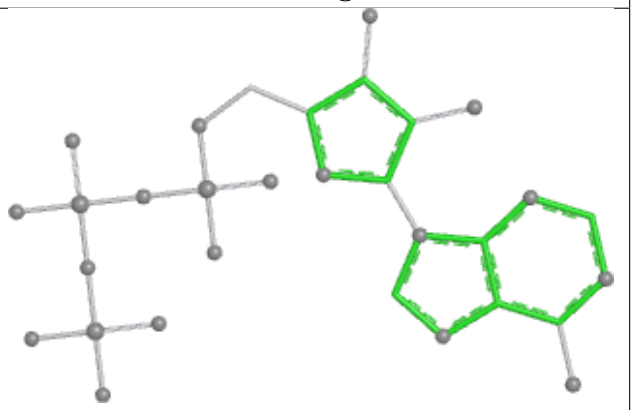
Bond lengths



Bond angles

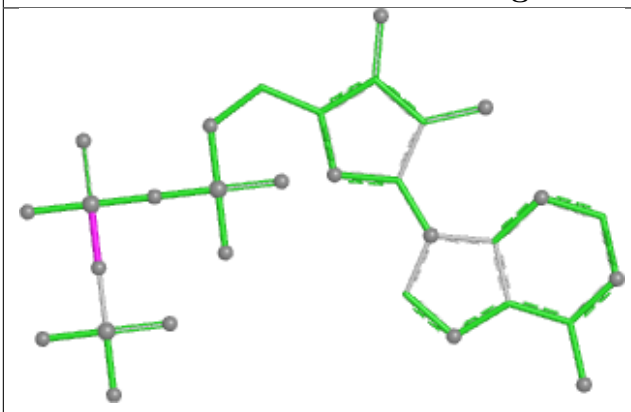


Torsions

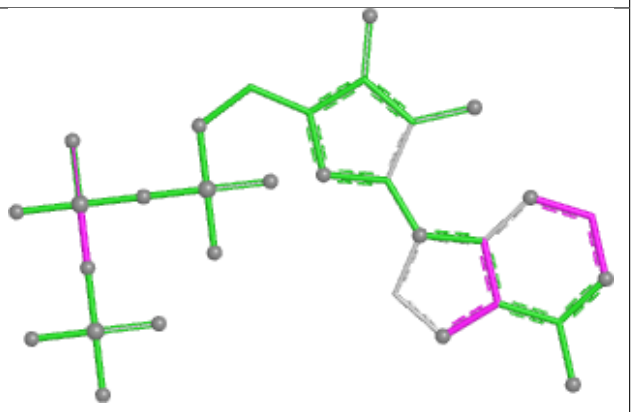


Rings

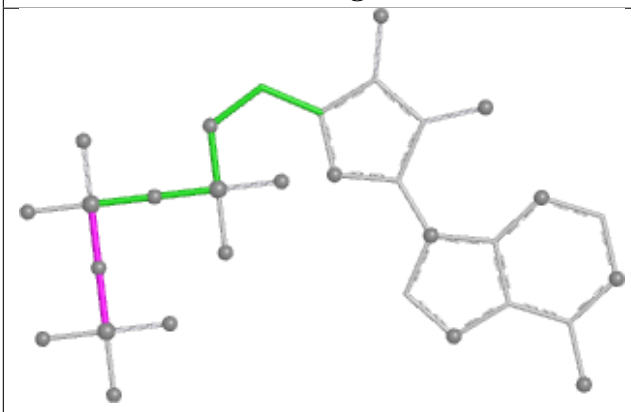
Ligand ATP Mk 502



Bond lengths



Bond angles



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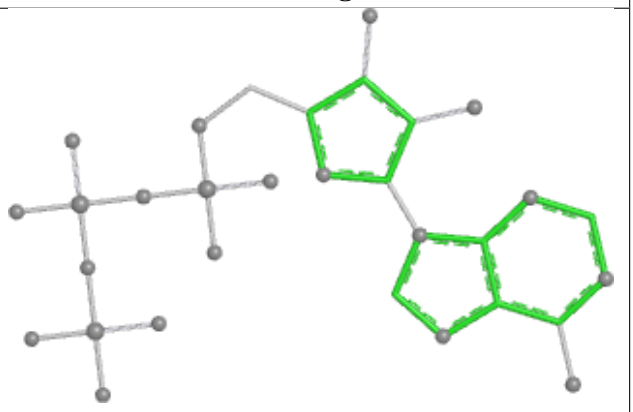
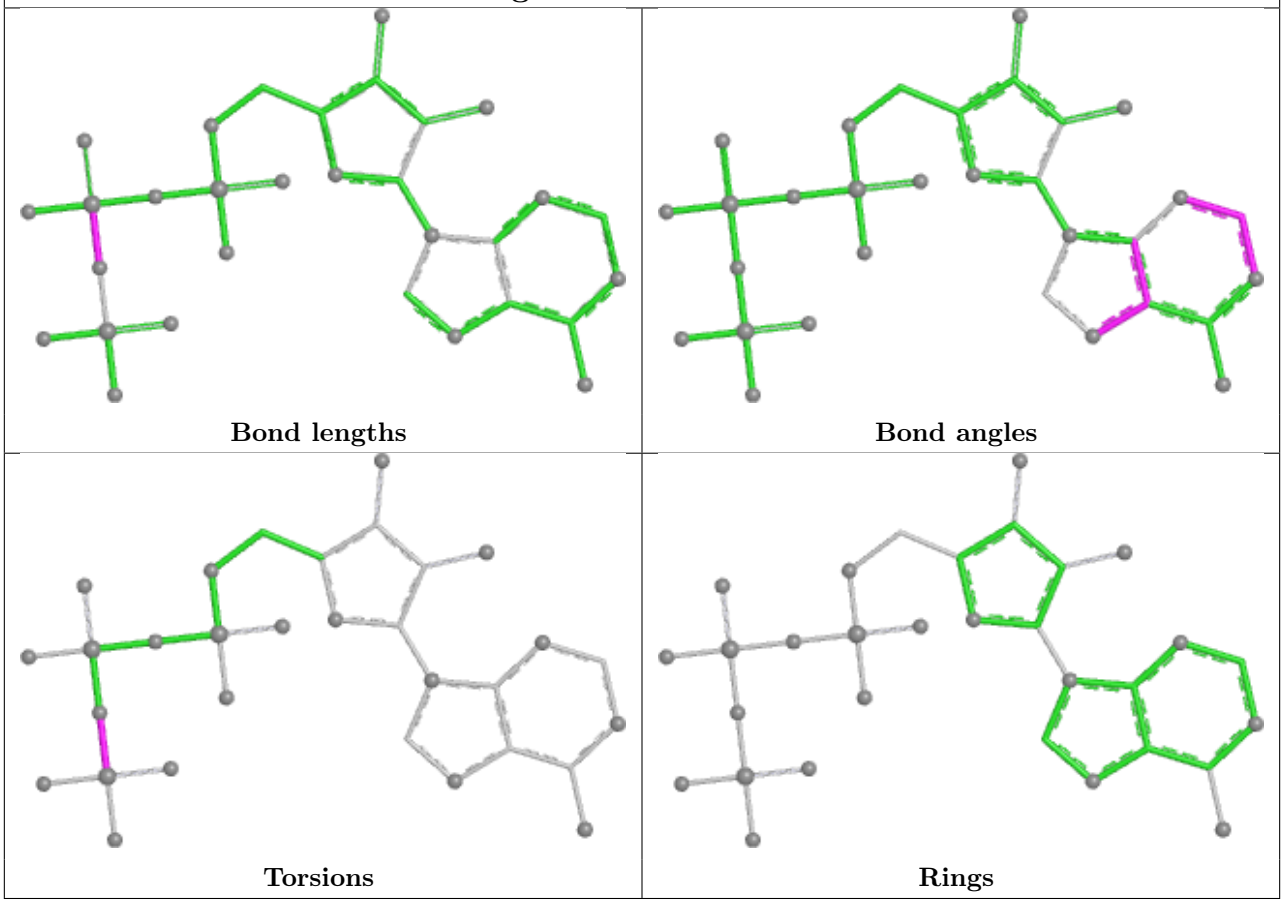


Rings

Ligand ATP Md 502



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Tomogram visualisation

This section contains visualisations of the EMDB entry EMD-3260. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Mask visualisation

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

7 Tomogram analysis (i)

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

7.1 Map-value distribution (i)

This section was not generated.

8 Map-model fit

This section was not generated.