



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 01:12 AM UTC

PDB ID : 3JC9 / pdb_00003jc9
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

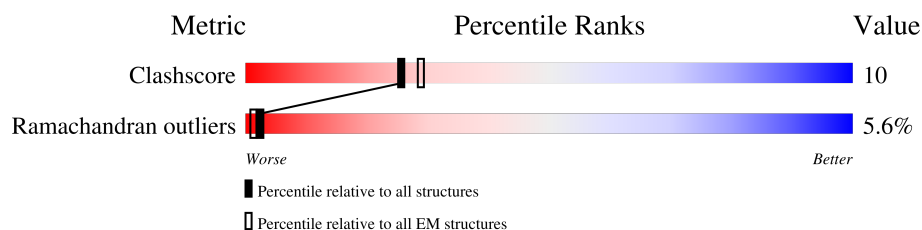
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	Aa	158	 82% 14% .
1	Ab	158	 86% 10% .
1	Ac	158	 85% 11% .
1	Ad	158	 86% 10% .
1	Ae	158	 85% 11% .
2	Ca	417	 68% 6% . 24%
2	Cb	417	 68% 6% . 24%
3	Na	225	 84% 11% ..
3	Nb	225	 84% 12% ..
3	Nc	225	 84% 12% ..

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Mol	Chain	Length	Quality of chain
3	Nd	225	 84% 12% ..
3	Ne	225	 83% 13% ..
3	Nf	225	 84% 11% ..
3	Ng	225	 85% 11% ..
3	Nh	225	 84% 11% ..
3	Ni	225	 84% 11% ..
3	Nj	225	 84% 12% ..
3	Nk	225	 84% 11% ..
3	Nl	225	 84% 12% ..
4	Oa	205	 80% 8% .. 8%
4	Ob	205	 80% 8% . 8%
4	Oc	205	 80% 8% .. 8%
4	Od	205	 80% 8% . 8%
4	Oe	205	 80% 8% . 8%
4	Of	205	 80% 9% .. 8%
4	Og	205	 80% 8% .. 8%
4	Oh	205	 81% 7% .. 8%
4	Oi	205	 78% 10% . 8%
4	Oj	205	 79% 9% .. 8%
4	Ok	205	 80% 8% . 8%
4	Ol	205	 80% 9% . 8%
5	Ma	395	 81% 8% . 10%
5	Mb	395	 81% 8% . 10%
5	Mc	395	 81% 8% . 10%
5	Md	395	 82% 8% . 10%

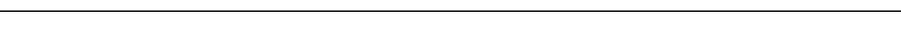
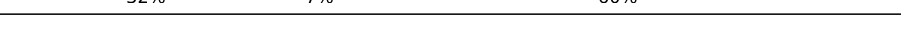
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Mol	Chain	Length	Quality of chain
5	Me	395	 81% 8% • 10%
5	Mf	395	 81% 8% • 10%
5	Mg	395	 81% 8% • 10%
5	Mh	395	 82% 8% • 10%
5	Mi	395	 81% 8% • 10%
5	Mj	395	 81% 8% • 10%
5	Mk	395	 81% 9% • 10%
5	Ml	395	 81% 8% • 10%
6	Qa	901	 40% 5% • 54%
6	Qb	901	 40% 5% • 54%
6	Qc	901	 40% 5% • 54%
6	Qd	901	 40% 5% • 54%
6	Qe	901	 40% 5% • 54%
6	Qf	901	 40% 5% • 54%
6	Qg	901	 40% 5% • 54%
6	Qh	901	 40% 5% • 54%
6	Qi	901	 40% 5% • 54%
6	Qj	901	 40% 5% • 54%
6	Qk	901	 40% 5% • 54%
6	Ql	901	 40% 5% • 54%
7	Pa	172	 67% 15% 6% • 10%
7	Pb	172	 67% 16% 5% • 10%
7	Pc	172	 67% 17% • • 10%
7	Pd	172	 67% 16% 5% • 10%
7	Pe	172	 67% 16% 5% • 10%

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Mol	Chain	Length	Quality of chain
7	Pf	172	
7	Pg	172	
7	Ph	172	
7	Pi	172	
7	Pj	172	
7	Pk	172	
7	Pl	172	
8	Ta	411	
8	Tb	411	
8	Tc	411	
8	Td	411	
8	Te	411	
8	Tf	411	
8	Tg	411	
8	Th	411	
8	Ti	411	
8	Tj	411	
8	Tk	411	
8	Tl	411	

2 Entry composition

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	C	N	O	0	0
			632	316	158	158		
1	Ab	158	Total	C	N	O	0	0
			632	316	158	158		
1	Ac	158	Total	C	N	O	0	0
			632	316	158	158		
1	Ad	158	Total	C	N	O	0	0
			632	316	158	158		
1	Ae	158	Total	C	N	O	0	0
			632	316	158	158		

- Molecule 2 is a protein called PilC.

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

- Molecule 3 is a protein called PilN.

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

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

- Molecule 4 is a protein called PilO.

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

- 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	MI	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	C	N	O	0	0
			1672	836	418	418		
6	Qj	418	Total	C	N	O	0	0
			1672	836	418	418		
6	Qk	418	Total	C	N	O	0	0
			1672	836	418	418		
6	Ql	418	Total	C	N	O	0	0
			1672	836	418	418		

- Molecule 7 is a protein called PilP.

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

- Molecule 8 is a protein called TsaP.

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

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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 (CCD ID: MG) (formula: Mg).

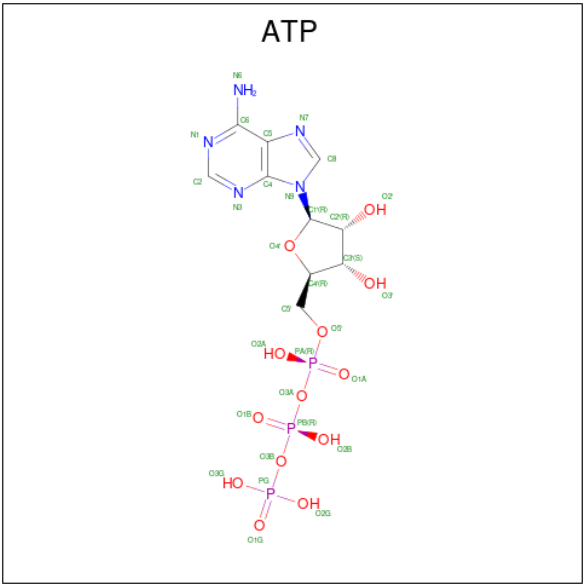
Mol	Chain	Residues	Atoms		AltConf
9	Ma	1	Total 1	Mg 1	0
9	Mb	1	Total 1	Mg 1	0
9	Mc	1	Total 1	Mg 1	0
9	Md	1	Total 1	Mg 1	0
9	Me	1	Total 1	Mg 1	0
9	Mf	1	Total 1	Mg 1	0
9	Mg	1	Total 1	Mg 1	0
9	Mh	1	Total 1	Mg 1	0

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

- Molecule 10 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

3 Residue-property plots [i](#)

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

• Molecule 1: PilA

Chain Aa:  82% 14% .



• Molecule 1: PilA

Chain Ab:  86% 10% .



• Molecule 1: PilA

Chain Ac:  85% 11% .



• Molecule 1: PilA

Chain Ad:  86% 10% .



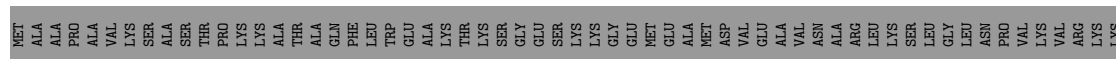
• Molecule 1: PilA

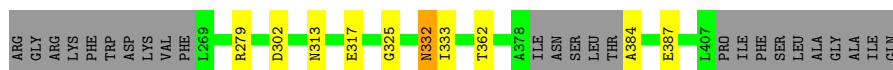
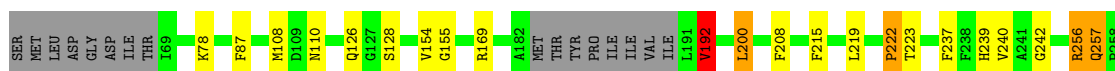
Chain Ae:  85% 11% .



• Molecule 2: PilC

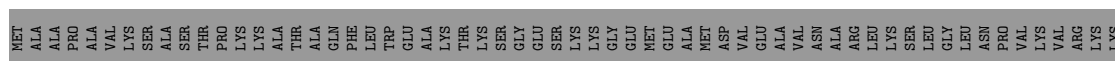
Chain Ca:  68% 6% 24% .





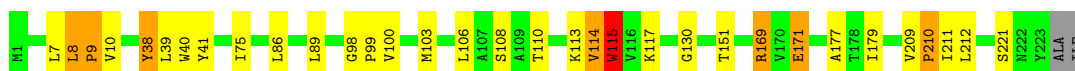
• Molecule 2: PiIC

Chain Cb: 68% 6% 24%



• Molecule 3: PiIN

Chain Na: 84% 11% 5%



• Molecule 3: PiIN

Chain Nb: 84% 12% 4%



• Molecule 3: PiIN

Chain Nc: 84% 12% 4%



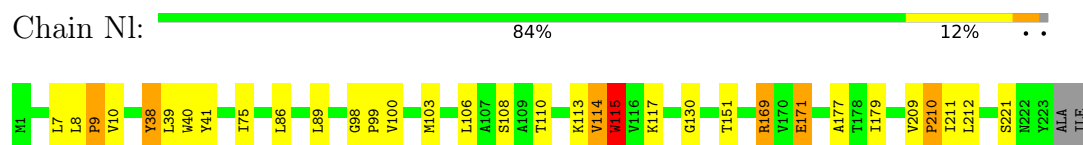
• Molecule 3: PiIN

Chain Nd: 84% 12% 4%

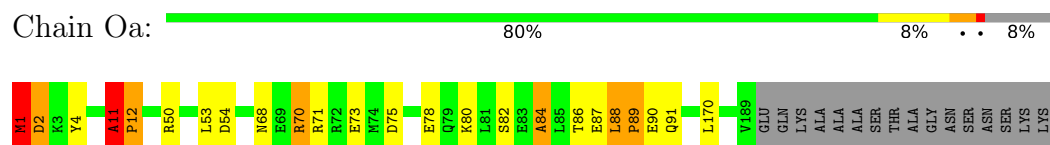


M1		L7	L8	P9	V10		X38	L39	W40	Y41		I75	L86		L89	G98	P99	V100		M103		L106	A107	S108	A109	T110	K113	V114	V115	W116	K117		G130		T151		R169	V170	E171		T178	A179	I179		V209	P210	T211	L212		S221	N222	V223	ALE	ALA	I1E
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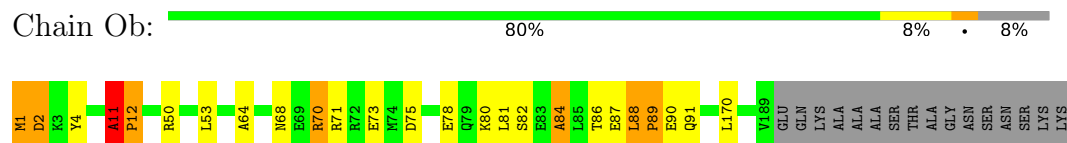
- Molecule 3: PiLN



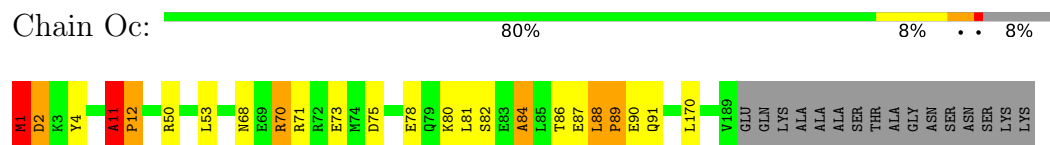
- Molecule 4: PiLO



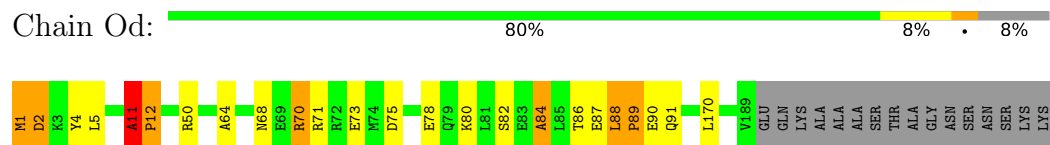
- Molecule 4: PiLO



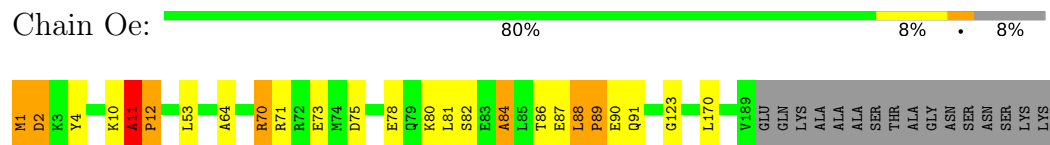
- Molecule 4: PiLO



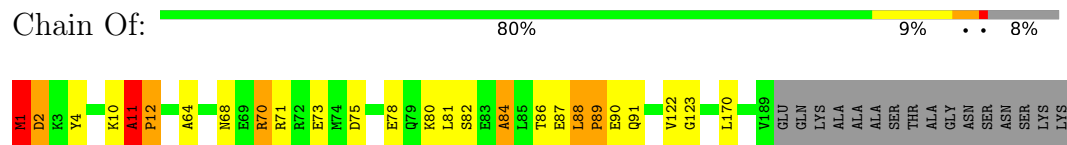
- Molecule 4: PiLO



- Molecule 4: PiLO



- Molecule 4: PiLO



- Molecule 4: PiLO

Chain Og:  80% 8% 8%



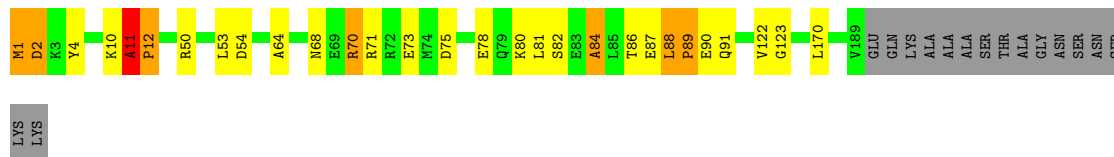
• Molecule 4: PiLO

Chain Oh:  81% 7% 8%



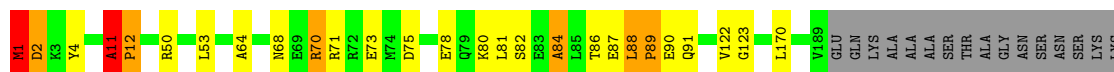
• Molecule 4: PiLO

Chain Oi:  78% 10% 8%



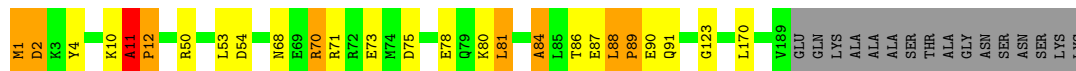
• Molecule 4: PiLO

Chain Oj:  79% 9% 8%



• Molecule 4: PiLO

Chain Ok:  80% 8% 8%



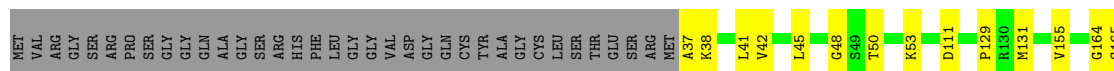
• Molecule 4: PiLO

Chain Ol:  80% 9% 8%



• Molecule 5: PiLM

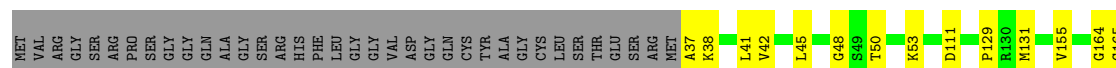
Chain Ma:  81% 8% 10%





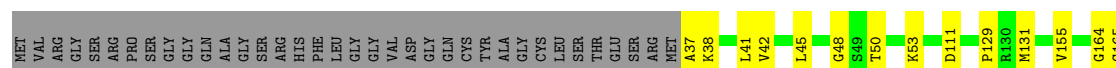
- Molecule 5: PiIM

Chain Mb: 81% 8% 10%



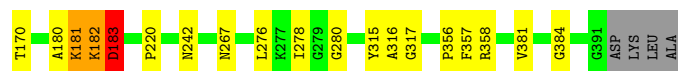
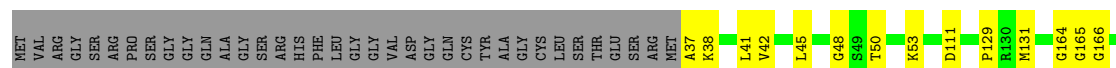
- Molecule 5: PiIM

Chain Mc: 81% 8% 10%



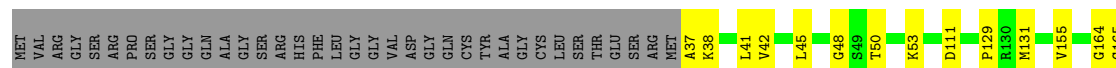
- Molecule 5: PiIM

Chain Md: 82% 8% 10%



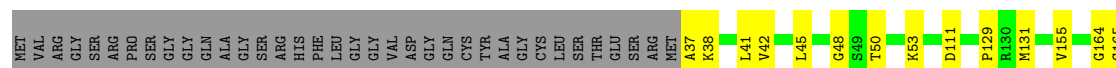
- Molecule 5: PiIM

Chain Me: 81% 8% 10%



- Molecule 5: PiIM

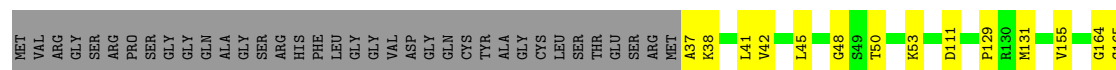
Chain Mf: 81% 8% 10%





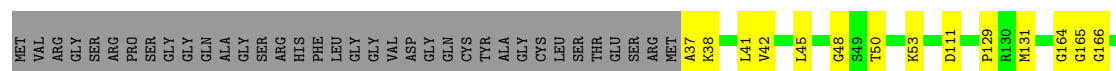
- Molecule 5: PiIM

Chain Mg: 81% 8% 10%



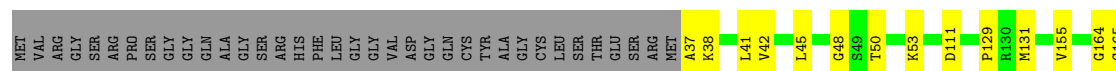
- Molecule 5: PiIM

Chain Mh: 82% 8% 10%



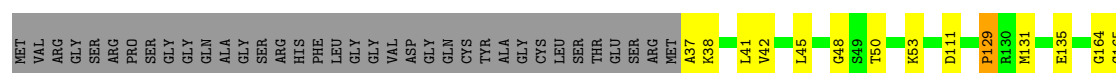
- Molecule 5: PiIM

Chain Mi: 81% 8% 10%



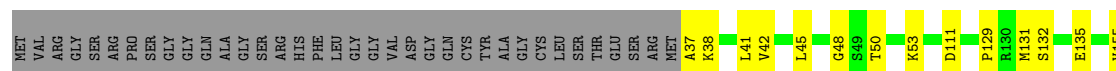
- Molecule 5: PiIM

Chain Mj: 81% 8% 10%

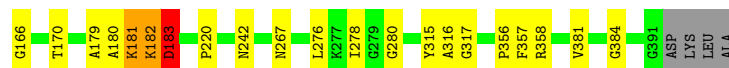
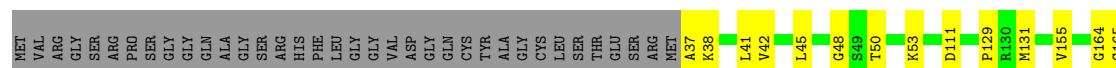
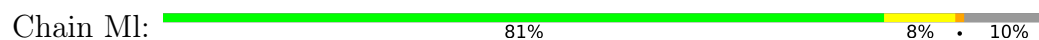


- Molecule 5: PiIM

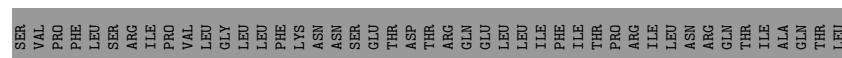
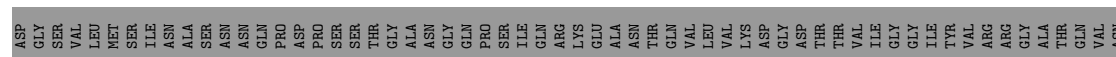
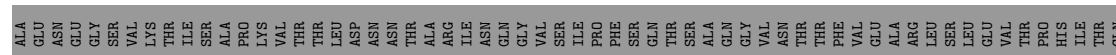
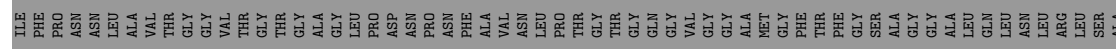
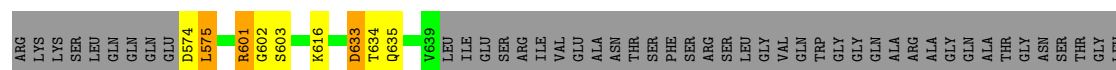
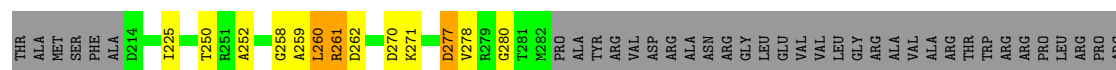
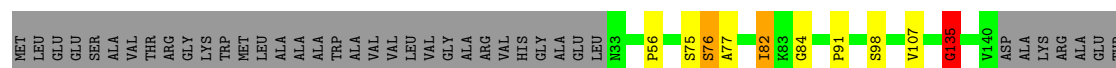
Chain Mk: 81% 9% 10%



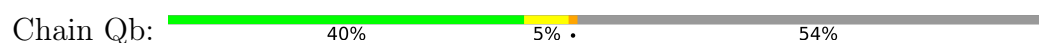
- Molecule 5: PiM

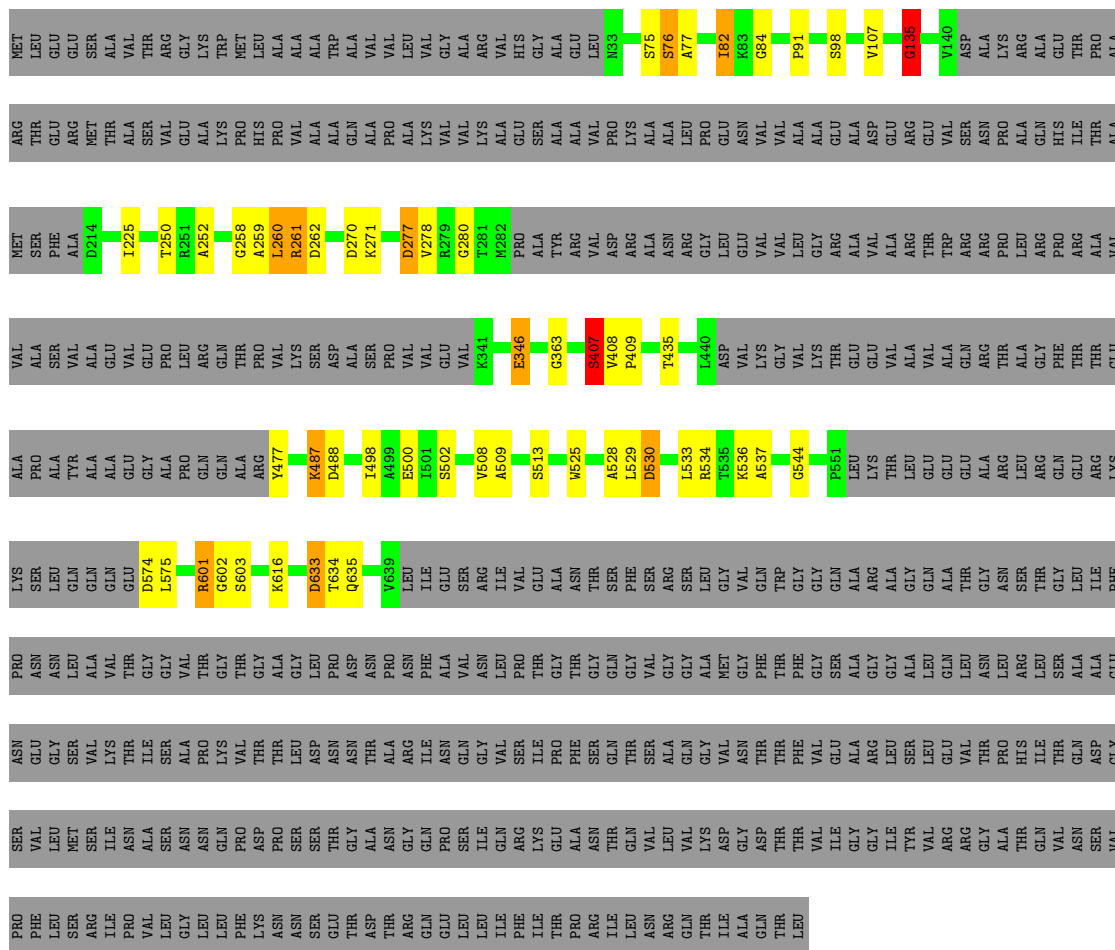


- Molecule 6: PilQ

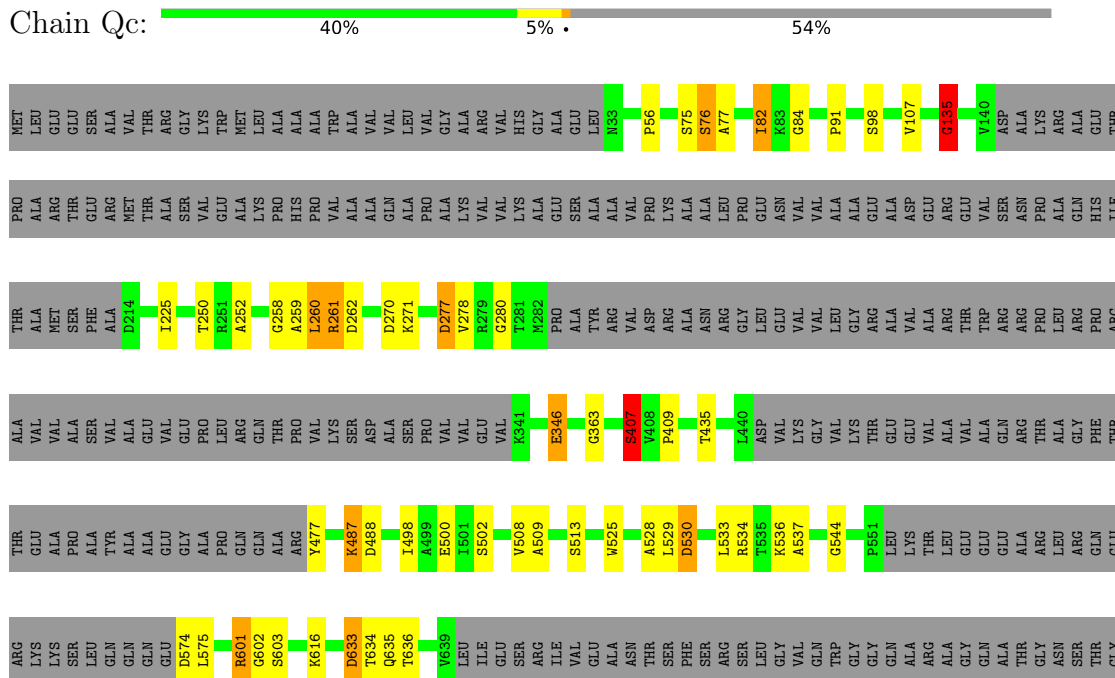


- Molecule 6: PilQ



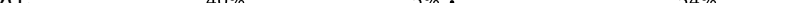


- Molecule 6: PilQ



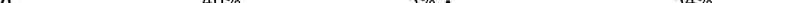
[illegible]

- Molecule 6: PilQ

Chain Qd: 

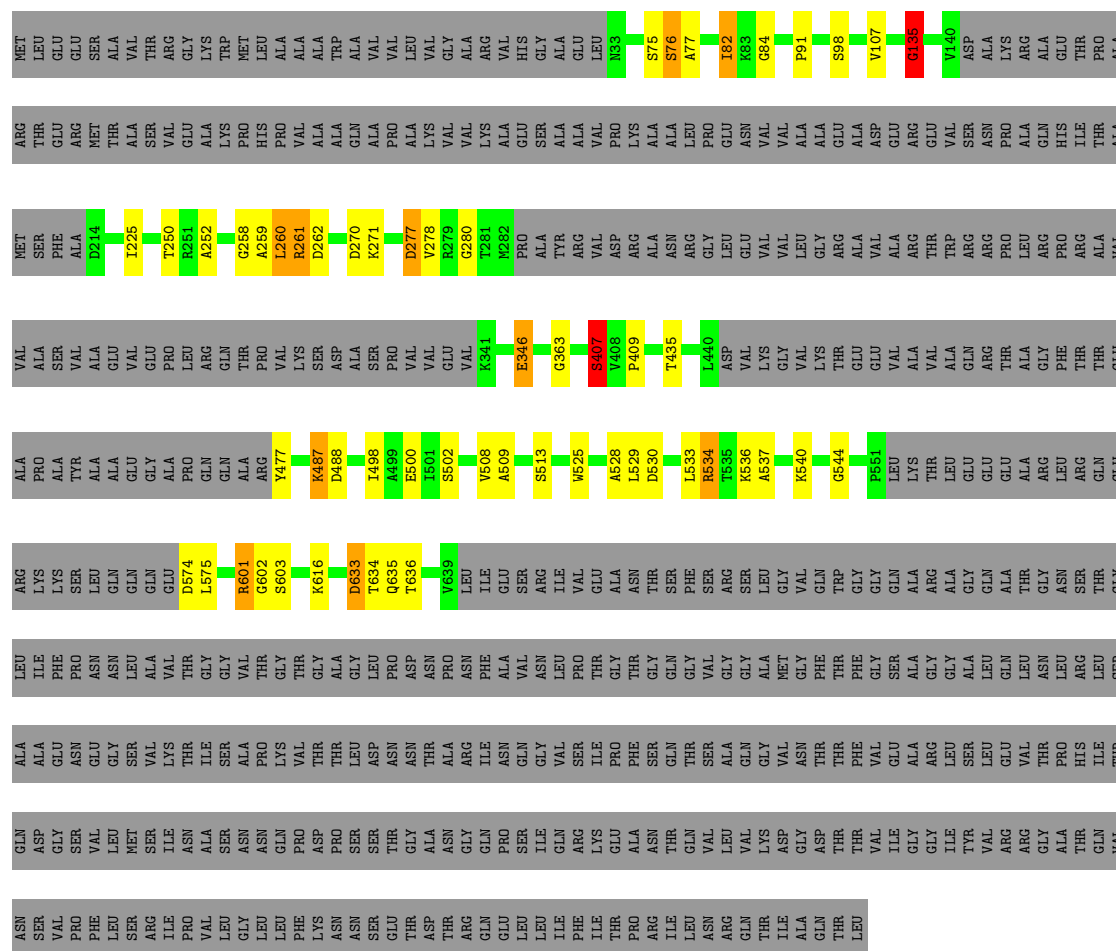
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- Molecule 6: PilQ

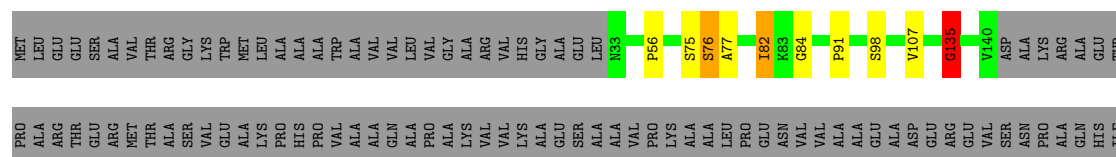
Chain Qe: 

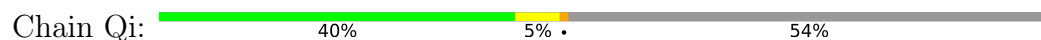
MET	LEU	GLU	GLU	GLU	SER	ALA	ALA	VAL	THR	ARG	GLY	LYS	TRP	MET	LEU	ALA	ALA	ALA	ALA	TRP	VAL	ALA	VAL	VAL	VAL	VAL	GLY	ALA	ALA	GLU	LEU	GLU	N33	S75	S76	A17	T82	K83	G84	P91	S98	V107	G135	V140	ASP	ALA	LYS	ARG	ALA	ALA	GLU	THR	PRO
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- Molecule 6: PilQ



- Molecule 6: PilQ





- Molecule 6: PilQ

Chain Qj:

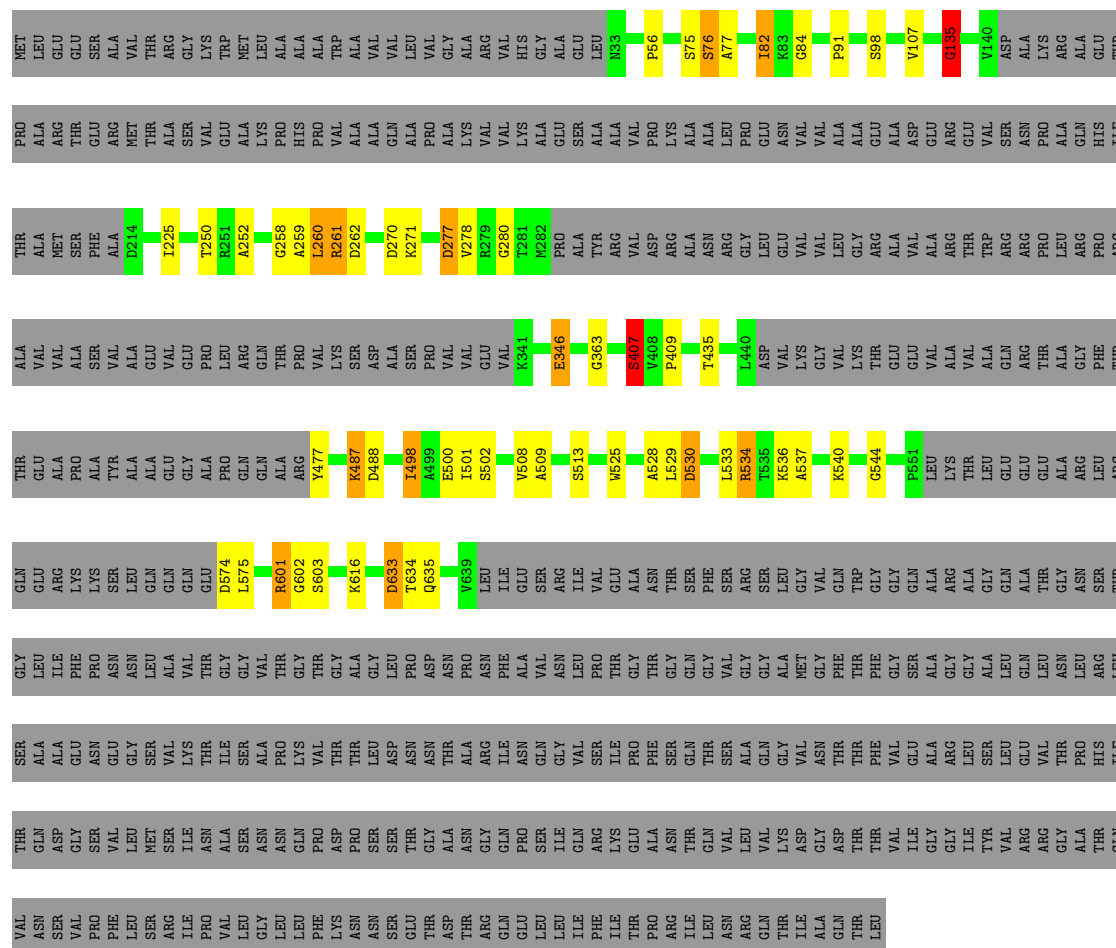
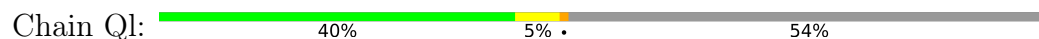


SER	VAL	PRO	PHE	LEU	SER	ARG	ILE	PRO	VAL	LEU	GLY	LEU	LEU	PHE	LYS	ASN	ASN	SER	GLU	THR	ASP	THR	ARG	ARG	GLN	GLU	LEU	LEU	ILE	PHE	ILE	THR	PRO	ARG	ILE	ILE	LEU	ASN	ARG	GLN	THR	THR	ILE	ALA	GLN	THR	LEU
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- Molecule 6: PilQ

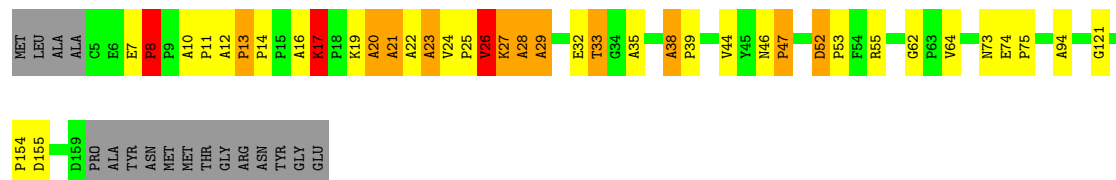
Chain Q_k :

- Molecule 6: PilQ



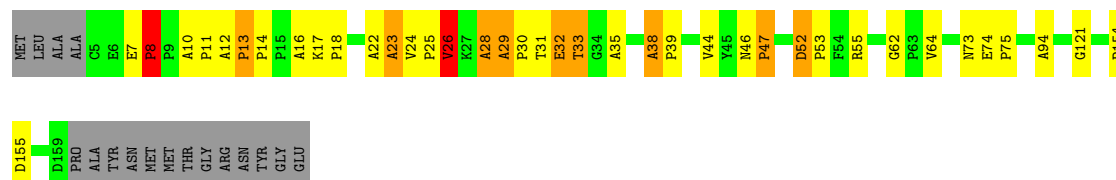
- Molecule 7: PilP

Chain Pa: 



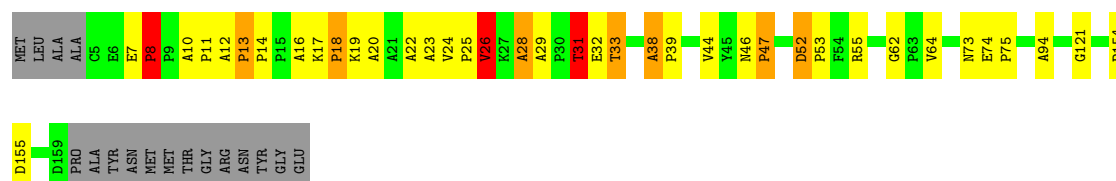
- Molecule 7: PilP

Chain Pb: 



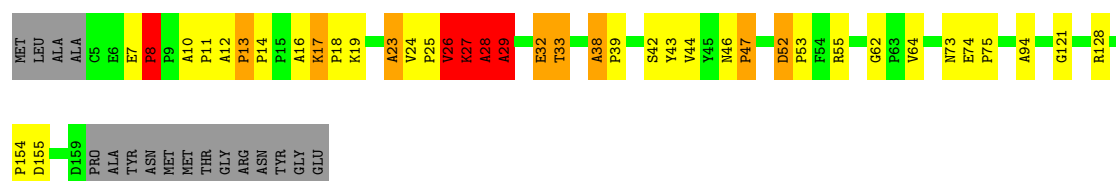
- Molecule 7: PilP

Chain Pc: 



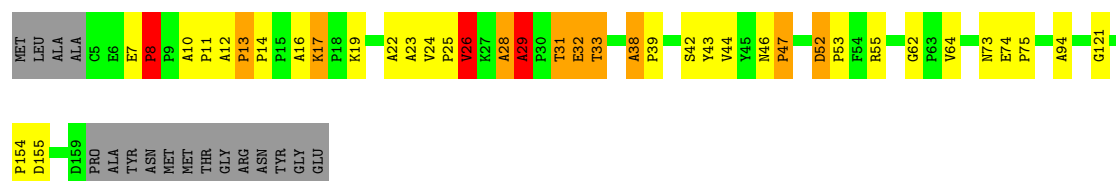
- Molecule 7: PilP

Chain Pd: 



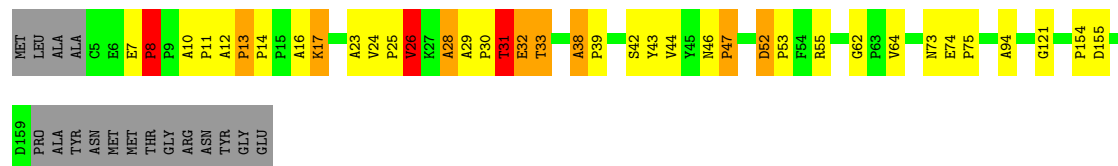
- Molecule 7: PilP

Chain Pe: 



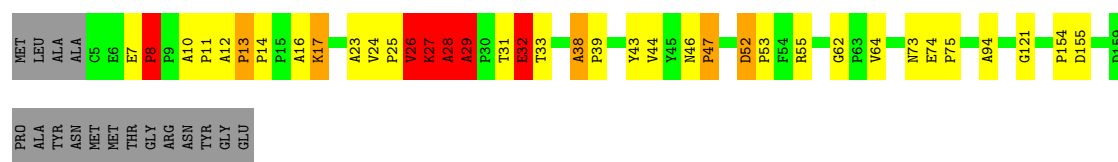
- Molecule 7: PilP

Chain Pf:  68% 16% 5% • 10%



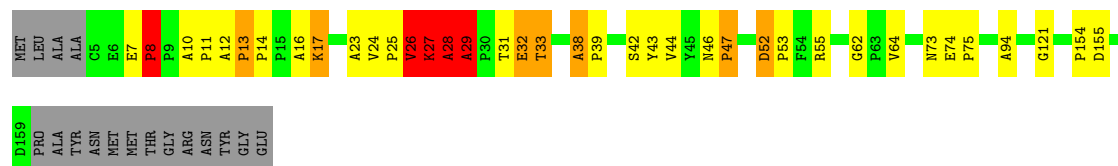
- Molecule 7: PilP

Chain Pg:  69% 15% • • 10%



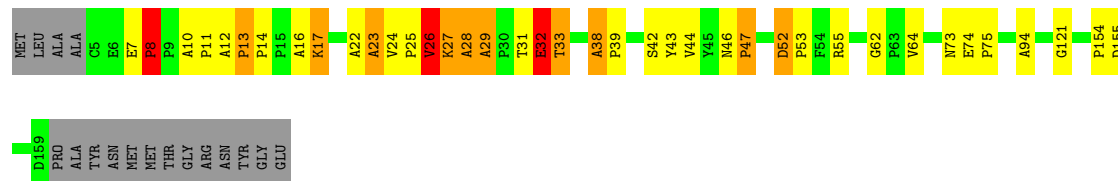
- Molecule 7: PilP

Chain Ph:  68% 15% • • 10%



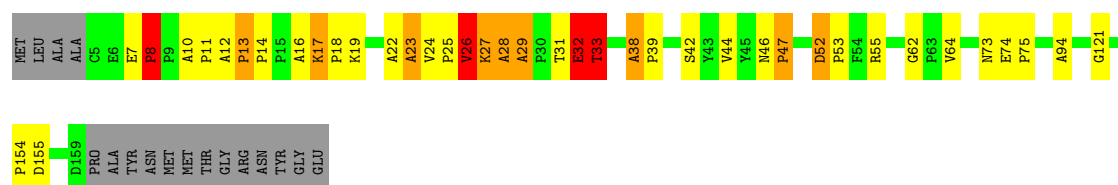
- Molecule 7: PilP

Chain Pi:  67% 15% 6% • 10%

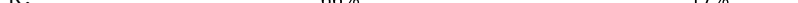


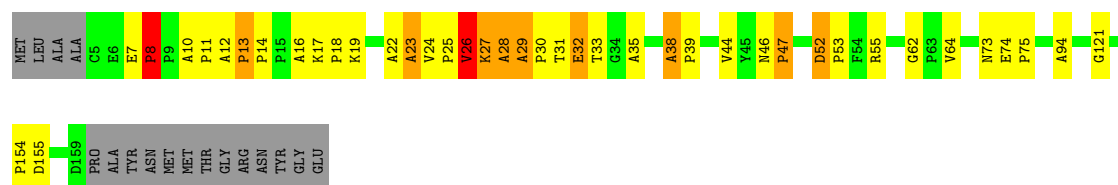
- Molecule 7: PilP

Chain Pj:  67% 16% 5% • 10%



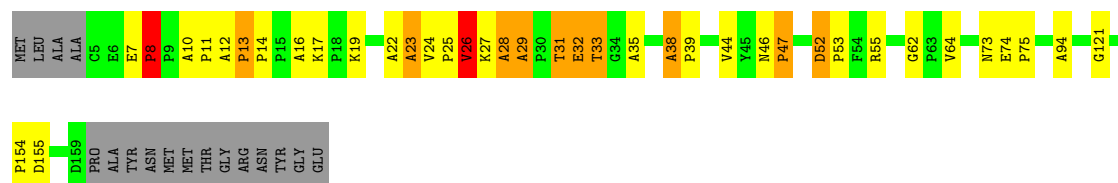
- Molecule 7: PilP

Chain Pk: 

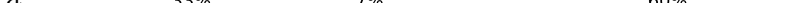


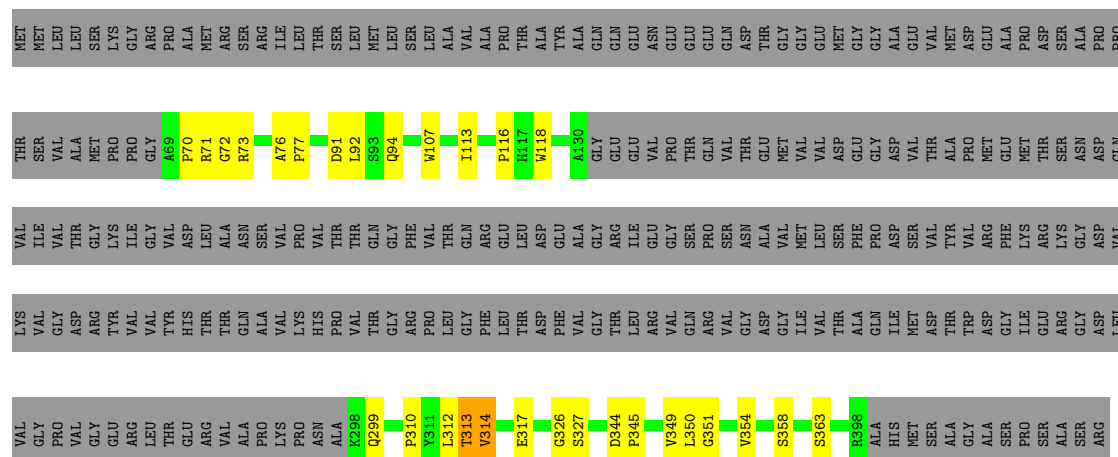
- Molecule 7: PilP

Chain Pl:

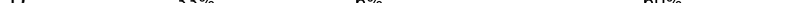


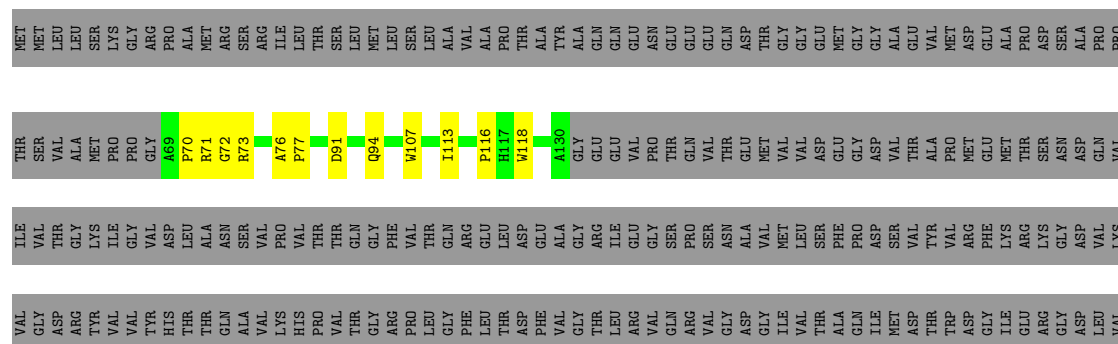
- Molecule 8: TsaP

Chain Ta: 



- Molecule 8: TsaP

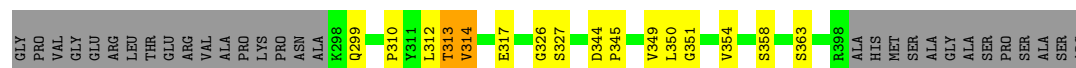
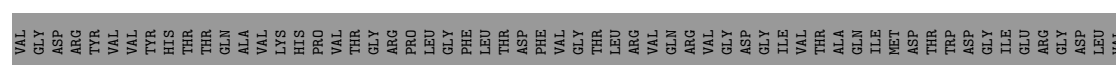
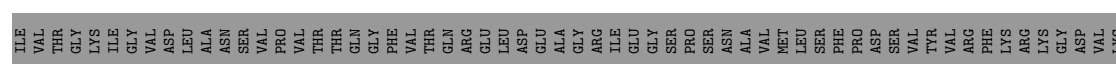
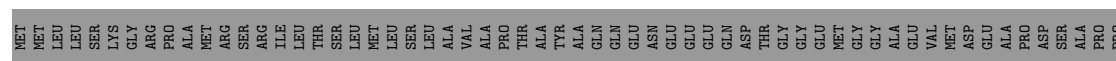
Chain Tb:  33% 6% 60%





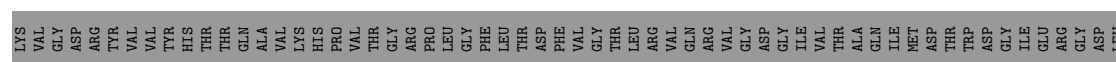
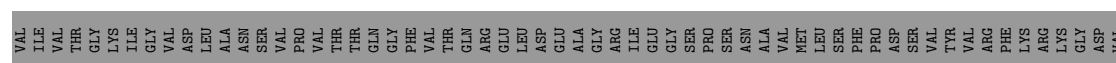
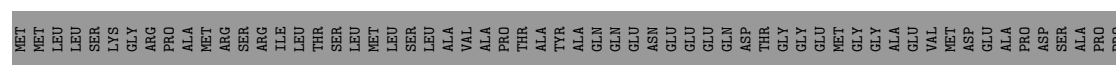
• Molecule 8: TsaP

Chain Tc:  33% 6% 60%



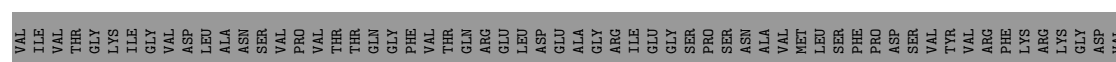
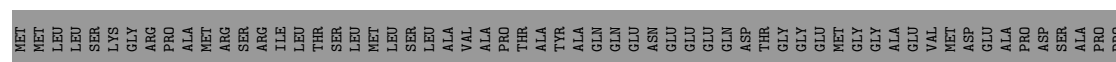
• Molecule 8: TsaP

Chain Td:  33% 7% 60%



• Molecule 8: TsaP

Chain Te:  33% 7% 60%



LYS	VAL	GLY	PRO	ASP	ARG	TYR	VAL	VAL	VAL	THR	THR	HIS	ALA	ALA	GLN	THR	VAL	LYS	VAL	LYS	ASN	HIS	PRO	VAL	THR	GLY	PRO	ARG	PRO	LEU	GLY	PHE	THR	THR	ASP	PHE	VAL	GLY	THR	THR	ARG	GLN	GLN	ARG	VAL	GLY	ASP	GLY	GLY	ILE	VAL	THR	ALA	GLN	ILE	ILE	MET	ASP	THR	THR	ASP	GLY	ILE	ARG	GLU	ILE	PRO	ASP	SER	ALA	GLY	PRO	ASP	LEU
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VAL	GLY	PRO	VAL	VAL	GLY	GLU	ARG	LEU	THR	THR	HIS	ARG	VAL	ALA	PRO	LYS	VAL	ASN	ALA	K298	K299	P310	Y311	L312	T313	V314	E317	G326	S327	D344	P345	V349	L350	G351	V354	S358	S363	K398	ALA	HIS	MET	SER	SER	ALA	GLY	THR	THR	ASP	GLY	ALA	GLN	ASP	GLU	VAL	VAL	MET	GLY	GLY	ALA	THR	VAL	ASP	GLY	THR	PRO	ASP	SER	ALA	GLY	PRO	ASP	ARG
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• Molecule 8: TsaP



MET	MET	LEU	LEU	SER	SER	LYS	ARG	GLY	PRO	ALA	MET	ARG	SER	ARG	ILE	THR	SER	LEU	THR	SER	ALA	K298	K299	P310	Y311	L312	T313	V314	E317	G326	S327	D344	P345	V349	L350	G351	V354	S358	S363	K398	ALA	HIS	MET	SER	SER	ALA	GLY	THR	THR	ASP	GLY	ALA	GLN	ASP	GLU	VAL	VAL	MET	GLY	GLY	ALA	THR	VAL	ASP	GLY	THR	PRO	ASP	SER	ALA	GLY	PRO	ASP	LEU
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THR	SER	VAL	ALA	MET	PRO	GLY	ARG	GLY	THR	LYS	ILE	GLY	VAL	VAL	ASP	LEU	ALA	SER	PRO	VAL	VAL	K298	K299	P310	Y311	L312	T313	V314	E317	G326	S327	D344	P345	V349	L350	G351	V354	S358	S363	K398	ALA	HIS	MET	SER	SER	ALA	GLY	THR	THR	ASP	GLY	ALA	GLN	ASP	GLU	VAL	VAL	MET	GLY	GLY	ALA	THR	VAL	ASP	GLY	THR	PRO	ASP	SER	ALA	GLY	PRO	ASP	LEU
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ASN	ASP	GLN	VAL	ILE	VAL	THR	GLY	THR	LYS	ILE	GLY	VAL	VAL	ASP	LEU	ALA	SER	PRO	VAL	VAL	VAL	K298	K299	P310	Y311	L312	T313	V314	E317	G326	S327	D344	P345	V349	L350	G351	V354	S358	S363	K398	ALA	HIS	MET	SER	SER	ALA	GLY	THR	THR	ASP	GLY	ALA	GLN	ASP	GLU	VAL	VAL	MET	GLY	GLY	ALA	THR	VAL	ASP	GLY	THR	PRO	ASP	SER	ALA	GLY	PRO	ASP	LEU
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GLY	ASP	VAL	VAL	VAL	VAL	ASP	ARG	THR	LYS	ILE	GLY	VAL	VAL	ASP	LEU	ALA	SER	PRO	VAL	VAL	VAL	K298	K299	P310	Y311	L312	T313	V314	E317	G326	S327	D344	P345	V349	L350	G351	V354	S358	S363	K398	ALA	HIS	MET	SER	SER	ALA	GLY	THR	THR	ASP	GLY	ALA	GLN	ASP	GLU	VAL	VAL	MET	GLY	GLY	ALA	THR	VAL	ASP	GLY	THR	PRO	ASP	SER	ALA	GLY	PRO	ASP	LEU
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GLY	ASP	LEU	VAL	VAL	GLY	PRO	VAL	GLY	THR	LYS	ILE	GLY	VAL	VAL	ASP	LEU	ALA	SER	PRO	VAL	VAL	K298	K299	P310	Y311	L312	T313	V314	E317	G326	S327	D344	P345	V349	L350	G351	V354	S358	S363	K398	ALA	HIS	MET	SER	SER	ALA	GLY	THR	THR	ASP	GLY	ALA	GLN	ASP	GLU	VAL	VAL	MET	GLY	GLY	ALA	THR	VAL	ASP	GLY	THR	PRO	ASP	SER	ALA	GLY	PRO	ASP	LEU
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SER	ARG
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• Molecule 8: TsaP



MET	MET	LEU	LEU	VAL	VAL	GLY	ARG	THR	LYS	ILE	GLY	VAL	VAL	ASP	LEU	ALA	SER	PRO	VAL	VAL	VAL	K298	K299	P310	Y311	L312	T313	V314	E317	G326	S327	D344	P345	V349	L350	G351	V354	S358	S363	K398	ALA	HIS	MET	SER	SER	ALA	GLY	THR	THR	ASP	GLY	ALA	GLN	ASP	GLU	VAL	VAL	MET	GLY	GLY	ALA	THR	VAL	ASP	GLY	THR	PRO	ASP	SER	ALA	GLY	PRO	ASP	LEU
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THR	SER	VAL	ALA	MET	PRO	GLY	ARG	GLY	THR	LYS	ILE	GLY	VAL	VAL	ASP	LEU	ALA	SER	PRO	VAL	VAL	K298	K299	P310	Y311	L312	T313	V314	E317	G326	S327	D344	P345	V349	L350	G351	V354	S358	S363	K398	ALA	HIS	MET	SER	SER	ALA	GLY	THR	THR	ASP	GLY	ALA	GLN	ASP	GLU	VAL	VAL	MET	GLY	GLY	ALA	THR	VAL	ASP	GLY	THR	PRO	ASP	SER	ALA	GLY	PRO	ASP	LEU
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VAL	ILE	THR	THR	THR	LYS	ILE	GLY	THR	LYS	ILE	GLY	VAL	VAL	ASP	LEU	ALA	SER	PRO	VAL	VAL	VAL	K298	K299	P310	Y311	L312	T313	V314	E317	G326	S327	D344	P345	V349	L350	G351	V354	S358	S363	K398	ALA	HIS	MET	SER	SER	ALA	GLY	THR	THR	ASP	GLY	ALA	GLN	ASP	GLU	VAL	VAL	MET	GLY	GLY	ALA	THR	VAL	ASP	GLY	THR	PRO	ASP	SER	ALA	GLY	PRO	ASP	LEU
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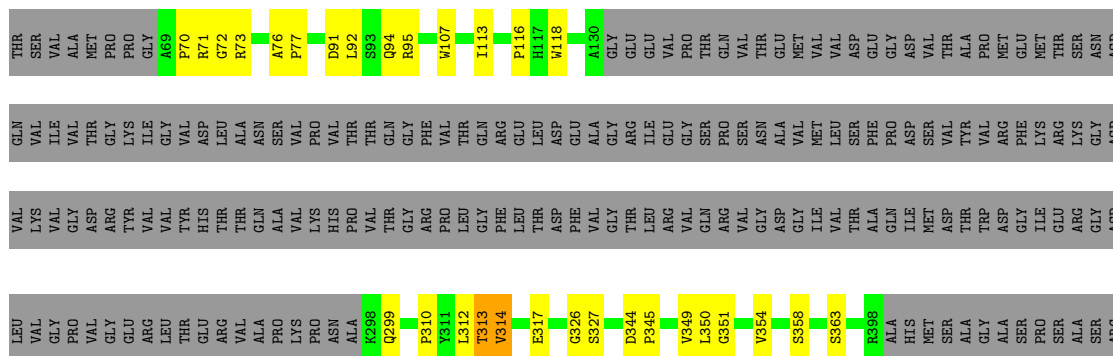
LYS	VAL	GLY	ASP	ARG	TYR	VAL	VAL	VAL	THR	THR	HIS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	K298	K299	P310	Y311	L312	T313	V314	E317	G326	S327	D344	P345	V349	L350	G351	V354	S358	S363	K398	ALA	HIS	MET	SER	SER	ALA	GLY	THR	THR	ASP	GLY	ALA	GLN	ASP	GLU	VAL	VAL	MET	GLY	GLY	ALA	THR	VAL	ASP	GLY	THR	PRO	ASP	SER	ALA	GLY	PRO	ASP	LEU
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VAL	GLY	PRO	VAL	VAL	GLY	GLU	ARG	LEU	THR	THR	HIS	ARG	VAL	ALA	PRO	LYS	VAL	ASN	ALA	K298	K299	P310	Y311	L312	T313	V314	E317	G326	S327	D344	P345	V349	L350	G351	V354	S358	S363	K398	ALA	HIS	MET	SER	SER	ALA	GLY	THR	THR	ASP	GLY	ALA	GLN	ASP	GLU	VAL	VAL	MET	GLY	GLY	ALA	THR	VAL	ASP	GLY	THR	PRO	ASP	SER	ALA	GLY	PRO	ASP	LEU
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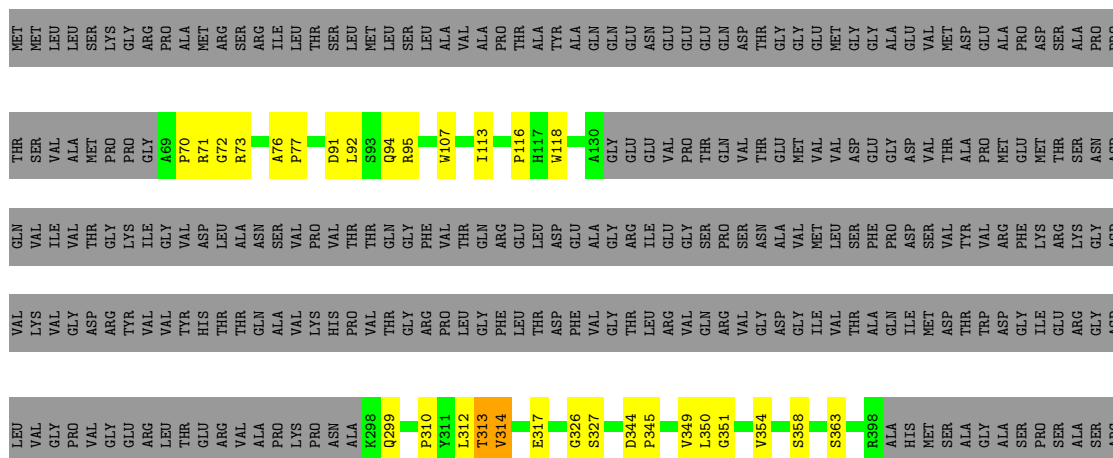
• Molecule 8: TsaP



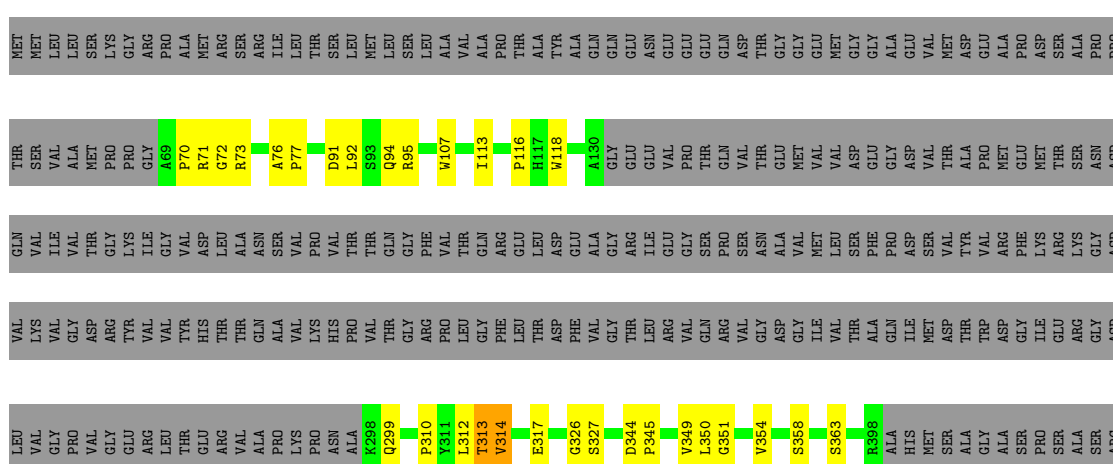
MET	MET	LEU	LEU	VAL	VAL	GLY	ARG	THR	LYS	ILE	GLY	VAL	VAL	ASP	LEU	ALA	SER	PRO	VAL	VAL	VAL	K298	K299	P310	Y311	L312	T313	V314	E317	G326	S327	D344	P345	V349	L350	G351	V354	S358	S363	K398	ALA	HIS	MET	SER	SER	ALA	GLY	THR	THR	ASP	GLY	ALA	GLN	ASP	GLU	VAL	VAL	MET	GLY	GLY	ALA	THR	VAL	ASP	GLY	THR	PRO	ASP	SER	ALA	GLY	PRO	ASP	LEU
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- Molecule 8: TsaP



- Molecule 8: TsaP



- Molecule 8: TsaP



MET	THR	GLN	VAL	LEU
MET	SER	VAL	LYS	VAL
LEU	VAL	ILE	VAL	GLY
LEU	ALA	THR	GLY	ASP
SER	MET	THR	ARG	VAL
LYS	PRO	GLY	TYR	VAL
GLY	PRO	ILE	VAL	ARG
ARG	GLY	GLY	VAL	LEU
PRO	A69	VAL	THR	THR
ALA	P70	VAL	HIS	GLU
MET	R71	ASP	ASP	ARG
ARG	G72	LEU	THR	VAL
SER	R73	ALA	THR	ALA
ARG		ASN	GLN	ALA
ILE	A76	SER	ALA	PRO
LEU	P77	VAL	LYS	PRO
THR		PRO	ASN	ALA
SER	D91	VAL	HIS	VAL
LEU	L92	THR	PRO	VAL
MET	S93	THR	VAL	THR
LEU	Q94	GLN	GLY	THR
SER	R95	THR	ARG	GLY
LEU		PHE	VAL	PRO
ALA	W107	VAL	LEU	GLY
VAL		THR	GLN	PHE
ALA	I113	ARG	THR	VAL
PRO		GLU	LEU	THR
THR	P116	LEU	THR	D344
ALA	H117	LEU	THR	P345
TYR	W118	ASP	ASP	V349
ALA		GLY	PHE	L350
GLN	A130	ALA	VAL	G351
GLY		GLY	VAL	V354
GLU	GLY	ILE	THR	V358
ASN	GLU	VAL	GLY	S358
GLU	THR	MET	ILE	S363
GLN	VAL	LEU	VAL	R398
GLY	ASP	SER	THR	ALA
ASP	GLY	PHE	GLN	HIS
THR	ALA	PRO	GLN	THR
GLY	VAL	ASP	ILE	MET
GLY	THR	SER	ASP	SER
VAL	VAL	VAL	THR	ALA
MET	THR	VAL	TYR	GLY
ASP	ALA	THR	VAL	ASP
PRO	MET	ARG	ASP	PRO
ALA	GLU	PHE	GLY	ILE
SER	MET	LYS	THR	GLU
ASP	THR	ARG	ARG	ALA
PRO	SER	LYS	GLY	SER
PRO	ASN	THR	GLY	ALA
PRO	ASP	ASP	ASP	ARG

● Molecule 8: TsaP



MET	THR	GLN	VAL	LEU
MET	SER	VAL	LYS	VAL
LEU	VAL	ILE	VAL	GLY
LEU	ALA	THR	GLY	ASP
SER	MET	THR	ARG	VAL
LYS	PRO	GLY	TYR	VAL
GLY	PRO	ILE	VAL	ARG
ARG	GLY	GLY	VAL	LEU
PRO	A69	VAL	THR	THR
ALA	P70	VAL	HIS	GLU
MET	R71	ASP	ASP	ARG
ARG	G72	LEU	THR	VAL
SER	R73	ALA	THR	ALA
ARG		ASN	GLN	ALA
ILE	A76	SER	ALA	PRO
LEU	P77	VAL	LYS	PRO
THR		PRO	ASN	ALA
SER	D91	VAL	HIS	VAL
LEU	L92	THR	PRO	VAL
MET	S93	THR	VAL	THR
LEU	Q94	GLN	GLY	THR
SER	R95	THR	ARG	GLY
LEU		PHE	VAL	PRO
ALA	W107	VAL	LEU	GLY
VAL		THR	GLN	PHE
ALA	I113	ARG	THR	VAL
PRO		GLU	LEU	THR
THR	P116	LEU	THR	D344
ALA	H117	LEU	THR	P345
TYR	W118	ASP	ASP	V349
ALA		GLY	PHE	L350
GLN	A130	ALA	VAL	G351
GLY		GLY	VAL	V354
GLU	GLY	ILE	THR	V358
ASN	GLU	VAL	GLY	S358
GLU	THR	MET	ILE	S363
GLN	VAL	LEU	VAL	R398
GLY	ASP	SER	THR	ALA
ASP	GLY	PHE	GLN	HIS
THR	ALA	PRO	GLN	THR
GLY	VAL	ASP	ILE	MET
GLY	THR	SER	ASP	SER
VAL	VAL	VAL	THR	ALA
MET	THR	VAL	TYR	GLY
ASP	ALA	THR	VAL	ASP
PRO	MET	ARG	ASP	PRO
ALA	GLU	PHE	GLY	ILE
SER	MET	LYS	THR	GLU
ASP	THR	ARG	ARG	ALA
PRO	SER	LYS	GLY	SER
PRO	ASN	THR	GLY	ALA
PRO	ASP	ASP	ASP	ARG

4 Experimental information

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, 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	Aa	1.14	1/627 (0.2%)	1.43	10/782 (1.3%)
1	Ab	1.14	1/627 (0.2%)	1.44	10/782 (1.3%)
1	Ac	1.13	1/627 (0.2%)	1.43	11/782 (1.4%)
1	Ad	1.14	1/627 (0.2%)	1.44	10/782 (1.3%)
1	Ae	1.14	1/627 (0.2%)	1.43	10/782 (1.3%)
2	Ca	1.09	1/1260 (0.1%)	1.71	10/1568 (0.6%)
2	Cb	1.10	1/1260 (0.1%)	1.71	10/1568 (0.6%)
3	Na	1.05	2/891 (0.2%)	1.11	11/1112 (1.0%)
3	Nb	1.03	1/891 (0.1%)	1.12	11/1112 (1.0%)
3	Nc	1.03	1/891 (0.1%)	1.11	11/1112 (1.0%)
3	Nd	1.03	1/891 (0.1%)	1.10	11/1112 (1.0%)
3	Ne	1.04	2/891 (0.2%)	1.11	11/1112 (1.0%)
3	Nf	1.03	1/891 (0.1%)	1.12	12/1112 (1.1%)
3	Ng	1.03	1/891 (0.1%)	1.08	9/1112 (0.8%)
3	Nh	1.03	2/891 (0.2%)	1.12	11/1112 (1.0%)
3	Ni	1.03	1/891 (0.1%)	1.11	12/1112 (1.1%)
3	Nj	1.03	1/891 (0.1%)	1.12	11/1112 (1.0%)
3	Nk	1.03	1/891 (0.1%)	1.11	12/1112 (1.1%)
3	Nl	1.03	1/891 (0.1%)	1.12	11/1112 (1.0%)
4	Oa	0.50	1/755 (0.1%)	1.06	8/942 (0.8%)
4	Ob	0.51	1/755 (0.1%)	1.02	6/942 (0.6%)
4	Oc	0.50	1/755 (0.1%)	1.05	8/942 (0.8%)
4	Od	0.49	1/755 (0.1%)	1.05	8/942 (0.8%)
4	Oe	0.49	1/755 (0.1%)	1.03	6/942 (0.6%)
4	Of	0.50	1/755 (0.1%)	1.08	8/942 (0.8%)
4	Og	0.51	1/755 (0.1%)	1.06	8/942 (0.8%)
4	Oh	0.50	1/755 (0.1%)	1.07	8/942 (0.8%)
4	Oi	0.50	1/755 (0.1%)	1.04	6/942 (0.6%)
4	Oj	0.50	1/755 (0.1%)	1.06	8/942 (0.8%)
4	Ok	0.50	1/755 (0.1%)	1.00	5/942 (0.5%)
4	Ol	0.56	2/755 (0.3%)	1.03	6/942 (0.6%)
5	Ma	0.38	0/1419	0.84	4/1772 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	Mb	0.38	0/1419	0.85	4/1772 (0.2%)
5	Mc	0.37	0/1419	0.84	4/1772 (0.2%)
5	Md	0.37	0/1419	0.85	4/1772 (0.2%)
5	Me	0.37	0/1419	0.84	4/1772 (0.2%)
5	Mf	0.37	0/1419	0.84	4/1772 (0.2%)
5	Mg	0.37	0/1419	0.85	4/1772 (0.2%)
5	Mh	0.37	0/1419	0.84	4/1772 (0.2%)
5	Mi	0.37	0/1419	0.85	4/1772 (0.2%)
5	Mj	0.37	0/1419	0.85	4/1772 (0.2%)
5	Mk	0.37	0/1419	0.84	4/1772 (0.2%)
5	ML	0.37	0/1419	0.85	4/1772 (0.2%)
6	Qa	1.05	7/1667 (0.4%)	2.32	28/2075 (1.3%)
6	Qb	1.05	5/1667 (0.3%)	2.32	29/2075 (1.4%)
6	Qc	1.05	6/1667 (0.4%)	2.32	31/2075 (1.5%)
6	Qd	1.04	7/1667 (0.4%)	2.32	28/2075 (1.3%)
6	Qe	1.04	5/1667 (0.3%)	2.32	28/2075 (1.3%)
6	Qf	1.05	6/1667 (0.4%)	2.31	28/2075 (1.3%)
6	Qg	1.05	5/1667 (0.3%)	2.32	30/2075 (1.4%)
6	Qh	1.05	6/1667 (0.4%)	2.32	29/2075 (1.4%)
6	Qi	1.04	5/1667 (0.3%)	2.32	30/2075 (1.4%)
6	Qj	1.05	6/1667 (0.4%)	2.32	28/2075 (1.3%)
6	Qk	1.05	6/1667 (0.4%)	2.32	29/2075 (1.4%)
6	Ql	1.05	7/1667 (0.4%)	2.32	30/2075 (1.4%)
7	Pa	1.01	1/619 (0.2%)	1.70	8/772 (1.0%)
7	Pb	1.00	1/619 (0.2%)	1.73	8/772 (1.0%)
7	Pc	1.02	1/619 (0.2%)	1.75	8/772 (1.0%)
7	Pd	1.05	1/619 (0.2%)	1.73	10/772 (1.3%)
7	Pe	1.05	0/619	1.77	9/772 (1.2%)
7	Pf	1.04	1/619 (0.2%)	1.77	8/772 (1.0%)
7	Pg	1.04	1/619 (0.2%)	1.74	8/772 (1.0%)
7	Ph	1.04	1/619 (0.2%)	1.73	8/772 (1.0%)
7	Pi	1.05	1/619 (0.2%)	1.73	8/772 (1.0%)
7	Pj	1.04	1/619 (0.2%)	1.72	8/772 (1.0%)
7	Pk	0.99	1/619 (0.2%)	1.70	8/772 (1.0%)
7	Pl	0.98	1/619 (0.2%)	1.69	8/772 (1.0%)
8	Ta	0.38	0/650	0.91	0/809
8	Tb	0.38	0/650	0.91	0/809
8	Tc	0.40	0/650	0.91	0/809
8	Td	0.39	0/650	0.92	0/809
8	Te	0.41	0/650	0.91	0/809
8	Tf	0.41	0/650	0.91	0/809
8	Tg	0.39	0/650	0.91	0/809
8	Th	0.39	0/650	0.91	0/809

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	Ti	0.38	0/650	0.92	0/809
8	Tj	0.39	0/650	0.91	0/809
8	Tk	0.38	0/650	0.90	0/809
8	Tl	0.40	0/650	0.90	0/809
All	All	0.83	117/77667 (0.2%)	1.54	784/96830 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	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 117 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Ng	169	ARG	CA-C	28.21	1.89	1.52
3	Nl	169	ARG	CA-C	28.08	1.89	1.52
3	Na	169	ARG	CA-C	28.01	1.89	1.52
3	Nj	169	ARG	CA-C	27.93	1.89	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Nc	169	ARG	CA-C	27.90	1.89	1.52

The worst 5 of 784 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Qf	407	SER	O-C-N	-64.94	36.22	122.59
6	Qg	407	SER	O-C-N	-64.94	36.22	122.59
6	Qk	407	SER	O-C-N	-64.93	36.23	122.59
6	Qh	407	SER	O-C-N	-64.93	36.23	122.59
6	Qb	407	SER	O-C-N	-64.93	36.23	122.59

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 ⓘ

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	26	0
1	Ab	632	0	174	12	0
1	Ac	632	0	174	11	0
1	Ad	632	0	174	11	0
1	Ae	632	0	174	15	0
2	Ca	1264	0	354	6	0
2	Cb	1264	0	354	20	0
3	Na	892	0	248	12	0
3	Nb	892	0	248	12	0
3	Nc	892	0	248	16	0
3	Nd	892	0	248	17	0
3	Ne	892	0	248	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Nf	892	0	248	11	0
3	Ng	892	0	248	12	0
3	Nh	892	0	248	12	0
3	Ni	892	0	248	12	0
3	Nj	892	0	248	12	0
3	Nk	892	0	248	12	0
3	Nl	892	0	248	11	0
4	Oa	756	0	207	18	0
4	Ob	756	0	207	20	0
4	Oc	756	0	207	18	0
4	Od	756	0	207	12	0
4	Oe	756	0	207	14	0
4	Of	756	0	207	16	0
4	Og	756	0	207	16	0
4	Oh	756	0	207	16	0
4	Oi	756	0	207	23	0
4	Oj	756	0	206	23	0
4	Ok	756	0	207	28	0
4	Ol	756	0	207	24	0
5	Ma	1420	0	396	13	0
5	Mb	1420	0	396	13	0
5	Mc	1420	0	396	13	0
5	Md	1420	0	396	12	0
5	Me	1420	0	396	14	0
5	Mf	1420	0	396	13	0
5	Mg	1420	0	396	13	0
5	Mh	1420	0	396	12	0
5	Mi	1420	0	396	13	0
5	Mj	1420	0	396	15	0
5	Mk	1420	0	396	15	0
5	Ml	1420	0	396	13	0
6	Qa	1672	0	462	36	0
6	Qb	1672	0	462	35	0
6	Qc	1672	0	462	34	0
6	Qd	1672	0	462	35	0
6	Qe	1672	0	462	34	0
6	Qf	1672	0	462	36	0
6	Qg	1672	0	462	35	0
6	Qh	1672	0	462	35	0
6	Qi	1672	0	462	35	0
6	Qj	1672	0	462	33	0
6	Qk	1672	0	462	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Ql	1672	0	462	35	0
7	Pa	620	0	155	17	0
7	Pb	620	0	155	18	0
7	Pc	620	0	155	19	0
7	Pd	620	0	155	18	0
7	Pe	620	0	155	16	0
7	Pf	620	0	155	15	0
7	Pg	620	0	155	12	0
7	Ph	620	0	155	20	0
7	Pi	620	0	155	19	0
7	Pj	620	0	155	18	0
7	Pk	620	0	155	22	0
7	Pl	620	0	155	22	0
8	Ta	652	0	177	11	0
8	Tb	652	0	177	11	0
8	Tc	652	0	177	12	0
8	Td	652	0	177	11	0
8	Te	652	0	177	10	0
8	Tf	652	0	177	10	0
8	Tg	652	0	177	10	0
8	Th	652	0	177	10	0
8	Ti	652	0	177	10	0
8	Tj	652	0	177	10	0
8	Tk	652	0	177	10	0
8	Tl	652	0	177	11	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	MI	31	0	12	0	0
All	All	78216	0	21461	1023	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.

The worst 5 of 1023 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ac:26:ASP:N	1:Ac:26:ASP:CA	1.76	1.49
1:Ac:26:ASP:N	1:Ac:26:ASP:CA	1.76	1.48
1:Aa:26:ASP:N	1:Aa:26:ASP:CA	1.76	1.48
1:Ad:26:ASP:N	1:Ad:26:ASP:CA	1.76	1.47
1:Ab:26:ASP:N	1:Ab:26:ASP:CA	1.76	1.46

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
5	MI	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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 ⓘ

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 ⓘ

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	Ad	1	1	3,3,13	1.01	0	1,2,16	0.33	0
1	MEA	Ab	1	1	3,3,13	0.97	0	1,2,16	0.35	0
1	MEA	Ae	1	1	3,3,13	0.98	0	1,2,16	0.34	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	Ad	1	1	-	0/0/1/10	-
1	MEA	Ab	1	1	-	0/0/1/10	-
1	MEA	Ae	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.

1 monomer is involved in 4 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	32,33,33	1.43	6 (18%)	48,52,52	1.78	10 (20%)
10	ATP	Mg	502	9	32,33,33	1.42	5 (15%)	48,52,52	1.74	10 (20%)
10	ATP	Ma	502	9	32,33,33	1.45	5 (15%)	48,52,52	1.73	10 (20%)
10	ATP	Mc	502	9	32,33,33	1.43	5 (15%)	48,52,52	1.77	11 (22%)
10	ATP	Mk	502	9	32,33,33	1.40	5 (15%)	48,52,52	1.79	11 (22%)
10	ATP	Ml	502	9	32,33,33	1.41	5 (15%)	48,52,52	1.75	10 (20%)
10	ATP	Mb	502	9	32,33,33	1.37	5 (15%)	48,52,52	1.73	10 (20%)
10	ATP	Me	502	9	32,33,33	1.41	5 (15%)	48,52,52	1.73	10 (20%)
10	ATP	Md	502	9	32,33,33	1.41	5 (15%)	48,52,52	1.71	8 (16%)
10	ATP	Mf	502	9	32,33,33	1.42	5 (15%)	48,52,52	1.73	9 (18%)
10	ATP	Mh	502	9	32,33,33	1.40	5 (15%)	48,52,52	1.74	9 (18%)
10	ATP	Mi	502	9	32,33,33	1.43	5 (15%)	48,52,52	1.71	8 (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
10	ATP	Mj	502	9	-	3/22/38/38	0/3/3/3
10	ATP	Mg	502	9	-	1/22/38/38	0/3/3/3
10	ATP	Ma	502	9	-	4/22/38/38	0/3/3/3
10	ATP	Mc	502	9	-	2/22/38/38	0/3/3/3
10	ATP	Mk	502	9	-	4/22/38/38	0/3/3/3
10	ATP	Ml	502	9	-	4/22/38/38	0/3/3/3
10	ATP	Mb	502	9	-	4/22/38/38	0/3/3/3
10	ATP	Me	502	9	-	1/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	ATP	Md	502	9	-	1/22/38/38	0/3/3/3
10	ATP	Mf	502	9	-	1/22/38/38	0/3/3/3
10	ATP	Mh	502	9	-	1/22/38/38	0/3/3/3
10	ATP	Mi	502	9	-	2/22/38/38	0/3/3/3

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Mc	502	ATP	C5-C4	4.79	1.47	1.39
10	Mj	502	ATP	C5-C4	4.77	1.47	1.39
10	Md	502	ATP	C5-C4	4.75	1.47	1.39
10	Ma	502	ATP	C5-C4	4.73	1.47	1.39
10	Mh	502	ATP	C5-C4	4.69	1.47	1.39

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Mh	502	ATP	C5-C4-N3	-5.75	118.80	126.72
10	Mj	502	ATP	C5-C4-N3	-5.74	118.81	126.72
10	MI	502	ATP	C5-C4-N3	-5.71	118.85	126.72
10	Md	502	ATP	C5-C4-N3	-5.70	118.87	126.72
10	Mk	502	ATP	C5-C4-N3	-5.70	118.87	126.72

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

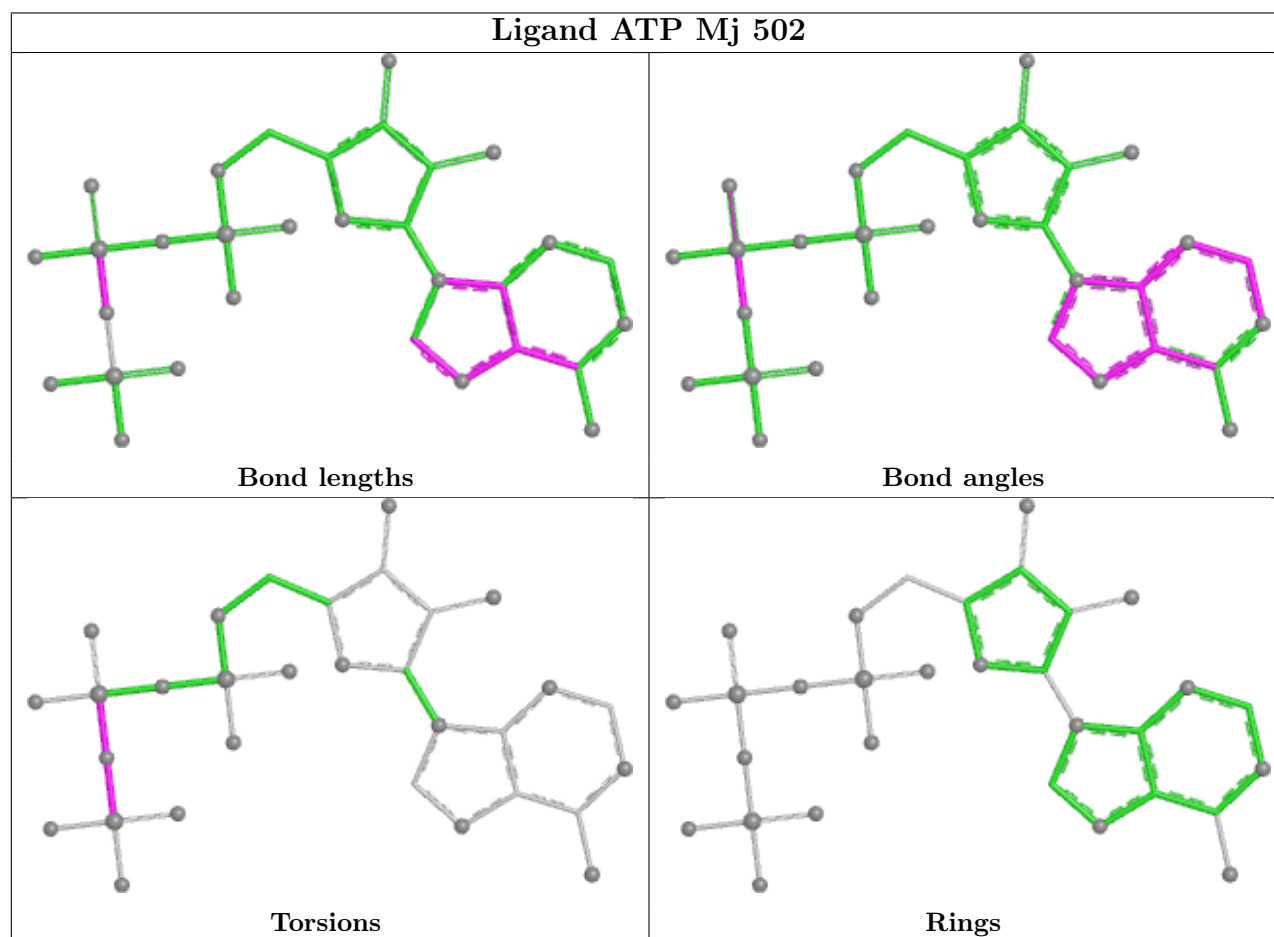
Mol	Chain	Res	Type	Atoms
10	Ma	502	ATP	PB-O3B-PG-O3G
10	Mb	502	ATP	PB-O3B-PG-O3G
10	Mi	502	ATP	PB-O3B-PG-O3G
10	Mj	502	ATP	PB-O3B-PG-O3G
10	Mk	502	ATP	PB-O3B-PG-O3G

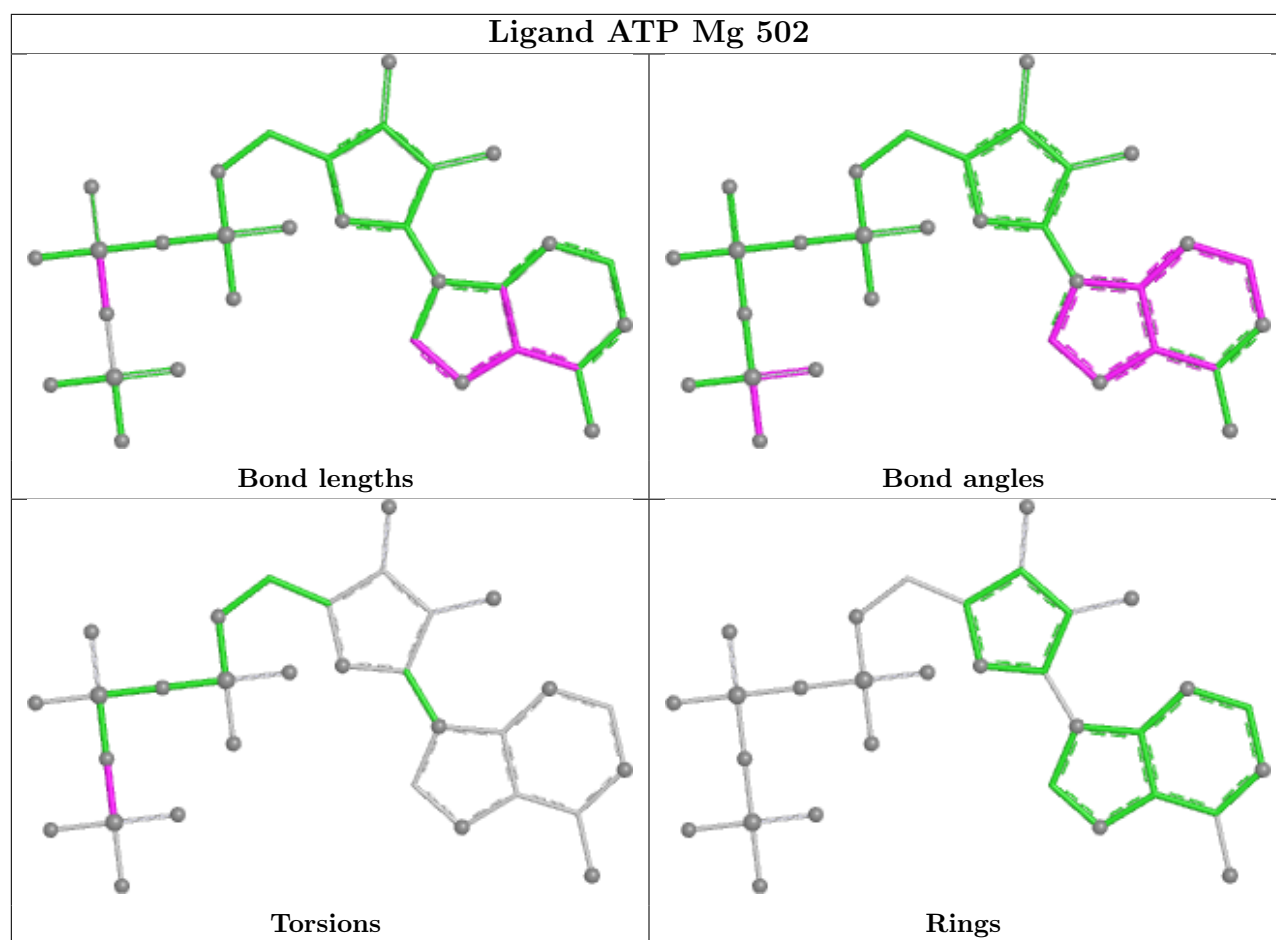
There are no ring outliers.

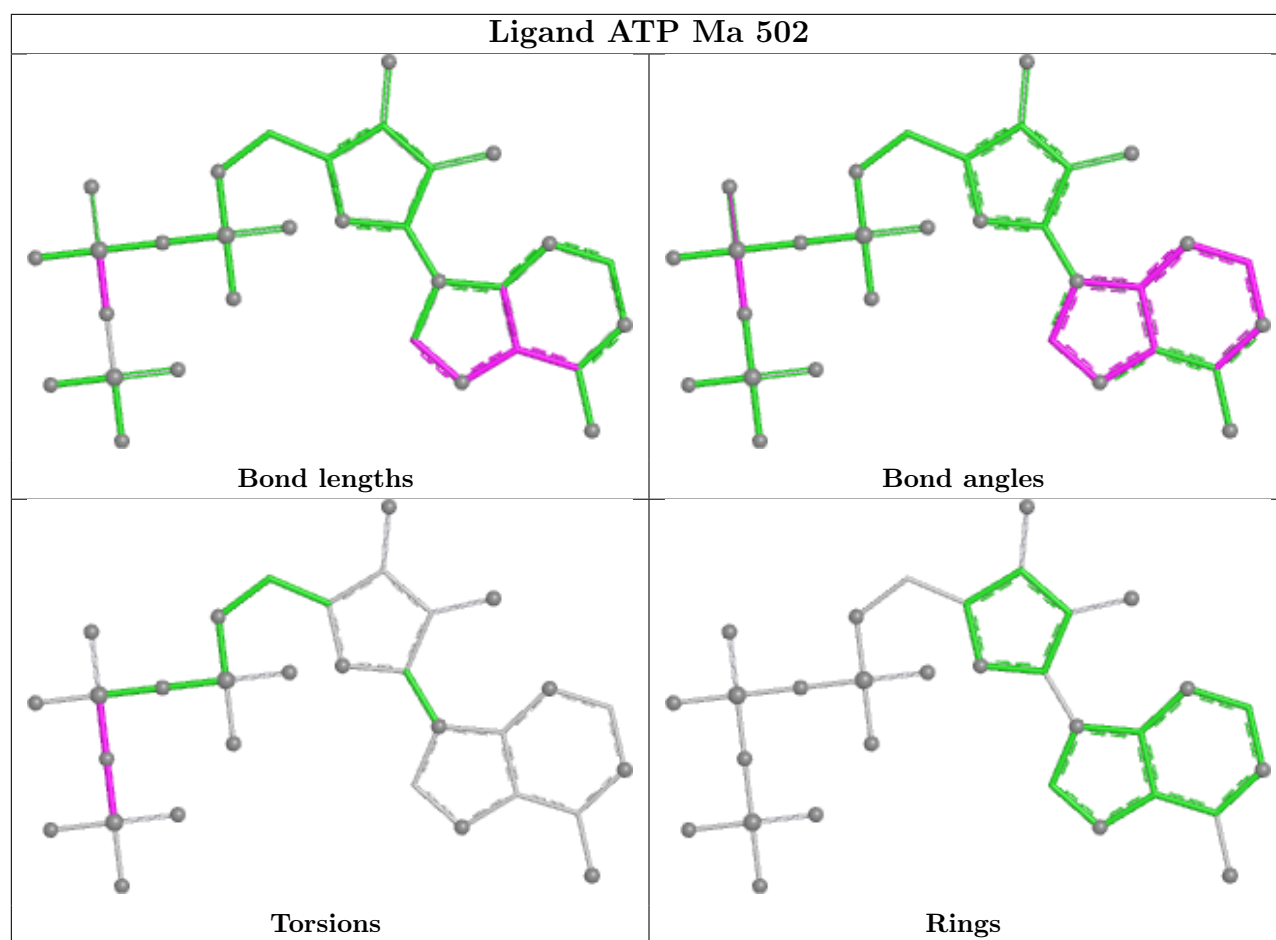
No monomer is involved in short contacts.

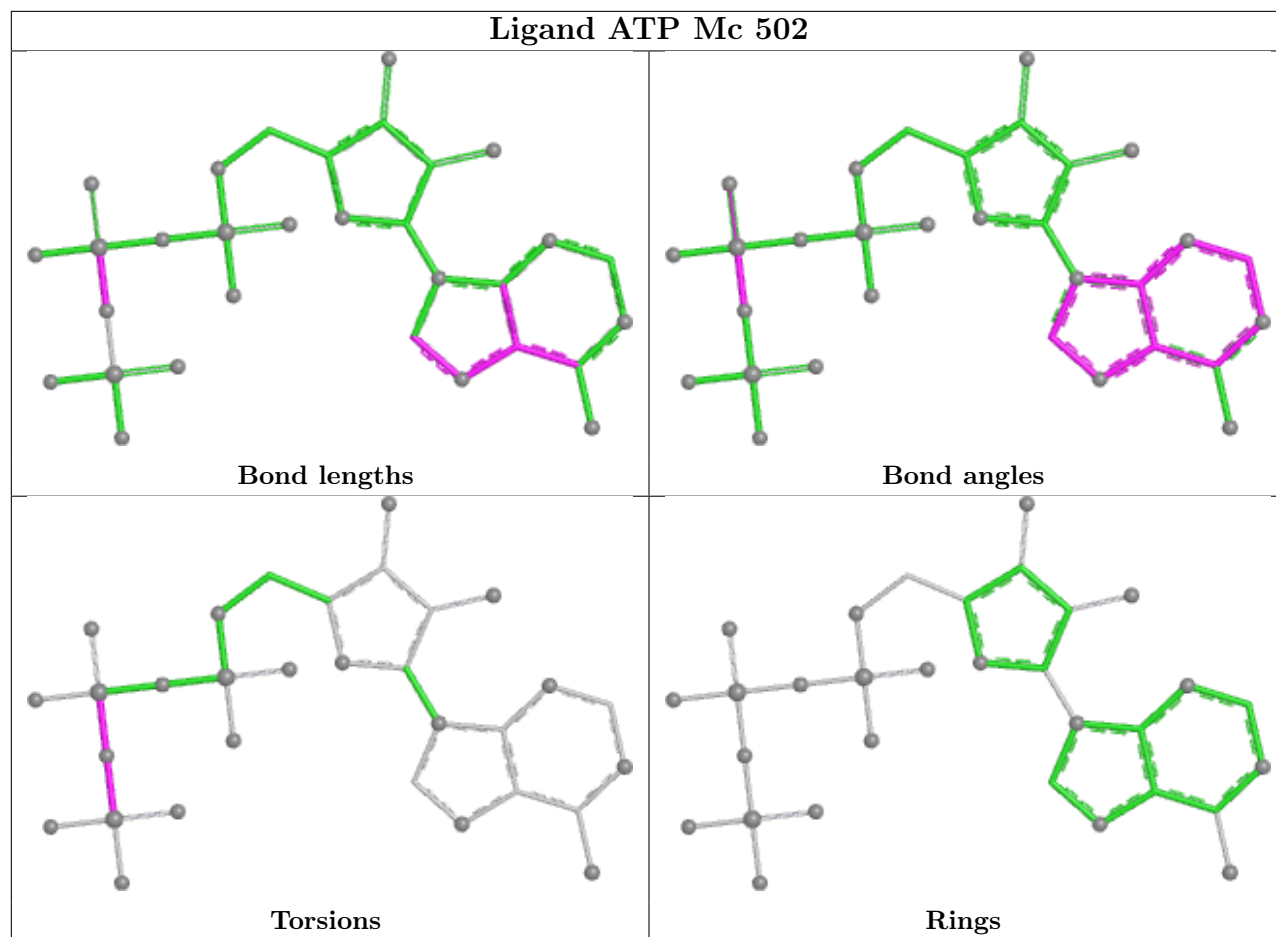
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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

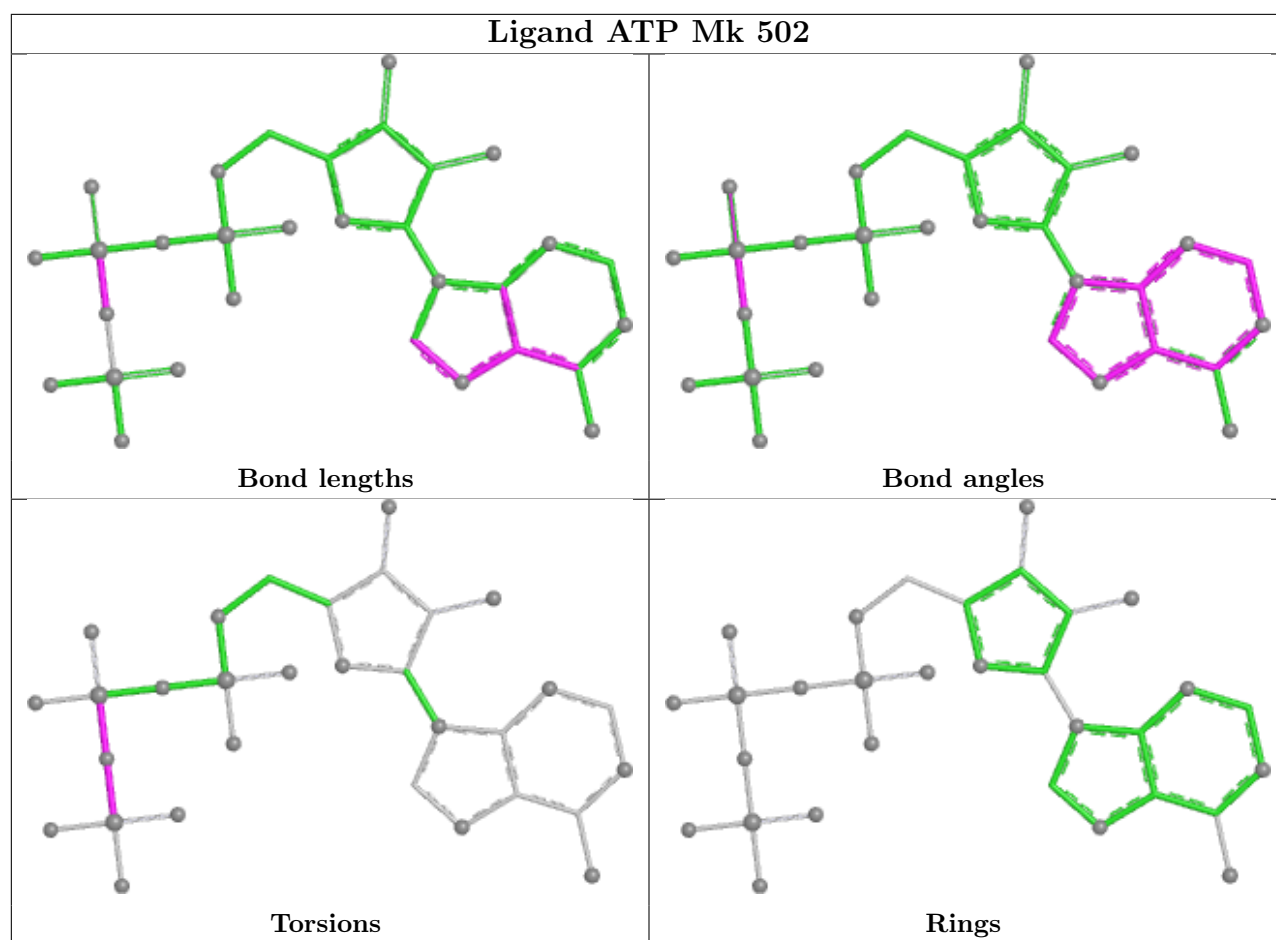
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

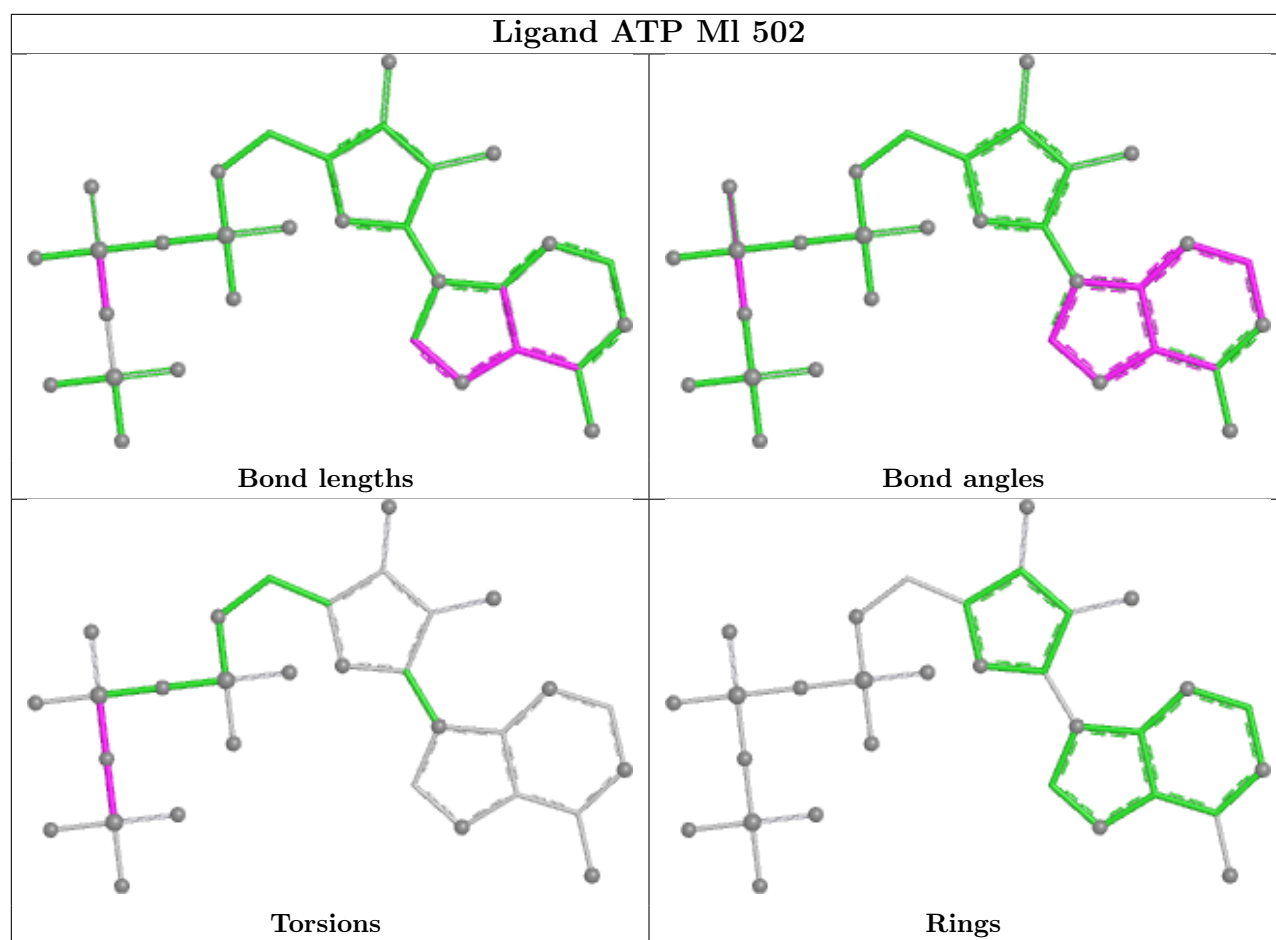


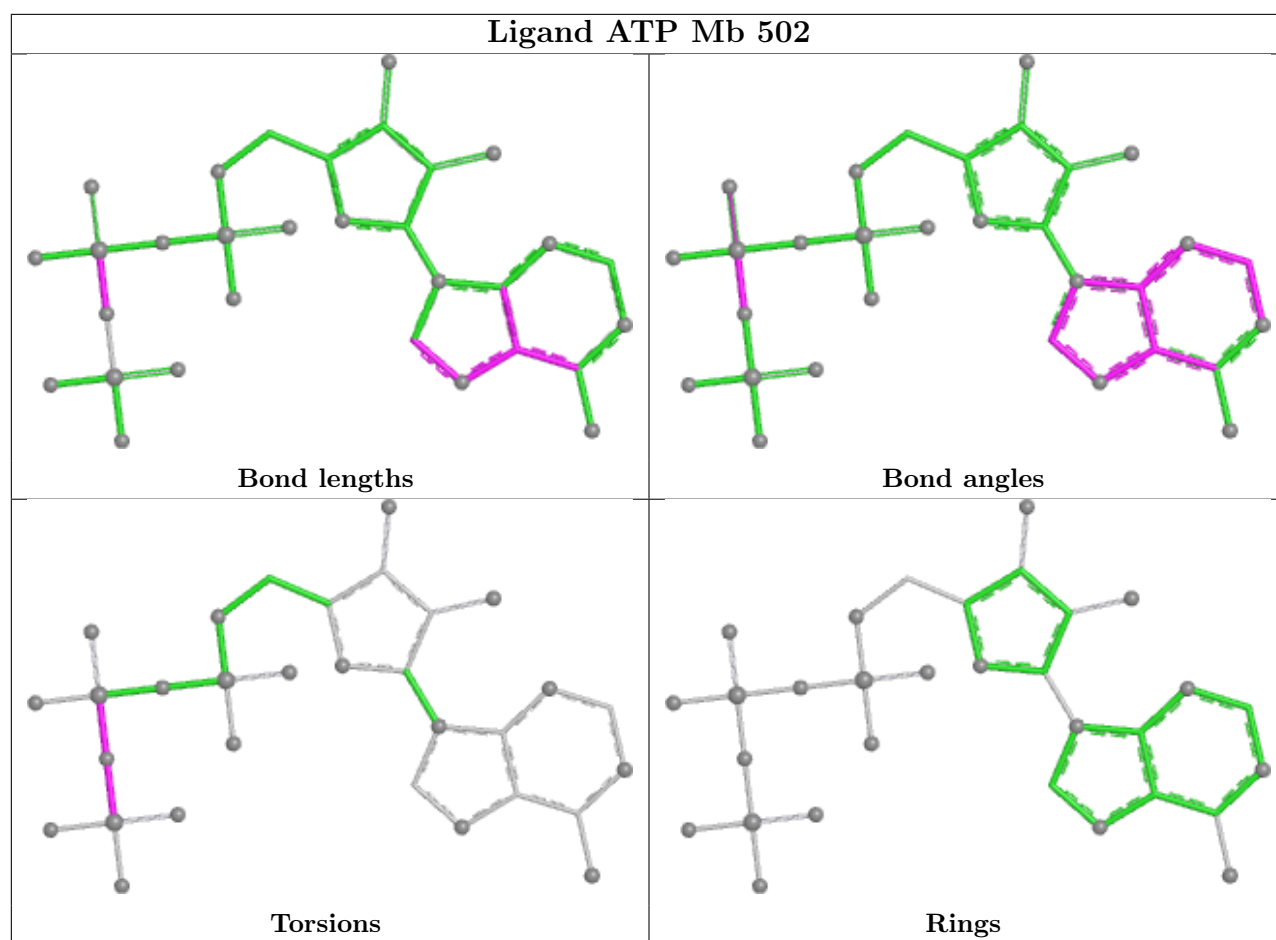


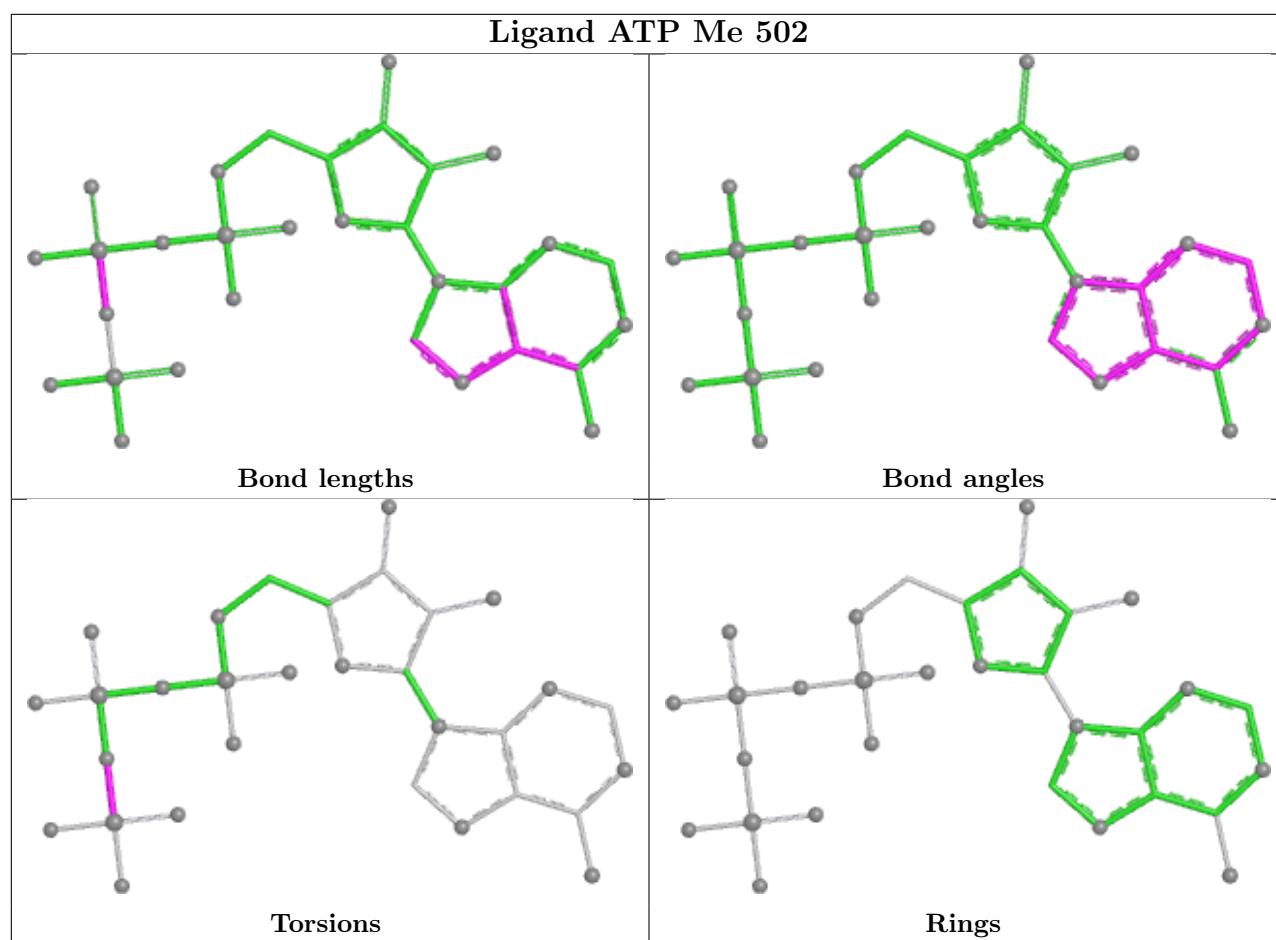


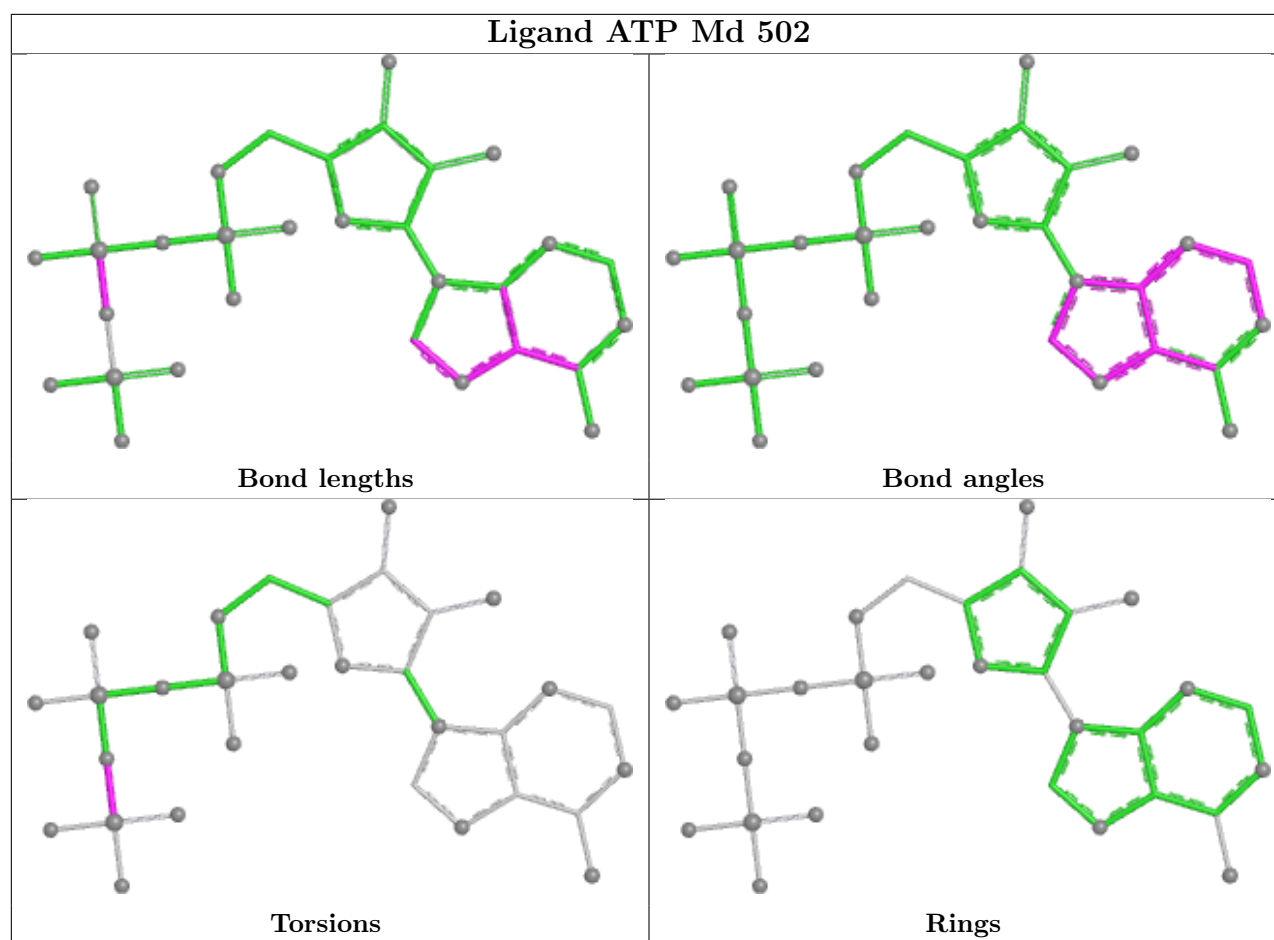


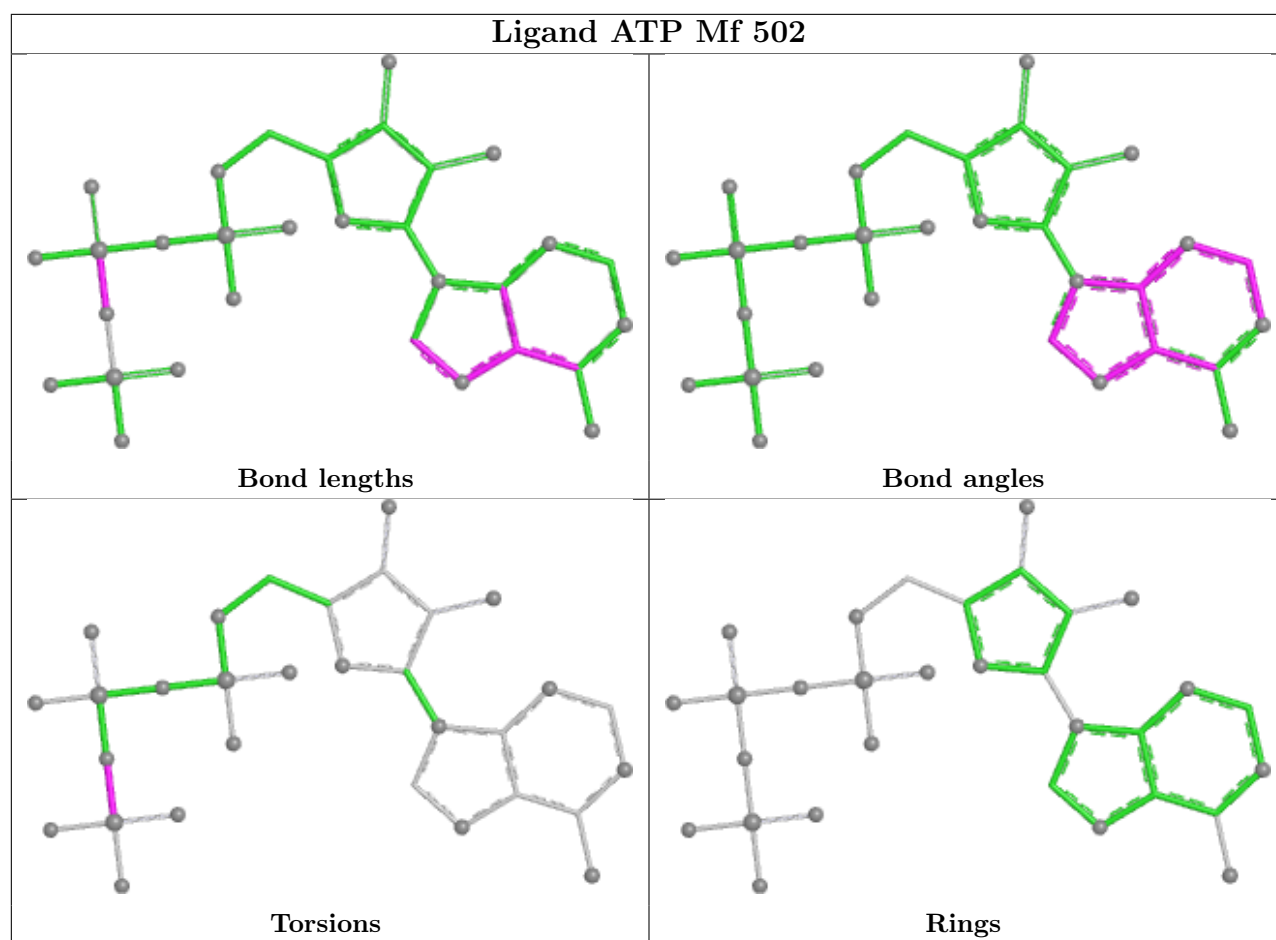


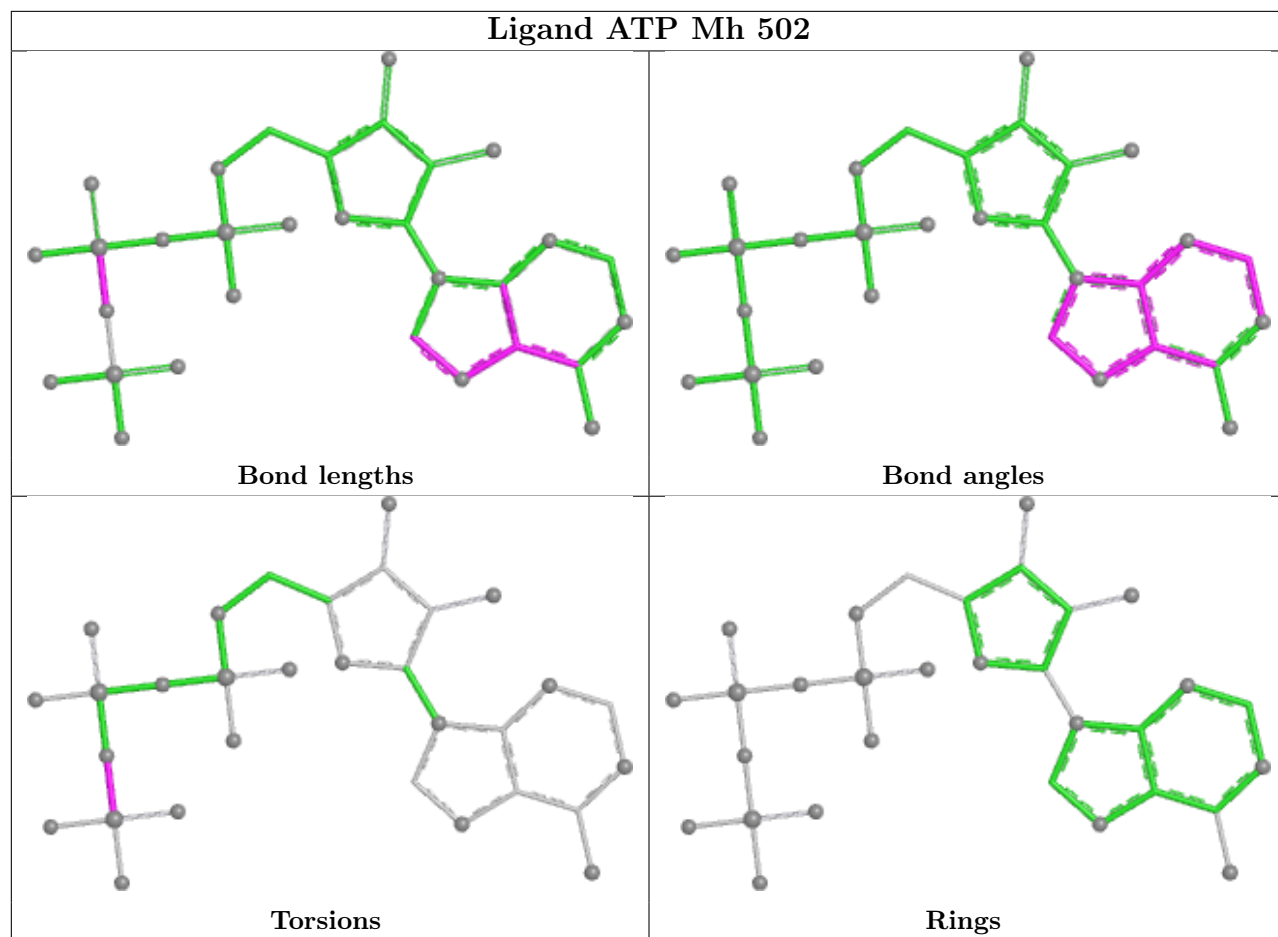


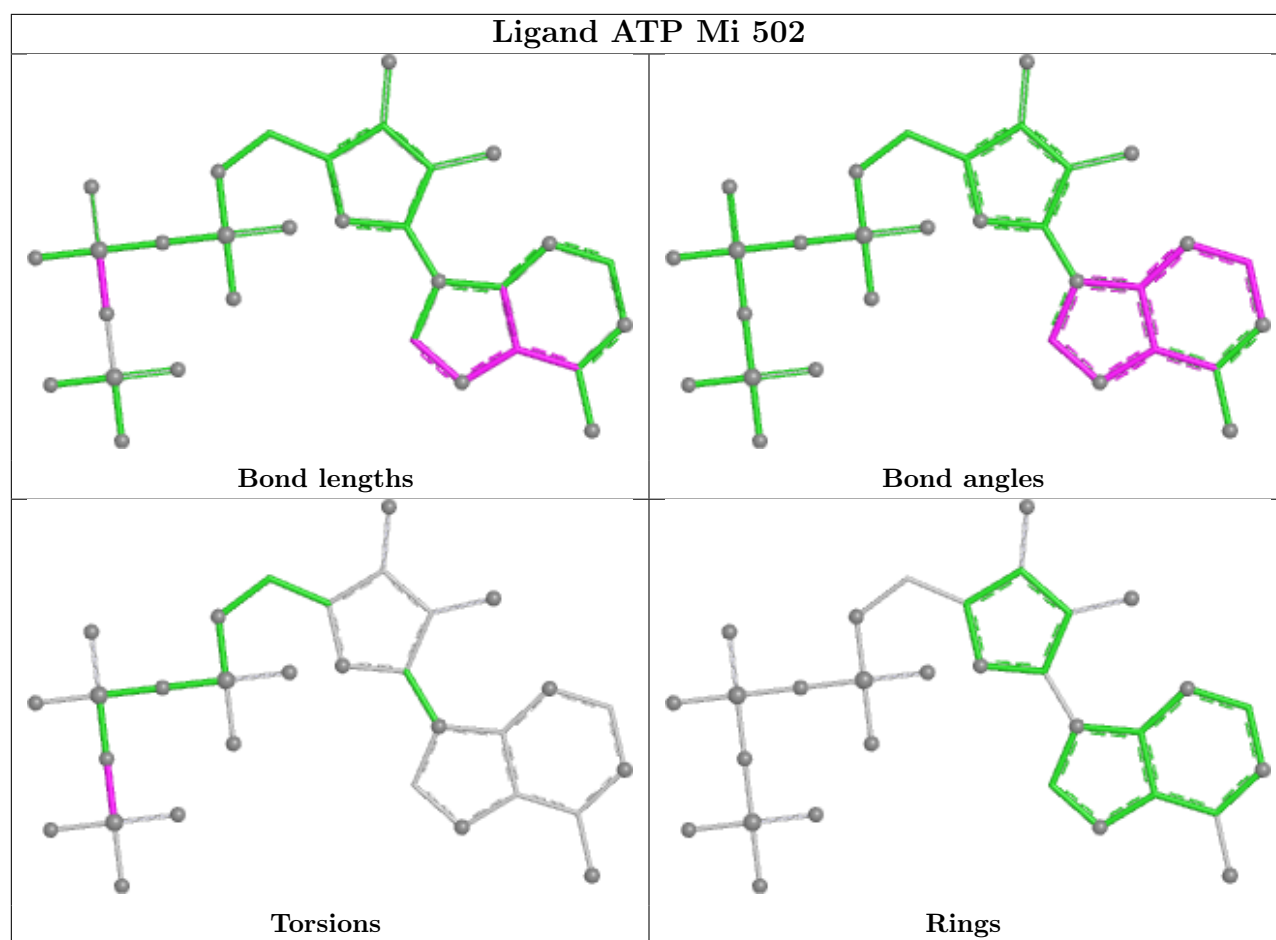












5.7 Other polymers [i](#)

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

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.