



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 22, 2018 – 08:14 PM EST

PDB ID : 5LER
EMDB ID: : EMD-4044
Title : Structure of the bacterial sex F pilus (13.2 Angstrom rise)
Authors : Costa, T.R.D.; Ilangovan, I.; Ukleja, M.; Redzej, A.; Santini, J.M.; Smith, T.K.; Egelman, E.H.; Waksman, G.
Deposited on : 2016-06-30
Resolution : 5.00 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

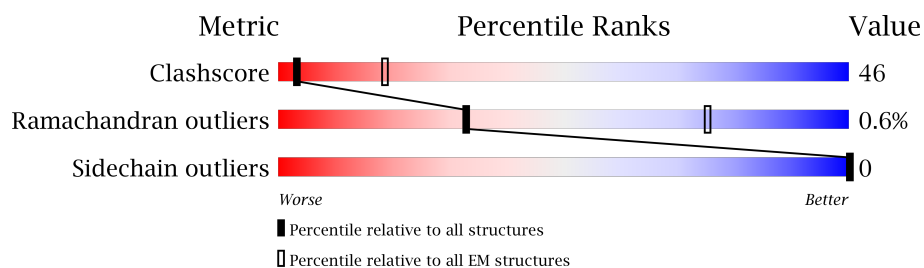
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.00 Å.

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.



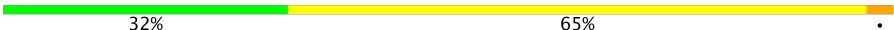

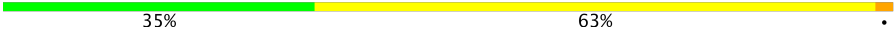








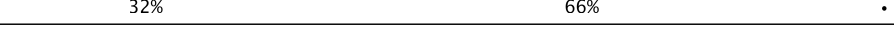







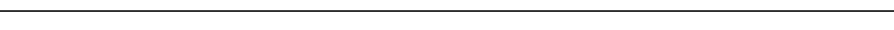

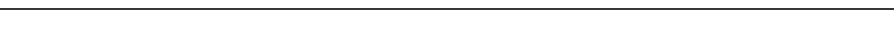
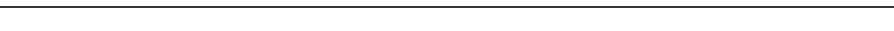


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	1A	65	32% 66% .
1	1B	65	34% 65% .
1	1C	65	34% 65% .
1	1D	65	31% 66% .
1	1E	65	34% 65% .
1	1F	65	32% 65% .
1	1G	65	35% 62% .
1	1H	65	32% 66% .
1	1I	65	34% 65% .





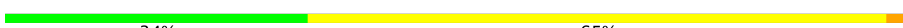
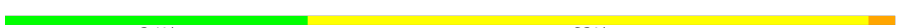







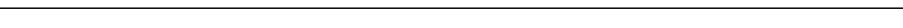











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Mol	Chain	Length	Quality of chain
1	1J	65	 32% 65% .
1	1K	65	 34% 63% .
1	1L	65	 35% 63% .
1	1M	65	 32% 65% .
1	1N	65	 37% 62% .
1	1O	65	 40% 57% .
1	2A	65	 32% 66% .
1	2B	65	 34% 65% .
1	2C	65	 32% 66% .
1	2D	65	 31% 68% .
1	2E	65	 34% 65% .
1	2F	65	 32% 66% .
1	2G	65	 35% 63% .
1	2H	65	 32% 66% .
1	2I	65	 34% 65% .
1	2J	65	 34% 65% .
1	2K	65	 35% 63% .
1	2L	65	 35% 63% .
1	2M	65	 32% 66% .
1	2N	65	 37% 60% .
1	2O	65	 40% 58% .
1	3A	65	 32% 66% .
1	3B	65	 34% 65% .
1	3C	65	 32% 66% .
1	3D	65	 31% 68% .


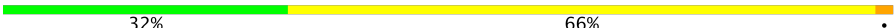
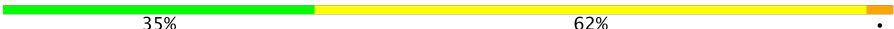
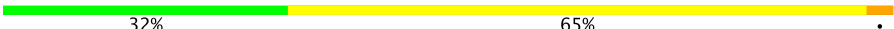
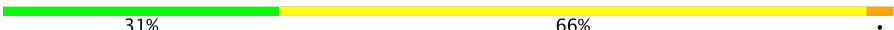
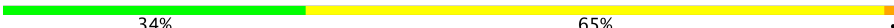

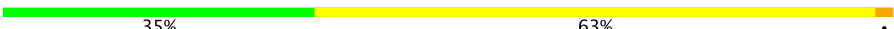
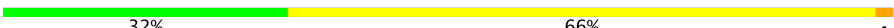
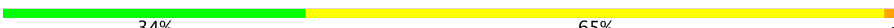




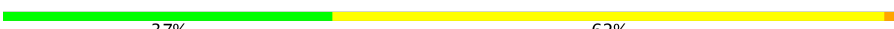
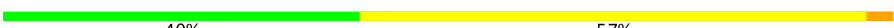
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Mol	Chain	Length	Quality of chain
1	3E	65	 34% 65% .
1	3F	65	 32% 66% .
1	3G	65	 35% 63% .
1	3H	65	 32% 66% .
1	3I	65	 34% 65% .
1	3J	65	 34% 63% .
1	3K	65	 35% 62% .
1	3L	65	 35% 63% .
1	3M	65	 32% 65% .
1	3N	65	 37% 60% .
1	3O	65	 40% 57% .
1	4A	65	 32% 65% .
1	4B	65	 34% 65% .
1	4C	65	 32% 66% .
1	4D	65	 32% 66% .
1	4E	65	 34% 65% .
1	4F	65	 32% 66% .
1	4G	65	 35% 63% .
1	4H	65	 32% 66% .
1	4I	65	 34% 65% .
1	4J	65	 34% 63% .
1	4K	65	 35% 62% .
1	4L	65	 35% 63% .
1	4M	65	 32% 66% .
1	4N	65	 37% 60% .

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Mol	Chain	Length	Quality of chain
1	4O	65	 40%57%.
1	5A	65	 32%66%.
1	5B	65	 35%62%.
1	5C	65	 32%65%.
1	5D	65	 31%66%.
1	5E	65	 34%65%.
1	5F	65	 32%65%.
1	5G	65	 35%63%.
1	5H	65	 32%66%.
1	5I	65	 34%65%.
1	5J	65	 34%63%.
1	5K	65	 35%62%.
1	5L	65	 34%65%.
1	5M	65	 31%66%.
1	5N	65	 37%62%.
1	5O	65	 40%57%.

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 36539 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 Pilin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	65	Total	C	N	O	S	0	0
			475	314	73	83	5		
1	1B	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1C	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1D	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1E	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1F	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1G	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1H	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1I	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1J	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1K	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1L	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1M	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1N	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1O	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	2A	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	2B	65	Total	C	N	O	S	0	0
			476	314	74	83	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	2C	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	2D	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	2E	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	2F	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	2G	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	2H	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	2I	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	2J	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	2K	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	2L	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	2M	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	2N	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	2O	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	3A	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	3B	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	3C	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	3D	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	3E	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	3F	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	3G	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	3H	65	Total 476	C 314	N 74	O 83	S 5	0	0

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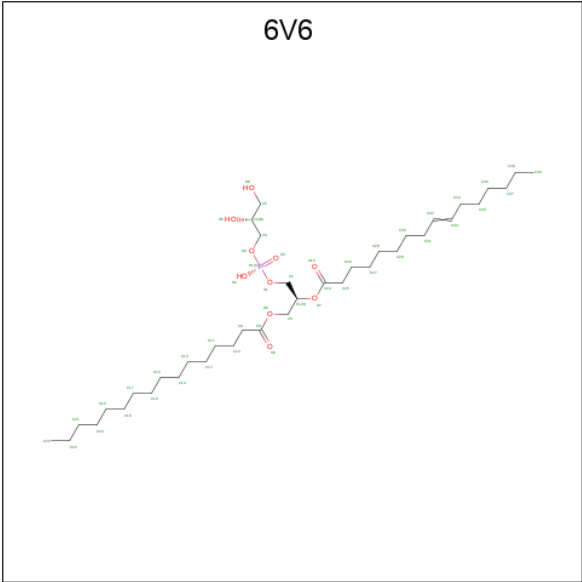
Mol	Chain	Residues	Atoms					AltConf	Trace
1	3I	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	3J	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	3K	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	3L	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	3M	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	3N	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	3O	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	4A	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	4B	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	4C	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	4D	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	4E	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	4F	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	4G	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	4H	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	4I	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	4J	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	4K	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	4L	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	4M	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	4N	65	Total 476	C 314	N 74	O 83	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	4O	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5A	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5B	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5C	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5D	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5E	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5F	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5G	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5H	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5I	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5J	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5K	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5L	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5M	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5N	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5O	65	Total	C	N	O	S	0	0
			476	314	74	83	5		

- Molecule 2 is [(2 {S})-3-[(2 {R})-2,3-bis(oxidanyl)propoxy]-oxidanyl-phosphoryl]oxy-2-hexadec-9-enoyloxy-propyl] hexadecanoate (three-letter code: 6V6) (formula: C₃₈H₇₃O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
2	1A	1	Total	C	O	P	0
			12	5	6	1	
2	1B	1	Total	C	O	P	0
			12	5	6	1	
2	1C	1	Total	C	O	P	0
			12	5	6	1	
2	1D	1	Total	C	O	P	0
			12	5	6	1	
2	1E	1	Total	C	O	P	0
			12	5	6	1	
2	1F	1	Total	C	O	P	0
			12	5	6	1	
2	1G	1	Total	C	O	P	0
			12	5	6	1	
2	1H	1	Total	C	O	P	0
			12	5	6	1	
2	1I	1	Total	C	O	P	0
			12	5	6	1	
2	1J	1	Total	C	O	P	0
			12	5	6	1	
2	1K	1	Total	C	O	P	0
			12	5	6	1	
2	1L	1	Total	C	O	P	0
			12	5	6	1	
2	1M	1	Total	C	O	P	0
			12	5	6	1	
2	1N	1	Total	C	O	P	0
			12	5	6	1	

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Mol	Chain	Residues	Atoms				AltConf
2	2A	1	Total	C	O	P	0
			12	5	6	1	
2	2B	1	Total	C	O	P	0
			12	5	6	1	
2	2C	1	Total	C	O	P	0
			12	5	6	1	
2	2D	1	Total	C	O	P	0
			12	5	6	1	
2	2E	1	Total	C	O	P	0
			12	5	6	1	
2	2F	1	Total	C	O	P	0
			12	5	6	1	
2	2G	1	Total	C	O	P	0
			12	5	6	1	
2	2H	1	Total	C	O	P	0
			12	5	6	1	
2	2I	1	Total	C	O	P	0
			12	5	6	1	
2	2J	1	Total	C	O	P	0
			12	5	6	1	
2	2K	1	Total	C	O	P	0
			12	5	6	1	
2	2L	1	Total	C	O	P	0
			12	5	6	1	
2	2M	1	Total	C	O	P	0
			12	5	6	1	
2	2N	1	Total	C	O	P	0
			12	5	6	1	
2	3A	1	Total	C	O	P	0
			12	5	6	1	
2	3B	1	Total	C	O	P	0
			12	5	6	1	
2	3C	1	Total	C	O	P	0
			12	5	6	1	
2	3D	1	Total	C	O	P	0
			12	5	6	1	
2	3E	1	Total	C	O	P	0
			12	5	6	1	
2	3F	1	Total	C	O	P	0
			12	5	6	1	
2	3G	1	Total	C	O	P	0
			12	5	6	1	

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Mol	Chain	Residues	Atoms				AltConf
2	3H	1	Total	C	O	P	0
			12	5	6	1	
2	3I	1	Total	C	O	P	0
			12	5	6	1	
2	3J	1	Total	C	O	P	0
			12	5	6	1	
2	3K	1	Total	C	O	P	0
			12	5	6	1	
2	3L	1	Total	C	O	P	0
			12	5	6	1	
2	3M	1	Total	C	O	P	0
			12	5	6	1	
2	3N	1	Total	C	O	P	0
			12	5	6	1	
2	4A	1	Total	C	O	P	0
			12	5	6	1	
2	4B	1	Total	C	O	P	0
			12	5	6	1	
2	4C	1	Total	C	O	P	0
			12	5	6	1	
2	4D	1	Total	C	O	P	0
			12	5	6	1	
2	4E	1	Total	C	O	P	0
			12	5	6	1	
2	4F	1	Total	C	O	P	0
			12	5	6	1	
2	4G	1	Total	C	O	P	0
			12	5	6	1	
2	4H	1	Total	C	O	P	0
			12	5	6	1	
2	4I	1	Total	C	O	P	0
			12	5	6	1	
2	4J	1	Total	C	O	P	0
			12	5	6	1	
2	4K	1	Total	C	O	P	0
			12	5	6	1	
2	4L	1	Total	C	O	P	0
			12	5	6	1	
2	4M	1	Total	C	O	P	0
			12	5	6	1	
2	4N	1	Total	C	O	P	0
			12	5	6	1	

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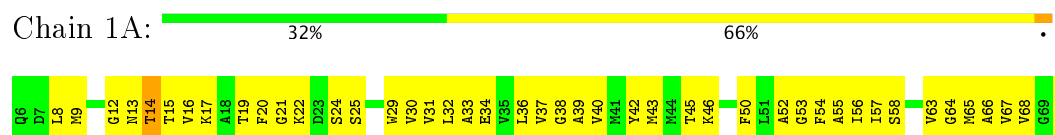
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Mol	Chain	Residues	Atoms				AltConf
2	5A	1	Total 12	C 5	O 6	P 1	0
2	5B	1	Total 12	C 5	O 6	P 1	0
2	5C	1	Total 12	C 5	O 6	P 1	0
2	5D	1	Total 12	C 5	O 6	P 1	0
2	5E	1	Total 12	C 5	O 6	P 1	0
2	5F	1	Total 12	C 5	O 6	P 1	0
2	5G	1	Total 12	C 5	O 6	P 1	0
2	5H	1	Total 12	C 5	O 6	P 1	0
2	5I	1	Total 12	C 5	O 6	P 1	0
2	5J	1	Total 12	C 5	O 6	P 1	0
2	5K	1	Total 12	C 5	O 6	P 1	0
2	5L	1	Total 12	C 5	O 6	P 1	0
2	5M	1	Total 12	C 5	O 6	P 1	0
2	5N	1	Total 12	C 5	O 6	P 1	0

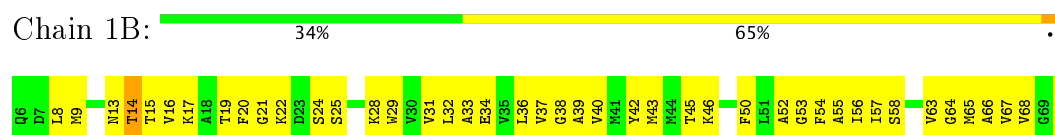
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

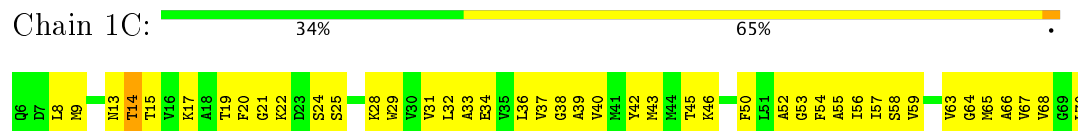
• Molecule 1: Pilin



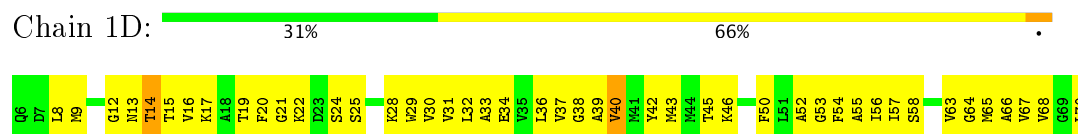
• Molecule 1: Pilin



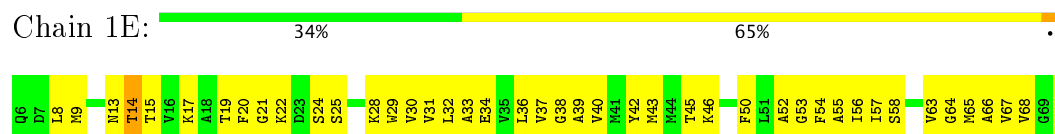
• Molecule 1: Pilin



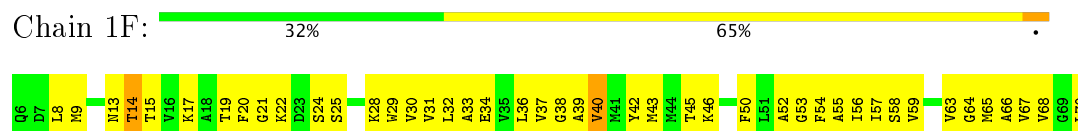
• Molecule 1: Pilin



• Molecule 1: Pilin



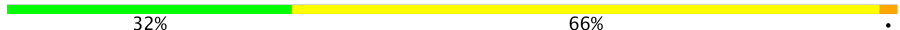
• Molecule 1: Pilin



• Molecule 1: Pilin

Chain 1G:  35% 62%

• Molecule 1: Pilin

Chain 1H:  32% 66%

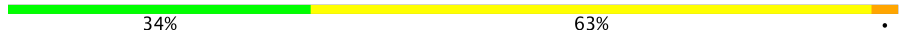
• Molecule 1: Pilin

Chain 1I:  34% 65%

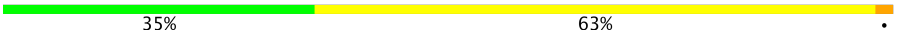
• Molecule 1: Pilin

Chain 1J:  32% 65%

• Molecule 1: Pilin

Chain 1K:  34% 63%

• Molecule 1: Pilin

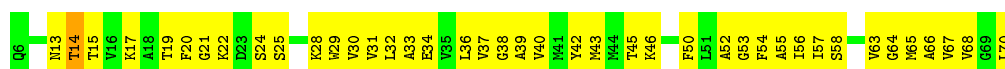
Chain 1L:  35% 63%

• Molecule 1: Pilin

Chain 1M:  32% 65%

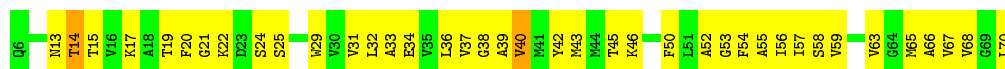
• Molecule 1: Pilin

Chain 1N:  37% 62%



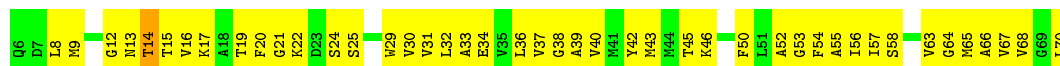
- Molecule 1: Pilin

Chain 1O: 40% 57%



- Molecule 1: Pilin

Chain 2A: 32% 66%



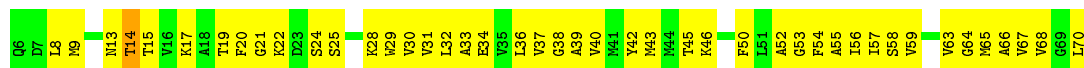
- Molecule 1: Pilin

Chain 2B: 34% 65%



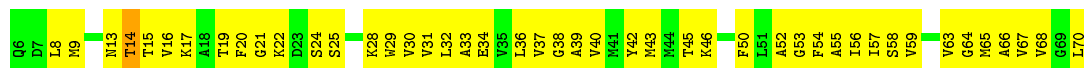
- Molecule 1: Pilin

Chain 2C: 32% 66%



- Molecule 1: Pilin

Chain 2D: 31% 68%



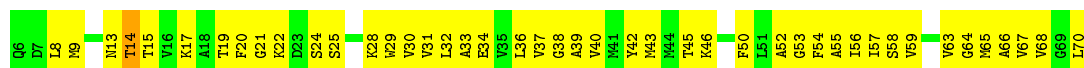
- Molecule 1: Pilin

Chain 2E: 34% 65%

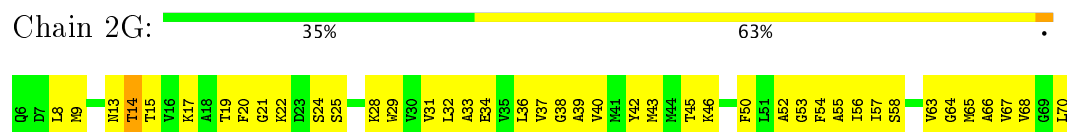


- Molecule 1: Pilin

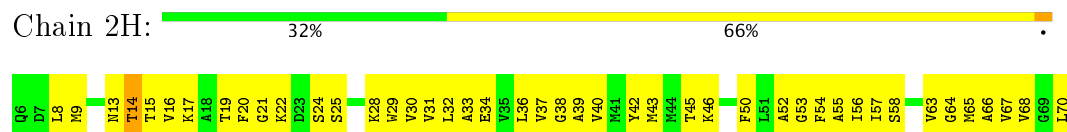
Chain 2F: 32% 66%



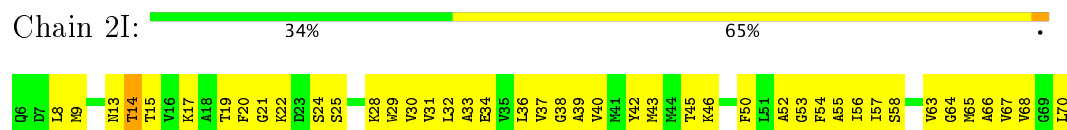
- Molecule 1: Pilin



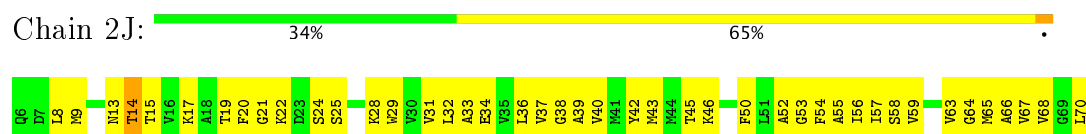
• Molecule 1: Pilin



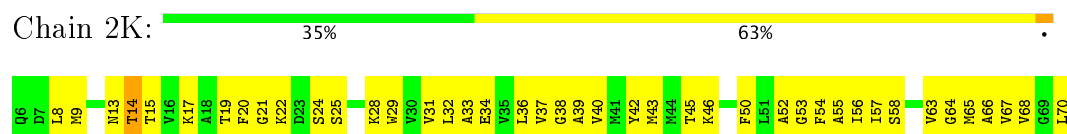
• Molecule 1: Pilin



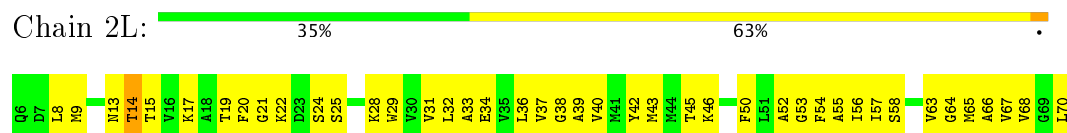
• Molecule 1: Pilin



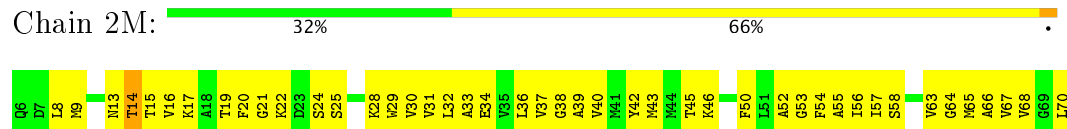
• Molecule 1: Pilin



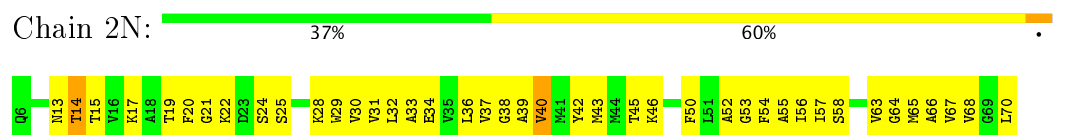
• Molecule 1: Pilin



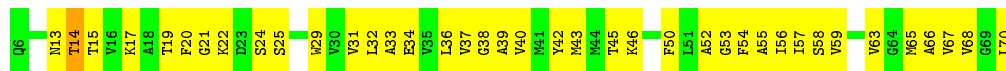
• Molecule 1: Pilin



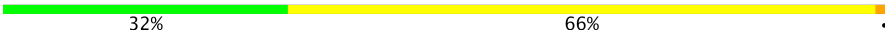
• Molecule 1: Pilin



• Molecule 1: Pilin

Chain 2O:  40% 58%

• Molecule 1: Pilin

Chain 3A:  32% 66%

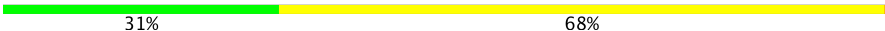
• Molecule 1: Pilin

Chain 3B:  34% 65%

• Molecule 1: Pilin

Chain 3C:  32% 66%

• Molecule 1: Pilin

Chain 3D:  31% 68%

• Molecule 1: Pilin

Chain 3E:  34% 65%

• Molecule 1: Pilin

Chain 3F:  32% 66%

• Molecule 1: Pilin

Chain 3G:  35% 63%



- Molecule 1: Pilin

Chain 3H: 32% 66%



- Molecule 1: Pilin

Chain 3I: 34% 65%



- Molecule 1: Pilin

Chain 3J: 34% 63%



- Molecule 1: Pilin

Chain 3K: 35% 62%



- Molecule 1: Pilin

Chain 3L: 35% 63%



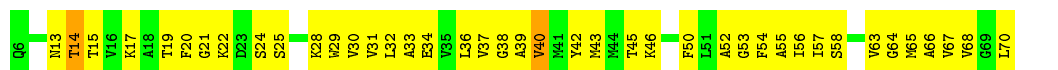
- Molecule 1: Pilin

Chain 3M: 32% 65%

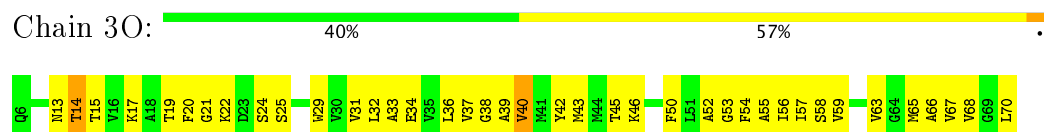


- Molecule 1: Pilin

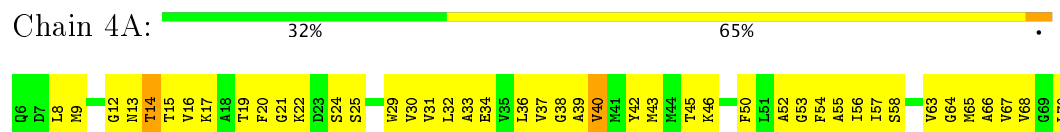
Chain 3N: 37% 60%



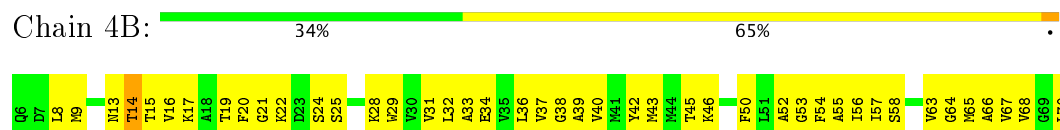
- Molecule 1: Pilin



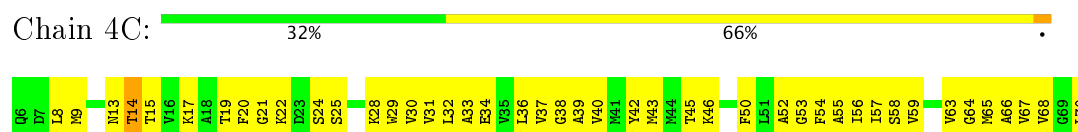
- Molecule 1: Pilin



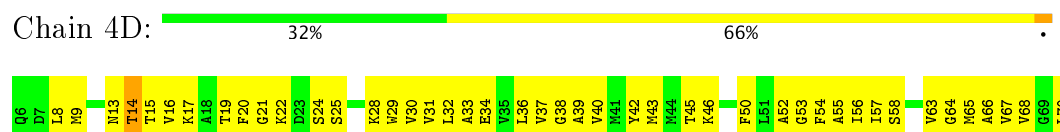
- Molecule 1: Pilin



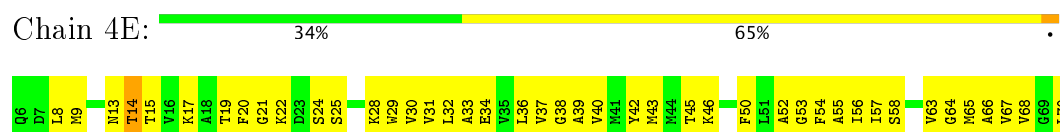
- Molecule 1: Pilin



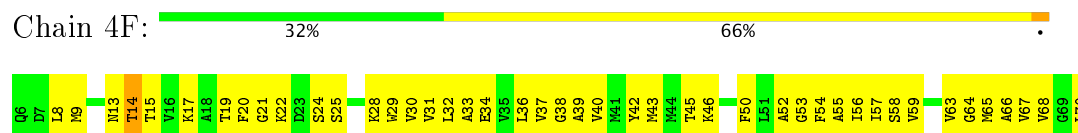
- Molecule 1: Pilin



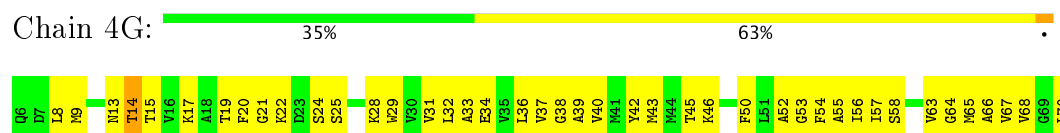
- Molecule 1: Pilin



- Molecule 1: Pilin



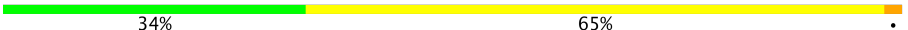
- Molecule 1: Pilin



• Molecule 1: Pilin

Chain 4H:  32% 66%

• Molecule 1: Pilin

Chain 4I:  34% 65%

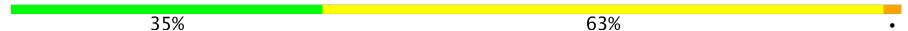
• Molecule 1: Pilin

Chain 4J:  34% 63%

• Molecule 1: Pilin

Chain 4K:  35% 62%

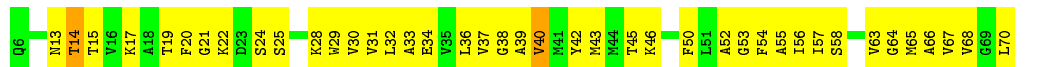
• Molecule 1: Pilin

Chain 4L:  35% 63%

• Molecule 1: Pilin

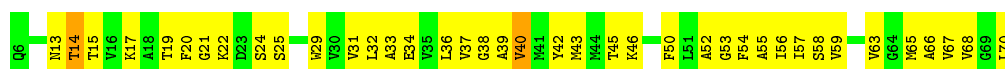
Chain 4M:  32% 66%

• Molecule 1: Pilin

Chain 4N:  37% 60%

• Molecule 1: Pilin

Chain 4O:  40% 57%



- Molecule 1: Pilin

Chain 5A: 32% 66%



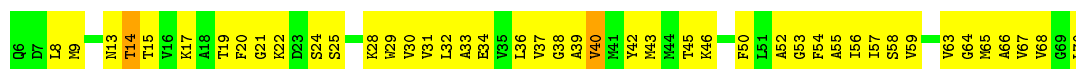
- Molecule 1: Pilin

Chain 5B: 35% 62%



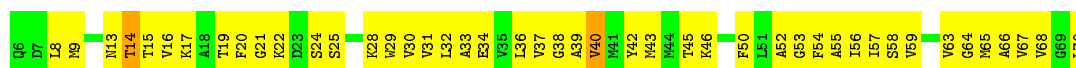
- Molecule 1: Pilin

Chain 5C: 32% 65%



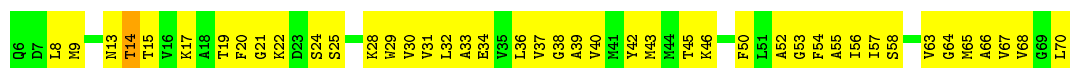
- Molecule 1: Pilin

Chain 5D: 31% 66%



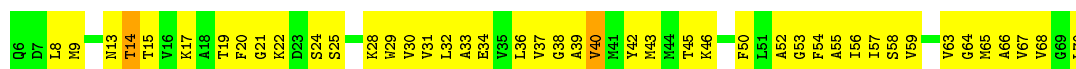
- Molecule 1: Pilin

Chain 5E: 34% 65%



- Molecule 1: Pilin

Chain 5F: 32% 65%

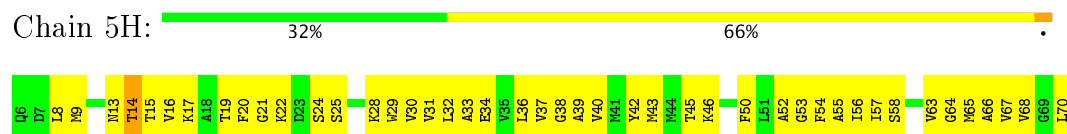


- Molecule 1: Pilin

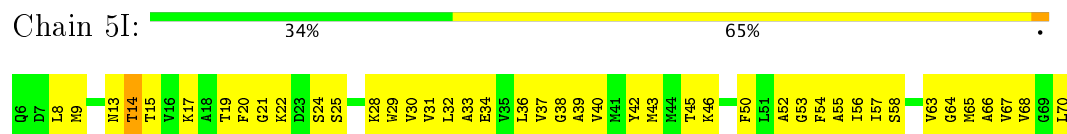
Chain 5G: 35% 63%



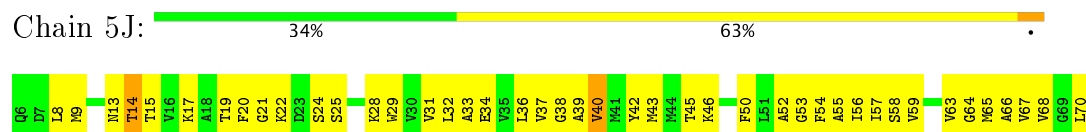
- Molecule 1: Pilin



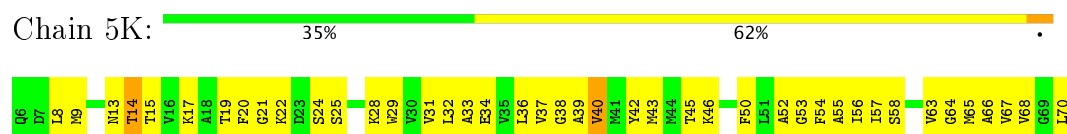
• Molecule 1: Pilin



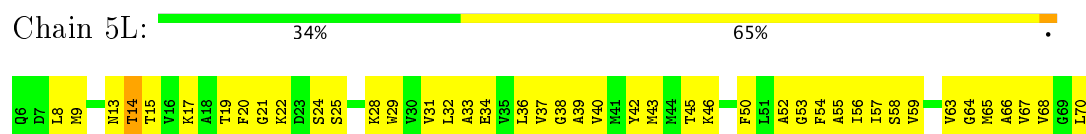
• Molecule 1: Pilin



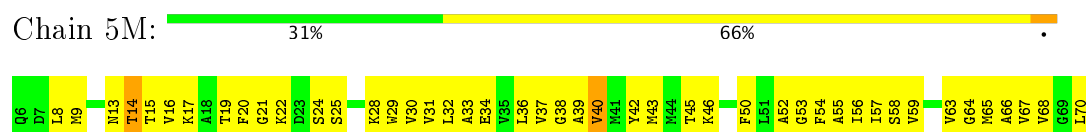
• Molecule 1: Pilin



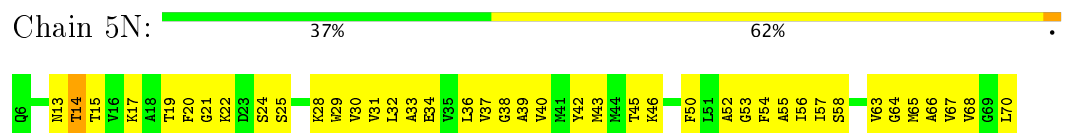
• Molecule 1: Pilin



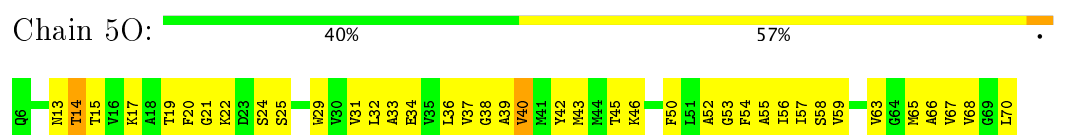
• Molecule 1: Pilin



• Molecule 1: Pilin



• Molecule 1: Pilin



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=27.9°, rise=13.2 Å, axial sym=C5	Depositor
Number of segments used	11969	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.67	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	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: 6V6

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	1A	0.52	0/481	0.61	0/649
1	1B	0.52	0/482	0.61	0/651
1	1C	0.52	0/482	0.61	0/651
1	1D	0.52	0/482	0.61	0/651
1	1E	0.52	0/482	0.61	0/651
1	1F	0.52	0/482	0.61	0/651
1	1G	0.52	0/482	0.61	0/651
1	1H	0.52	0/482	0.61	0/651
1	1I	0.52	0/482	0.61	0/651
1	1J	0.52	0/482	0.61	0/651
1	1K	0.52	0/482	0.61	0/651
1	1L	0.52	0/482	0.61	0/651
1	1M	0.52	0/482	0.61	0/651
1	1N	0.52	0/482	0.61	0/651
1	1O	0.52	0/482	0.61	0/651
1	2A	0.52	0/482	0.61	0/651
1	2B	0.52	0/482	0.61	0/651
1	2C	0.52	0/482	0.61	0/651
1	2D	0.52	0/482	0.61	0/651
1	2E	0.52	0/482	0.61	0/651
1	2F	0.52	0/482	0.61	0/651
1	2G	0.52	0/482	0.61	0/651
1	2H	0.52	0/482	0.61	0/651
1	2I	0.52	0/482	0.61	0/651
1	2J	0.52	0/482	0.61	0/651
1	2K	0.52	0/482	0.61	0/651
1	2L	0.52	0/482	0.61	0/651
1	2M	0.52	0/482	0.61	0/651
1	2N	0.52	0/482	0.61	0/651
1	2O	0.52	0/482	0.61	0/651
1	3A	0.52	0/482	0.61	0/651
1	3B	0.52	0/482	0.61	0/651

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	3C	0.52	0/482	0.61	0/651
1	3D	0.52	0/482	0.61	0/651
1	3E	0.52	0/482	0.61	0/651
1	3F	0.52	0/482	0.61	0/651
1	3G	0.52	0/482	0.61	0/651
1	3H	0.52	0/482	0.61	0/651
1	3I	0.52	0/482	0.61	0/651
1	3J	0.52	0/482	0.61	0/651
1	3K	0.52	0/482	0.61	0/651
1	3L	0.52	0/482	0.61	0/651
1	3M	0.52	0/482	0.61	0/651
1	3N	0.52	0/482	0.61	0/651
1	3O	0.52	0/482	0.61	0/651
1	4A	0.52	0/482	0.61	0/651
1	4B	0.52	0/482	0.61	0/651
1	4C	0.52	0/482	0.61	0/651
1	4D	0.52	0/482	0.61	0/651
1	4E	0.52	0/482	0.61	0/651
1	4F	0.52	0/482	0.61	0/651
1	4G	0.52	0/482	0.61	0/651
1	4H	0.52	0/482	0.61	0/651
1	4I	0.52	0/482	0.61	0/651
1	4J	0.52	0/482	0.61	0/651
1	4K	0.52	0/482	0.61	0/651
1	4L	0.52	0/482	0.61	0/651
1	4M	0.52	0/482	0.61	0/651
1	4N	0.52	0/482	0.61	0/651
1	4O	0.52	0/482	0.61	0/651
1	5A	0.52	0/482	0.61	0/651
1	5B	0.52	0/482	0.61	0/651
1	5C	0.52	0/482	0.61	0/651
1	5D	0.52	0/482	0.61	0/651
1	5E	0.52	0/482	0.61	0/651
1	5F	0.52	0/482	0.61	0/651
1	5G	0.52	0/482	0.61	0/651
1	5H	0.52	0/482	0.61	0/651
1	5I	0.52	0/482	0.61	0/651
1	5J	0.52	0/482	0.61	0/651
1	5K	0.52	0/482	0.61	0/651
1	5L	0.52	0/482	0.61	0/651
1	5M	0.52	0/482	0.61	0/651
1	5N	0.52	0/482	0.61	0/651
1	5O	0.52	0/482	0.61	0/651

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
All	All	0.52	0/36149	0.61	0/48823

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
1	1A	0	1
1	1B	0	1
1	1C	0	1
1	1D	0	1
1	1E	0	1
1	1F	0	1
1	1G	0	1
1	1H	0	1
1	1I	0	1
1	1J	0	1
1	1K	0	1
1	1L	0	1
1	1M	0	1
1	1N	0	1
1	1O	0	1
1	2A	0	1
1	2B	0	1
1	2C	0	1
1	2D	0	1
1	2E	0	1
1	2F	0	1
1	2G	0	1
1	2H	0	1
1	2I	0	1
1	2J	0	1
1	2K	0	1
1	2L	0	1
1	2M	0	1
1	2N	0	1
1	2O	0	1
1	3A	0	1
1	3B	0	1
1	3C	0	1
1	3D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	3E	0	1
1	3F	0	1
1	3G	0	1
1	3H	0	1
1	3I	0	1
1	3J	0	1
1	3K	0	1
1	3L	0	1
1	3M	0	1
1	3N	0	1
1	3O	0	1
1	4A	0	1
1	4B	0	1
1	4C	0	1
1	4D	0	1
1	4E	0	1
1	4F	0	1
1	4G	0	1
1	4H	0	1
1	4I	0	1
1	4J	0	1
1	4K	0	1
1	4L	0	1
1	4M	0	1
1	4N	0	1
1	4O	0	1
1	5A	0	1
1	5B	0	1
1	5C	0	1
1	5D	0	1
1	5E	0	1
1	5F	0	1
1	5G	0	1
1	5H	0	1
1	5I	0	1
1	5J	0	1
1	5K	0	1
1	5L	0	1
1	5M	0	1
1	5N	0	1
1	5O	0	1
All	All	0	75

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 75 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1A	14	THR	Peptide
1	1B	14	THR	Peptide
1	1C	14	THR	Peptide
1	1D	14	THR	Peptide
1	1E	14	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	475	0	508	55	0
1	1B	476	0	509	56	0
1	1C	476	0	509	65	0
1	1D	476	0	509	64	0
1	1E	476	0	509	60	0
1	1F	476	0	509	61	0
1	1G	476	0	509	58	0
1	1H	476	0	509	59	0
1	1I	476	0	509	59	0
1	1J	476	0	509	62	0
1	1K	476	0	509	57	0
1	1L	476	0	509	56	0
1	1M	476	0	509	65	0
1	1N	476	0	509	51	0
1	1O	476	0	509	52	0
1	2A	476	0	509	52	0
1	2B	476	0	509	53	0
1	2C	476	0	509	65	0
1	2D	476	0	509	61	0
1	2E	476	0	509	58	0
1	2F	476	0	509	61	0
1	2G	476	0	509	56	0
1	2H	476	0	509	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2I	476	0	509	57	0
1	2J	476	0	509	61	0
1	2K	476	0	509	56	0
1	2L	476	0	509	56	0
1	2M	476	0	509	66	0
1	2N	476	0	509	52	0
1	2O	476	0	509	51	0
1	3A	476	0	509	52	0
1	3B	476	0	509	56	0
1	3C	476	0	509	65	0
1	3D	476	0	509	64	0
1	3E	476	0	509	58	0
1	3F	476	0	509	61	0
1	3G	476	0	509	57	0
1	3H	476	0	509	59	0
1	3I	476	0	509	57	0
1	3J	476	0	509	61	0
1	3K	476	0	509	58	0
1	3L	476	0	509	56	0
1	3M	476	0	509	63	0
1	3N	476	0	509	53	0
1	3O	476	0	509	50	0
1	4A	476	0	509	53	0
1	4B	476	0	509	55	0
1	4C	476	0	509	63	0
1	4D	476	0	509	65	0
1	4E	476	0	509	59	0
1	4F	476	0	509	62	0
1	4G	476	0	509	59	0
1	4H	476	0	509	62	0
1	4I	476	0	509	60	0
1	4J	476	0	509	58	0
1	4K	476	0	509	55	0
1	4L	476	0	509	55	0
1	4M	476	0	509	63	0
1	4N	476	0	509	48	0
1	4O	476	0	509	51	0
1	5A	476	0	509	50	0
1	5B	476	0	509	53	0
1	5C	476	0	509	67	0
1	5D	476	0	509	66	0
1	5E	476	0	509	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5F	476	0	509	65	0
1	5G	476	0	509	59	0
1	5H	476	0	509	61	0
1	5I	476	0	509	58	0
1	5J	476	0	509	59	0
1	5K	476	0	509	57	0
1	5L	476	0	509	60	0
1	5M	476	0	509	67	0
1	5N	476	0	509	53	0
1	5O	476	0	509	50	0
2	1A	12	0	0	0	0
2	1B	12	0	0	1	0
2	1C	12	0	0	1	0
2	1D	12	0	0	1	0
2	1E	12	0	0	1	0
2	1F	12	0	0	1	0
2	1G	12	0	0	2	0
2	1H	12	0	0	1	0
2	1I	12	0	0	2	0
2	1J	12	0	0	1	0
2	1K	12	0	0	1	0
2	1L	12	0	0	1	0
2	1M	12	0	0	1	0
2	1N	12	0	0	1	0
2	2A	12	0	0	0	0
2	2B	12	0	0	1	0
2	2C	12	0	0	1	0
2	2D	12	0	0	1	0
2	2E	12	0	0	1	0
2	2F	12	0	0	1	0
2	2G	12	0	0	1	0
2	2H	12	0	0	1	0
2	2I	12	0	0	2	0
2	2J	12	0	0	1	0
2	2K	12	0	0	1	0
2	2L	12	0	0	1	0
2	2M	12	0	0	1	0
2	2N	12	0	0	1	0
2	3A	12	0	0	0	0
2	3B	12	0	0	1	0
2	3C	12	0	0	1	0
2	3D	12	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	3E	12	0	0	1	0
2	3F	12	0	0	1	0
2	3G	12	0	0	1	0
2	3H	12	0	0	1	0
2	3I	12	0	0	2	0
2	3J	12	0	0	1	0
2	3K	12	0	0	1	0
2	3L	12	0	0	1	0
2	3M	12	0	0	1	0
2	3N	12	0	0	1	0
2	4A	12	0	0	0	0
2	4B	12	0	0	1	0
2	4C	12	0	0	1	0
2	4D	12	0	0	1	0
2	4E	12	0	0	1	0
2	4F	12	0	0	1	0
2	4G	12	0	0	1	0
2	4H	12	0	0	1	0
2	4I	12	0	0	2	0
2	4J	12	0	0	1	0
2	4K	12	0	0	1	0
2	4L	12	0	0	1	0
2	4M	12	0	0	1	0
2	4N	12	0	0	1	0
2	5A	12	0	0	0	0
2	5B	12	0	0	1	0
2	5C	12	0	0	1	0
2	5D	12	0	0	1	0
2	5E	12	0	0	1	0
2	5F	12	0	0	1	0
2	5G	12	0	0	1	0
2	5H	12	0	0	1	0
2	5I	12	0	0	1	0
2	5J	12	0	0	1	0
2	5K	12	0	0	1	0
2	5L	12	0	0	1	0
2	5M	12	0	0	1	0
2	5N	12	0	0	1	0
All	All	36539	0	38174	3428	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 46.

The worst 5 of 3428 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)
1:3C:67:VAL:HG13	1:4A:9:MET:CE	1.15	1.63
1:2C:67:VAL:HG13	1:3A:9:MET:CE	1.15	1.61
1:4C:67:VAL:HG13	1:5A:9:MET:CE	1.17	1.60
1:1A:9:MET:CE	1:5C:67:VAL:HG13	1.15	1.60
1:3D:67:VAL:HG13	1:4B:9:MET:CE	1.39	1.53

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	1A	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	1B	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	1C	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	1D	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52
1	1E	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	1F	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52
1	1G	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52
1	1H	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	1I	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	1J	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52
1	1K	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52
1	1L	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	1M	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52
1	1N	63/65 (97%)	52 (82%)	11 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1O	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52
1	2A	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	2B	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	2C	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	2D	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	2E	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	2F	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	2G	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	2H	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	2I	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	2J	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	2K	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	2L	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	2M	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	2N	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52
1	2O	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	3A	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	3B	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	3C	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	3D	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	3E	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	3F	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	3G	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	3H	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	3I	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	3J	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52
1	3K	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52
1	3L	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	3M	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52
1	3N	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52
1	3O	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4A	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52
1	4B	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	4C	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	4D	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	4E	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	4F	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	4G	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	4H	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	4I	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	4J	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52
1	4K	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52
1	4L	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	4M	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	4N	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52
1	4O	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52
1	5A	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	5B	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52
1	5C	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52
1	5D	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52
1	5E	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	5F	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52
1	5G	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	5H	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	5I	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	5J	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52
1	5K	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52
1	5L	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	5M	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52
1	5N	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	5O	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	52
All	All	4725/4875 (97%)	3900 (82%)	799 (17%)	26 (1%)	33	70

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1D	40	VAL
1	1F	40	VAL
1	1G	40	VAL
1	1J	40	VAL
1	1K	40	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain 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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	50/51 (98%)	50 (100%)	0	100	100
1	1B	51/51 (100%)	51 (100%)	0	100	100
1	1C	51/51 (100%)	51 (100%)	0	100	100
1	1D	51/51 (100%)	51 (100%)	0	100	100
1	1E	51/51 (100%)	51 (100%)	0	100	100
1	1F	51/51 (100%)	51 (100%)	0	100	100
1	1G	51/51 (100%)	51 (100%)	0	100	100
1	1H	51/51 (100%)	51 (100%)	0	100	100
1	1I	51/51 (100%)	51 (100%)	0	100	100
1	1J	51/51 (100%)	51 (100%)	0	100	100
1	1K	51/51 (100%)	51 (100%)	0	100	100
1	1L	51/51 (100%)	51 (100%)	0	100	100
1	1M	51/51 (100%)	51 (100%)	0	100	100
1	1N	51/51 (100%)	51 (100%)	0	100	100
1	1O	51/51 (100%)	51 (100%)	0	100	100
1	2A	51/51 (100%)	51 (100%)	0	100	100
1	2B	51/51 (100%)	51 (100%)	0	100	100
1	2C	51/51 (100%)	51 (100%)	0	100	100
1	2D	51/51 (100%)	51 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2E	51/51 (100%)	51 (100%)	0	100	100
1	2F	51/51 (100%)	51 (100%)	0	100	100
1	2G	51/51 (100%)	51 (100%)	0	100	100
1	2H	51/51 (100%)	51 (100%)	0	100	100
1	2I	51/51 (100%)	51 (100%)	0	100	100
1	2J	51/51 (100%)	51 (100%)	0	100	100
1	2K	51/51 (100%)	51 (100%)	0	100	100
1	2L	51/51 (100%)	51 (100%)	0	100	100
1	2M	51/51 (100%)	51 (100%)	0	100	100
1	2N	51/51 (100%)	51 (100%)	0	100	100
1	2O	51/51 (100%)	51 (100%)	0	100	100
1	3A	51/51 (100%)	51 (100%)	0	100	100
1	3B	51/51 (100%)	51 (100%)	0	100	100
1	3C	51/51 (100%)	51 (100%)	0	100	100
1	3D	51/51 (100%)	51 (100%)	0	100	100
1	3E	51/51 (100%)	51 (100%)	0	100	100
1	3F	51/51 (100%)	51 (100%)	0	100	100
1	3G	51/51 (100%)	51 (100%)	0	100	100
1	3H	51/51 (100%)	51 (100%)	0	100	100
1	3I	51/51 (100%)	51 (100%)	0	100	100
1	3J	51/51 (100%)	51 (100%)	0	100	100
1	3K	51/51 (100%)	51 (100%)	0	100	100
1	3L	51/51 (100%)	51 (100%)	0	100	100
1	3M	51/51 (100%)	51 (100%)	0	100	100
1	3N	51/51 (100%)	51 (100%)	0	100	100
1	3O	51/51 (100%)	51 (100%)	0	100	100
1	4A	51/51 (100%)	51 (100%)	0	100	100
1	4B	51/51 (100%)	51 (100%)	0	100	100
1	4C	51/51 (100%)	51 (100%)	0	100	100
1	4D	51/51 (100%)	51 (100%)	0	100	100
1	4E	51/51 (100%)	51 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4F	51/51 (100%)	51 (100%)	0	100	100
1	4G	51/51 (100%)	51 (100%)	0	100	100
1	4H	51/51 (100%)	51 (100%)	0	100	100
1	4I	51/51 (100%)	51 (100%)	0	100	100
1	4J	51/51 (100%)	51 (100%)	0	100	100
1	4K	51/51 (100%)	51 (100%)	0	100	100
1	4L	51/51 (100%)	51 (100%)	0	100	100
1	4M	51/51 (100%)	51 (100%)	0	100	100
1	4N	51/51 (100%)	51 (100%)	0	100	100
1	4O	51/51 (100%)	51 (100%)	0	100	100
1	5A	51/51 (100%)	51 (100%)	0	100	100
1	5B	51/51 (100%)	51 (100%)	0	100	100
1	5C	51/51 (100%)	51 (100%)	0	100	100
1	5D	51/51 (100%)	51 (100%)	0	100	100
1	5E	51/51 (100%)	51 (100%)	0	100	100
1	5F	51/51 (100%)	51 (100%)	0	100	100
1	5G	51/51 (100%)	51 (100%)	0	100	100
1	5H	51/51 (100%)	51 (100%)	0	100	100
1	5I	51/51 (100%)	51 (100%)	0	100	100
1	5J	51/51 (100%)	51 (100%)	0	100	100
1	5K	51/51 (100%)	51 (100%)	0	100	100
1	5L	51/51 (100%)	51 (100%)	0	100	100
1	5M	51/51 (100%)	51 (100%)	0	100	100
1	5N	51/51 (100%)	51 (100%)	0	100	100
1	5O	51/51 (100%)	51 (100%)	0	100	100
All	All	3824/3825 (100%)	3824 (100%)	0	100	100

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

70 ligands 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	$\# Z > 2$
2	6V6	1A	101	-	11,11,48	0.50	0	11,14,54	0.53	0
2	6V6	1B	101	-	11,11,48	0.51	0	11,14,54	0.53	0
2	6V6	1C	101	-	11,11,48	0.50	0	11,14,54	0.53	0
2	6V6	1D	101	-	11,11,48	0.51	0	11,14,54	0.53	0
2	6V6	1E	101	-	11,11,48	0.50	0	11,14,54	0.52	0
2	6V6	1F	101	-	11,11,48	0.51	0	11,14,54	0.54	0
2	6V6	1G	101	-	11,11,48	0.51	0	11,14,54	0.52	0
2	6V6	1H	101	-	11,11,48	0.51	0	11,14,54	0.52	0
2	6V6	1I	101	-	11,11,48	0.50	0	11,14,54	0.53	0
2	6V6	1J	101	-	11,11,48	0.51	0	11,14,54	0.52	0
2	6V6	1K	101	-	11,11,48	0.50	0	11,14,54	0.51	0
2	6V6	1L	101	-	11,11,48	0.50	0	11,14,54	0.53	0
2	6V6	1M	101	-	11,11,48	0.51	0	11,14,54	0.52	0
2	6V6	1N	101	-	11,11,48	0.51	0	11,14,54	0.53	0
2	6V6	2A	101	-	11,11,48	0.50	0	11,14,54	0.53	0
2	6V6	2B	101	-	11,11,48	0.50	0	11,14,54	0.53	0
2	6V6	2C	101	-	11,11,48	0.50	0	11,14,54	0.53	0
2	6V6	2D	101	-	11,11,48	0.51	0	11,14,54	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	6V6	2E	101	-	11,11,48	0.51	0	11,14,54	0.52	0
2	6V6	2F	101	-	11,11,48	0.51	0	11,14,54	0.54	0
2	6V6	2G	101	-	11,11,48	0.51	0	11,14,54	0.52	0
2	6V6	2H	101	-	11,11,48	0.50	0	11,14,54	0.52	0
2	6V6	2I	101	-	11,11,48	0.50	0	11,14,54	0.53	0
2	6V6	2J	101	-	11,11,48	0.51	0	11,14,54	0.52	0
2	6V6	2K	101	-	11,11,48	0.50	0	11,14,54	0.51	0
2	6V6	2L	101	-	11,11,48	0.51	0	11,14,54	0.53	0
2	6V6	2M	101	-	11,11,48	0.50	0	11,14,54	0.51	0
2	6V6	2N	101	-	11,11,48	0.51	0	11,14,54	0.53	0
2	6V6	3A	101	-	11,11,48	0.51	0	11,14,54	0.53	0
2	6V6	3B	101	-	11,11,48	0.51	0	11,14,54	0.53	0
2	6V6	3C	101	-	11,11,48	0.50	0	11,14,54	0.53	0
2	6V6	3D	101	-	11,11,48	0.51	0	11,14,54	0.53	0
2	6V6	3E	101	-	11,11,48	0.51	0	11,14,54	0.52	0
2	6V6	3F	101	-	11,11,48	0.51	0	11,14,54	0.54	0
2	6V6	3G	101	-	11,11,48	0.51	0	11,14,54	0.52	0
2	6V6	3H	101	-	11,11,48	0.51	0	11,14,54	0.52	0
2	6V6	3I	101	-	11,11,48	0.51	0	11,14,54	0.53	0
2	6V6	3J	101	-	11,11,48	0.51	0	11,14,54	0.52	0
2	6V6	3K	101	-	11,11,48	0.51	0	11,14,54	0.51	0
2	6V6	3L	101	-	11,11,48	0.50	0	11,14,54	0.53	0
2	6V6	3M	101	-	11,11,48	0.51	0	11,14,54	0.52	0
2	6V6	3N	101	-	11,11,48	0.51	0	11,14,54	0.53	0
2	6V6	4A	101	-	11,11,48	0.50	0	11,14,54	0.53	0
2	6V6	4B	101	-	11,11,48	0.51	0	11,14,54	0.53	0
2	6V6	4C	101	-	11,11,48	0.50	0	11,14,54	0.53	0
2	6V6	4D	101	-	11,11,48	0.51	0	11,14,54	0.52	0
2	6V6	4E	101	-	11,11,48	0.51	0	11,14,54	0.52	0
2	6V6	4F	101	-	11,11,48	0.51	0	11,14,54	0.54	0
2	6V6	4G	101	-	11,11,48	0.51	0	11,14,54	0.52	0
2	6V6	4H	101	-	11,11,48	0.51	0	11,14,54	0.52	0
2	6V6	4I	101	-	11,11,48	0.50	0	11,14,54	0.52	0
2	6V6	4J	101	-	11,11,48	0.50	0	11,14,54	0.52	0
2	6V6	4K	101	-	11,11,48	0.50	0	11,14,54	0.51	0
2	6V6	4L	101	-	11,11,48	0.50	0	11,14,54	0.53	0
2	6V6	4M	101	-	11,11,48	0.50	0	11,14,54	0.51	0
2	6V6	4N	101	-	11,11,48	0.51	0	11,14,54	0.53	0
2	6V6	5A	101	-	11,11,48	0.50	0	11,14,54	0.53	0
2	6V6	5B	101	-	11,11,48	0.51	0	11,14,54	0.53	0
2	6V6	5C	101	-	11,11,48	0.51	0	11,14,54	0.53	0
2	6V6	5D	101	-	11,11,48	0.51	0	11,14,54	0.52	0
2	6V6	5E	101	-	11,11,48	0.50	0	11,14,54	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	6V6	5F	101	-	11,11,48	0.50	0	11,14,54	0.54	0
2	6V6	5G	101	-	11,11,48	0.50	0	11,14,54	0.52	0
2	6V6	5H	101	-	11,11,48	0.51	0	11,14,54	0.52	0
2	6V6	5I	101	-	11,11,48	0.50	0	11,14,54	0.53	0
2	6V6	5J	101	-	11,11,48	0.51	0	11,14,54	0.52	0
2	6V6	5K	101	-	11,11,48	0.51	0	11,14,54	0.52	0
2	6V6	5L	101	-	11,11,48	0.50	0	11,14,54	0.53	0
2	6V6	5M	101	-	11,11,48	0.51	0	11,14,54	0.52	0
2	6V6	5N	101	-	11,11,48	0.51	0	11,14,54	0.53	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
2	6V6	1A	101	-	-	0/12/12/53	0/0/0/0
2	6V6	1B	101	-	-	0/12/12/53	0/0/0/0
2	6V6	1C	101	-	-	0/12/12/53	0/0/0/0
2	6V6	1D	101	-	-	0/12/12/53	0/0/0/0
2	6V6	1E	101	-	-	0/12/12/53	0/0/0/0
2	6V6	1F	101	-	-	0/12/12/53	0/0/0/0
2	6V6	1G	101	-	-	0/12/12/53	0/0/0/0
2	6V6	1H	101	-	-	0/12/12/53	0/0/0/0
2	6V6	1I	101	-	-	0/12/12/53	0/0/0/0
2	6V6	1J	101	-	-	0/12/12/53	0/0/0/0
2	6V6	1K	101	-	-	0/12/12/53	0/0/0/0
2	6V6	1L	101	-	-	0/12/12/53	0/0/0/0
2	6V6	1M	101	-	-	0/12/12/53	0/0/0/0
2	6V6	1N	101	-	-	0/12/12/53	0/0/0/0
2	6V6	2A	101	-	-	0/12/12/53	0/0/0/0
2	6V6	2B	101	-	-	0/12/12/53	0/0/0/0
2	6V6	2C	101	-	-	0/12/12/53	0/0/0/0
2	6V6	2D	101	-	-	0/12/12/53	0/0/0/0
2	6V6	2E	101	-	-	0/12/12/53	0/0/0/0
2	6V6	2F	101	-	-	0/12/12/53	0/0/0/0
2	6V6	2G	101	-	-	0/12/12/53	0/0/0/0
2	6V6	2H	101	-	-	0/12/12/53	0/0/0/0
2	6V6	2I	101	-	-	0/12/12/53	0/0/0/0
2	6V6	2J	101	-	-	0/12/12/53	0/0/0/0
2	6V6	2K	101	-	-	0/12/12/53	0/0/0/0
2	6V6	2L	101	-	-	0/12/12/53	0/0/0/0
2	6V6	2M	101	-	-	0/12/12/53	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6V6	2N	101	-	-	0/12/12/53	0/0/0/0
2	6V6	3A	101	-	-	0/12/12/53	0/0/0/0
2	6V6	3B	101	-	-	0/12/12/53	0/0/0/0
2	6V6	3C	101	-	-	0/12/12/53	0/0/0/0
2	6V6	3D	101	-	-	0/12/12/53	0/0/0/0
2	6V6	3E	101	-	-	0/12/12/53	0/0/0/0
2	6V6	3F	101	-	-	0/12/12/53	0/0/0/0
2	6V6	3G	101	-	-	0/12/12/53	0/0/0/0
2	6V6	3H	101	-	-	0/12/12/53	0/0/0/0
2	6V6	3I	101	-	-	0/12/12/53	0/0/0/0
2	6V6	3J	101	-	-	0/12/12/53	0/0/0/0
2	6V6	3K	101	-	-	0/12/12/53	0/0/0/0
2	6V6	3L	101	-	-	0/12/12/53	0/0/0/0
2	6V6	3M	101	-	-	0/12/12/53	0/0/0/0
2	6V6	3N	101	-	-	0/12/12/53	0/0/0/0
2	6V6	4A	101	-	-	0/12/12/53	0/0/0/0
2	6V6	4B	101	-	-	0/12/12/53	0/0/0/0
2	6V6	4C	101	-	-	0/12/12/53	0/0/0/0
2	6V6	4D	101	-	-	0/12/12/53	0/0/0/0
2	6V6	4E	101	-	-	0/12/12/53	0/0/0/0
2	6V6	4F	101	-	-	0/12/12/53	0/0/0/0
2	6V6	4G	101	-	-	0/12/12/53	0/0/0/0
2	6V6	4H	101	-	-	0/12/12/53	0/0/0/0
2	6V6	4I	101	-	-	0/12/12/53	0/0/0/0
2	6V6	4J	101	-	-	0/12/12/53	0/0/0/0
2	6V6	4K	101	-	-	0/12/12/53	0/0/0/0
2	6V6	4L	101	-	-	0/12/12/53	0/0/0/0
2	6V6	4M	101	-	-	0/12/12/53	0/0/0/0
2	6V6	4N	101	-	-	0/12/12/53	0/0/0/0
2	6V6	5A	101	-	-	0/12/12/53	0/0/0/0
2	6V6	5B	101	-	-	0/12/12/53	0/0/0/0
2	6V6	5C	101	-	-	0/12/12/53	0/0/0/0
2	6V6	5D	101	-	-	0/12/12/53	0/0/0/0
2	6V6	5E	101	-	-	0/12/12/53	0/0/0/0
2	6V6	5F	101	-	-	0/12/12/53	0/0/0/0
2	6V6	5G	101	-	-	0/12/12/53	0/0/0/0
2	6V6	5H	101	-	-	0/12/12/53	0/0/0/0
2	6V6	5I	101	-	-	0/12/12/53	0/0/0/0
2	6V6	5J	101	-	-	0/12/12/53	0/0/0/0
2	6V6	5K	101	-	-	0/12/12/53	0/0/0/0
2	6V6	5L	101	-	-	0/12/12/53	0/0/0/0
2	6V6	5M	101	-	-	0/12/12/53	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6V6	5N	101	-	-	0/12/12/53	0/0/0/0

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.

65 monomers are involved in 70 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1B	101	6V6	1	0
2	1C	101	6V6	1	0
2	1D	101	6V6	1	0
2	1E	101	6V6	1	0
2	1F	101	6V6	1	0
2	1G	101	6V6	2	0
2	1H	101	6V6	1	0
2	1I	101	6V6	2	0
2	1J	101	6V6	1	0
2	1K	101	6V6	1	0
2	1L	101	6V6	1	0
2	1M	101	6V6	1	0
2	1N	101	6V6	1	0
2	2B	101	6V6	1	0
2	2C	101	6V6	1	0
2	2D	101	6V6	1	0
2	2E	101	6V6	1	0
2	2F	101	6V6	1	0
2	2G	101	6V6	1	0
2	2H	101	6V6	1	0
2	2I	101	6V6	2	0
2	2J	101	6V6	1	0
2	2K	101	6V6	1	0
2	2L	101	6V6	1	0
2	2M	101	6V6	1	0
2	2N	101	6V6	1	0
2	3B	101	6V6	1	0
2	3C	101	6V6	1	0
2	3D	101	6V6	1	0
2	3E	101	6V6	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	3F	101	6V6	1	0
2	3G	101	6V6	1	0
2	3H	101	6V6	1	0
2	3I	101	6V6	2	0
2	3J	101	6V6	1	0
2	3K	101	6V6	1	0
2	3L	101	6V6	1	0
2	3M	101	6V6	1	0
2	3N	101	6V6	1	0
2	4B	101	6V6	1	0
2	4C	101	6V6	1	0
2	4D	101	6V6	1	0
2	4E	101	6V6	1	0
2	4F	101	6V6	1	0
2	4G	101	6V6	1	0
2	4H	101	6V6	1	0
2	4I	101	6V6	2	0
2	4J	101	6V6	1	0
2	4K	101	6V6	1	0
2	4L	101	6V6	1	0
2	4M	101	6V6	1	0
2	4N	101	6V6	1	0
2	5B	101	6V6	1	0
2	5C	101	6V6	1	0
2	5D	101	6V6	1	0
2	5E	101	6V6	1	0
2	5F	101	6V6	1	0
2	5G	101	6V6	1	0
2	5H	101	6V6	1	0
2	5I	101	6V6	1	0
2	5J	101	6V6	1	0
2	5K	101	6V6	1	0
2	5L	101	6V6	1	0
2	5M	101	6V6	1	0
2	5N	101	6V6	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.