



## wwPDB EM Map/Model Validation Report ⓘ

Oct 25, 2016 – 04:51 PM EDT

PDB ID : 5LFB  
EMDB ID: : EMD-4046  
Title : Structure of the bacterial sex F pilus (12.5 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 EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

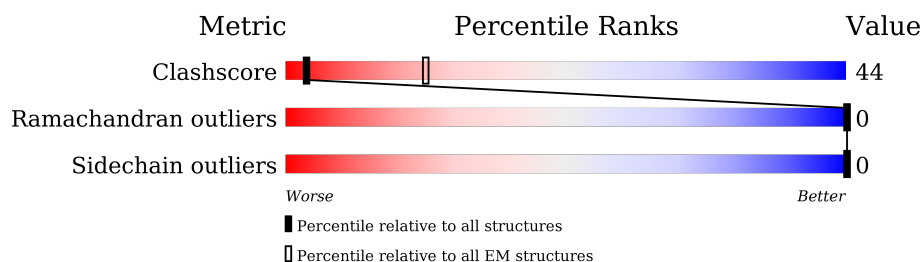
# 1 Overall quality at a glance

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.






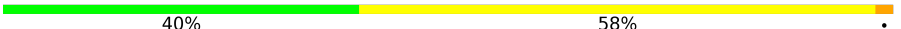
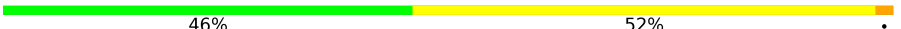

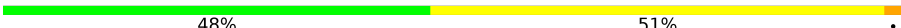


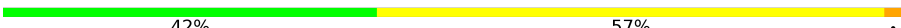
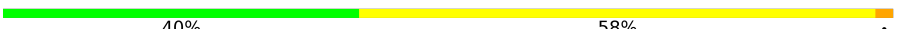
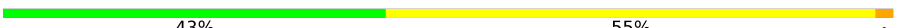




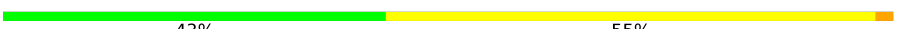
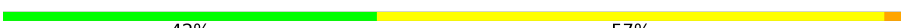

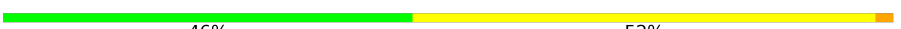


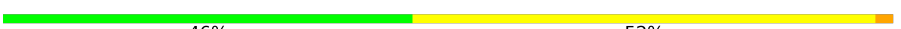


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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  $\geq 3$ , 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	48% 51% .
1	1B	65	45% 54% .
1	1C	65	35% 63% .
1	1D	65	42% 57% .
1	1E	65	40% 58% .
1	1F	65	40% 58% .
1	1G	65	38% 60% .
1	1H	65	42% 57% .
1	1I	65	45% 54% .


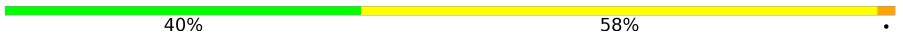
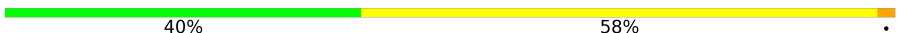


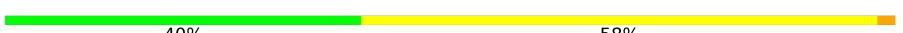
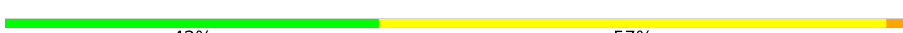




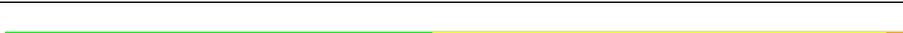













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Mol	Chain	Length	Quality of chain
1	1J	65	 40% 58%
1	1K	65	 45% 54%
1	1L	65	 38% 60%
1	1M	65	 40% 58%
1	1N	65	 46% 52%
1	1O	65	 49% 49%
1	2A	65	 48% 51%
1	2B	65	 45% 54%
1	2C	65	 34% 65%
1	2D	65	 42% 57%
1	2E	65	 40% 58%
1	2F	65	 43% 55%
1	2G	65	 40% 58%
1	2H	65	 42% 57%
1	2I	65	 43% 55%
1	2J	65	 42% 57%
1	2K	65	 43% 55%
1	2L	65	 42% 57%
1	2M	65	 46% 52%
1	2N	65	 46% 52%
1	2O	65	 51% 48%
1	3A	65	 51% 48%
1	3B	65	 46% 52%
1	3C	65	 37% 62%
1	3D	65	 43% 55%

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Mol	Chain	Length	Quality of chain	
1	3E	65		.
1	3F	65		.
1	3G	65		.
1	3H	65		.
1	3I	65		.
1	3J	65		.
1	3K	65		.
1	3L	65		.
1	3M	65		.
1	3N	65		.
1	3O	65		.
1	4A	65		.
1	4B	65		.
1	4C	65		.
1	4D	65		.
1	4E	65		.
1	4F	65		.
1	4G	65		.
1	4H	65		.
1	4I	65		.
1	4J	65		.
1	4K	65		.
1	4L	65		.
1	4M	65		.
1	4N	65		.

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Mol	Chain	Length	Quality of chain
1	4O	65	<div><div></div><div>51%</div><div>48%</div><div></div></div>
1	5A	65	<div><div></div><div>48%</div><div>51%</div><div></div></div>
1	5B	65	<div><div></div><div>42%</div><div>57%</div><div></div></div>
1	5C	65	<div><div></div><div>37%</div><div>62%</div><div></div></div>
1	5D	65	<div><div></div><div>43%</div><div>55%</div><div></div></div>
1	5E	65	<div><div></div><div>43%</div><div>55%</div><div></div></div>
1	5F	65	<div><div></div><div>43%</div><div>55%</div><div></div></div>
1	5G	65	<div><div></div><div>42%</div><div>57%</div><div></div></div>
1	5H	65	<div><div></div><div>43%</div><div>55%</div><div></div></div>
1	5I	65	<div><div></div><div>43%</div><div>55%</div><div></div></div>
1	5J	65	<div><div></div><div>42%</div><div>57%</div><div></div></div>
1	5K	65	<div><div></div><div>46%</div><div>52%</div><div></div></div>
1	5L	65	<div><div></div><div>43%</div><div>55%</div><div></div></div>
1	5M	65	<div><div></div><div>48%</div><div>51%</div><div></div></div>
1	5N	65	<div><div></div><div>48%</div><div>51%</div><div></div></div>
1	5O	65	<div><div></div><div>46%</div><div>52%</div><div></div></div>

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 36600 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
			476	314	74	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

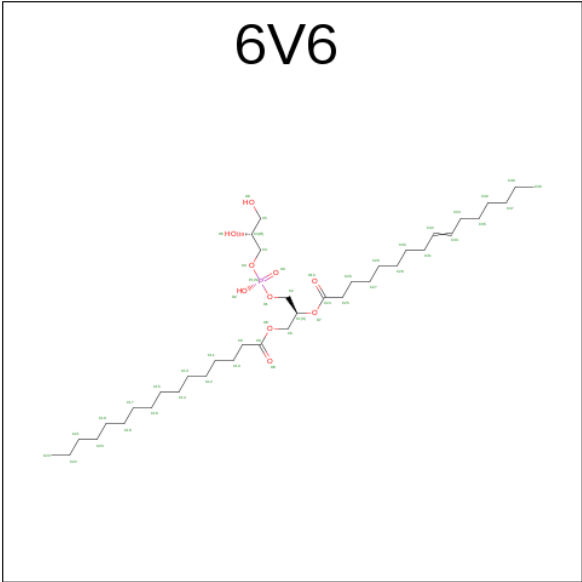
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	4O	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	5A	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	5B	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	5C	65	Total 476	C 314	N 74	O 83	S 5	0	0
1	5D	65	Total 476	C 314	N 74	O 83	S 5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

- 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: C<sub>38</sub>H<sub>73</sub>O<sub>10</sub>P).



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

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

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Mol	Chain	Residues	Atoms				AltConf
2	4L	1	Total 12	C 5	O 6	P 1	0
2	4M	1	Total 12	C 5	O 6	P 1	0
2	4N	1	Total 12	C 5	O 6	P 1	0
2	4O	1	Total 12	C 5	O 6	P 1	0
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
2	5O	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 errors 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

Chain 1A: 



- Molecule 1: Pilin

Chain 1B: 



- Molecule 1: Pilin

Chain 1C: 



- Molecule 1: Pilin

Chain 1D: 



- Molecule 1: Pilin

Chain 1E: 

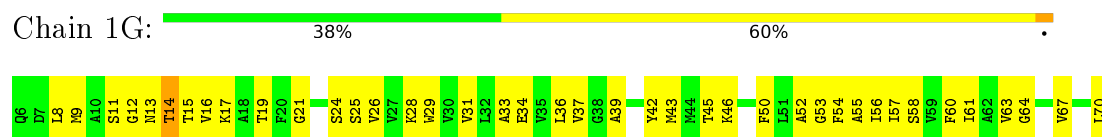


- Molecule 1: Pilin

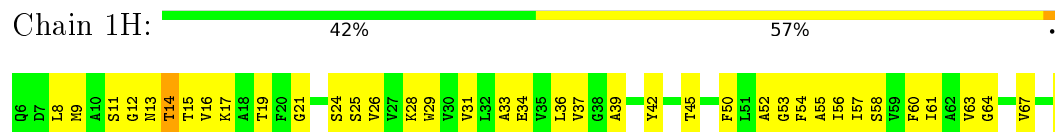
Chain 1F: 



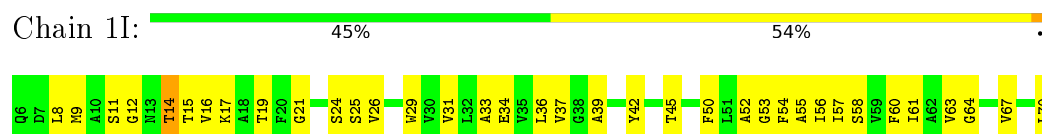
## • Molecule 1: Pilin



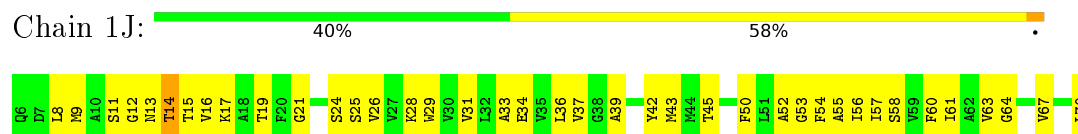
## • Molecule 1: Pilin



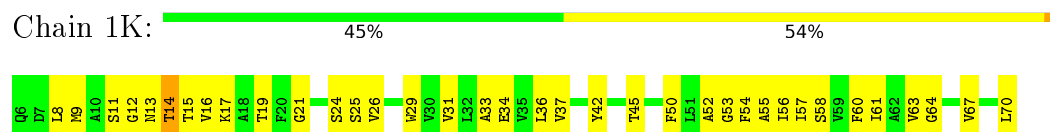
## • Molecule 1: Pilin



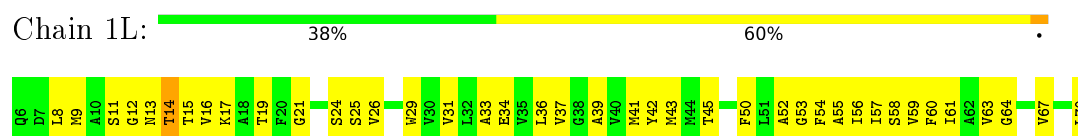
## • Molecule 1: Pilin



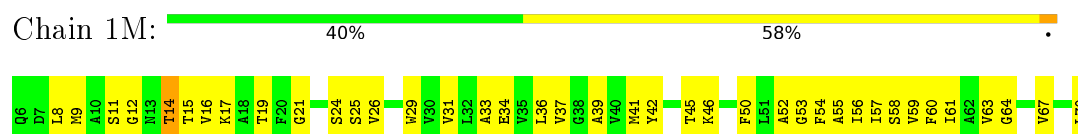
## • Molecule 1: Pilin



## • Molecule 1: Pilin

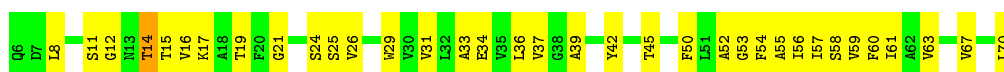


## • Molecule 1: Pilin



## • Molecule 1: Pilin





- Molecule 1: Pilin

Chain 1O: .



- Molecule 1: Pilin

Chain 2A: .



- Molecule 1: Pilin

Chain 2B: .



- Molecule 1: Pilin

Chain 2C: .



- Molecule 1: Pilin

Chain 2D: .



- Molecule 1: Pilin

Chain 2E: .



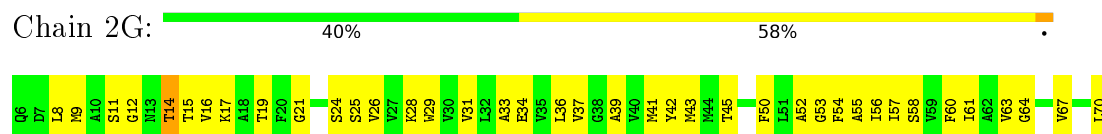
- Molecule 1: Pilin

Chain 2F: .

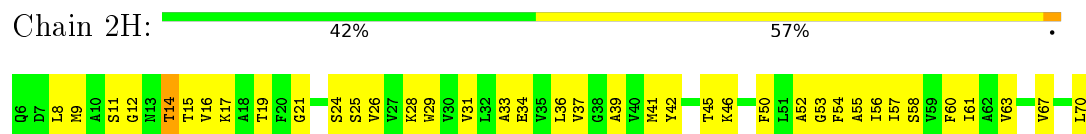


- Molecule 1: Pilin

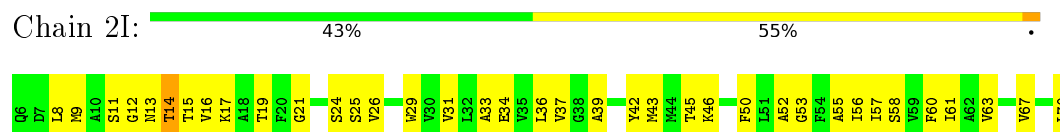




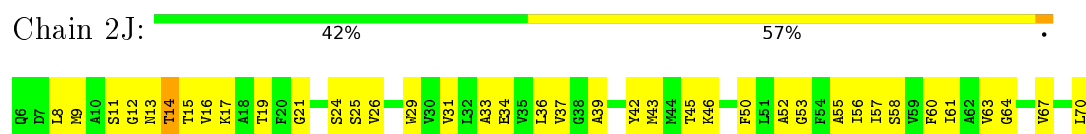
- Molecule 1: Pilin



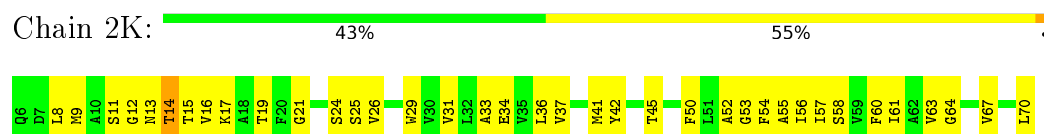
- Molecule 1: Pilin



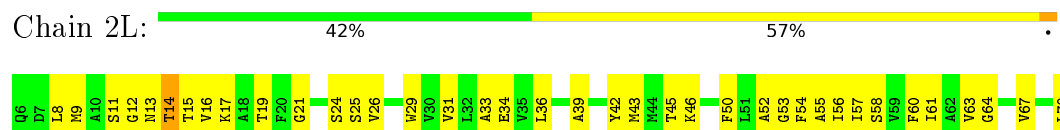
- Molecule 1: Pilin



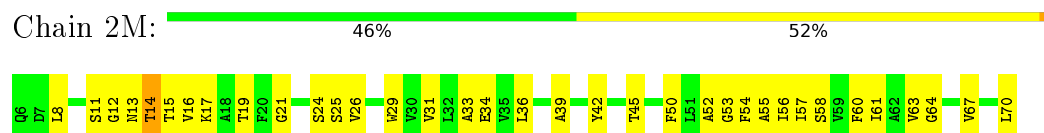
- Molecule 1: Pilin



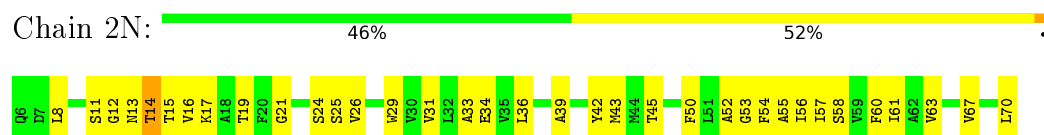
- Molecule 1: Pilin



- Molecule 1: Pilin



- Molecule 1: Pilin



## • Molecule 1: Pilin

Chain 2O:  51% 48%

## • Molecule 1: Pilin

Chain 3A:  51% 48%

## • Molecule 1: Pilin

Chain 3B:  46% 52%

## • Molecule 1: Pilin

Chain 3C:  37% 62%

## • Molecule 1: Pilin

Chain 3D:  43% 55%

## • Molecule 1: Pilin

Chain 3E:  40% 58%

## • Molecule 1: Pilin

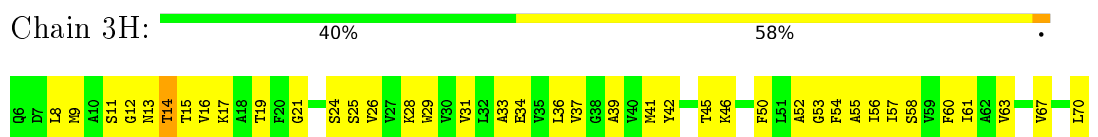
Chain 3F:  40% 58%

## • Molecule 1: Pilin

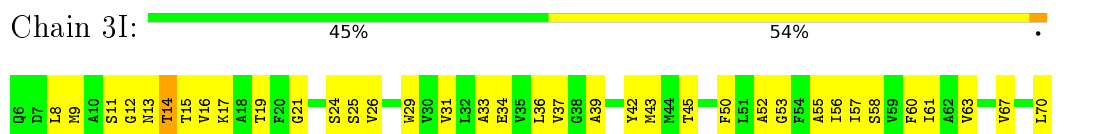
Chain 3G:  40% 58%



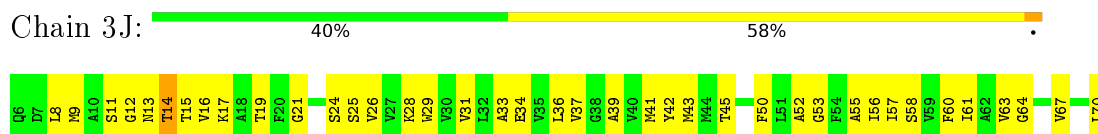
- Molecule 1: Pilin



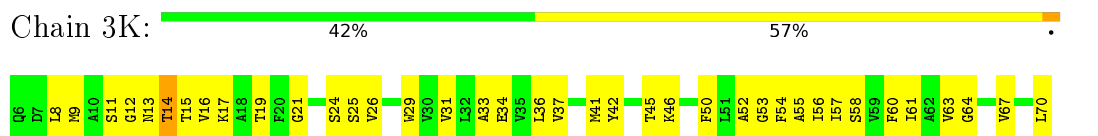
- Molecule 1: Pilin



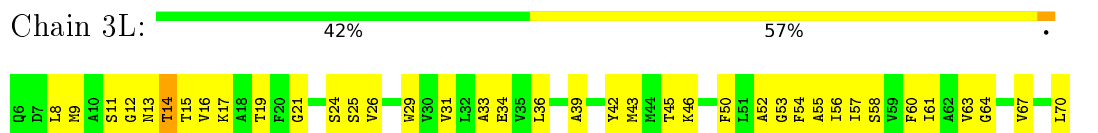
- Molecule 1: Pilin



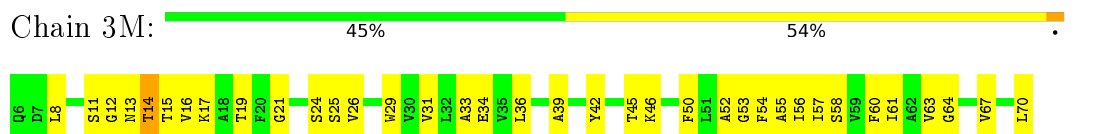
- Molecule 1: Pilin



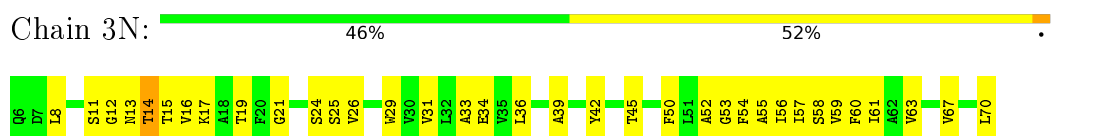
- Molecule 1: Pilin



- Molecule 1: Pilin



- Molecule 1: Pilin



- Molecule 1: Pilin

Chain 3O:  .



• Molecule 1: Pilin

Chain 4A:  .



• Molecule 1: Pilin

Chain 4B:  .



• Molecule 1: Pilin

Chain 4C:  .



• Molecule 1: Pilin

Chain 4D:  .



• Molecule 1: Pilin

Chain 4E:  .



• Molecule 1: Pilin

Chain 4F:  .



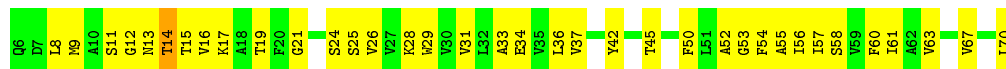
• Molecule 1: Pilin

Chain 4G:  .



- Molecule 1: Pilin

Chain 4H:  45% 54%



- Molecule 1: Pilin

Chain 4I:  43% 55%



- Molecule 1: Pilin

Chain 4J:  38% 60%



- Molecule 1: Pilin

Chain 4K:  42% 57%



- Molecule 1: Pilin

Chain 4L:  42% 57%



- Molecule 1: Pilin

Chain 4M:  46% 52%



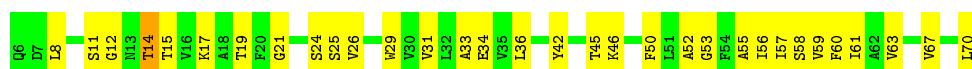
- Molecule 1: Pilin

Chain 4N:  45% 54%



- Molecule 1: Pilin

Chain 4O:  51% 48%



- Molecule 1: Pilin

Chain 5A: 48% 51%



- Molecule 1: Pilin

Chain 5B: 42% 57%



- Molecule 1: Pilin

Chain 5C: 37% 62%



- Molecule 1: Pilin

Chain 5D: 43% 55%



- Molecule 1: Pilin

Chain 5E: 43% 55%



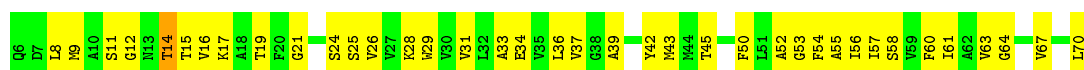
- Molecule 1: Pilin

Chain 5F: 43% 55%

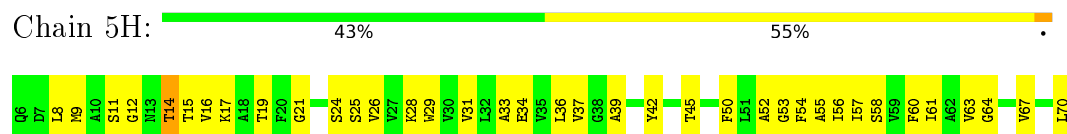


- Molecule 1: Pilin

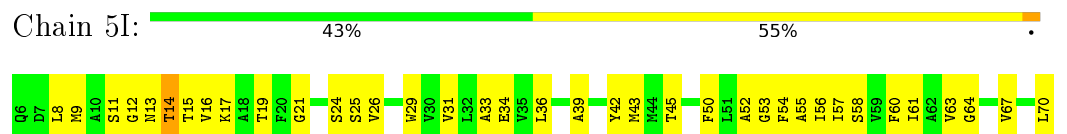
Chain 5G: 42% 57%



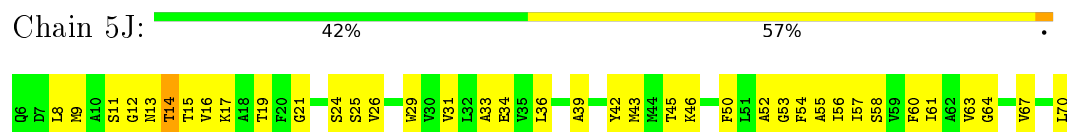
- Molecule 1: Pilin



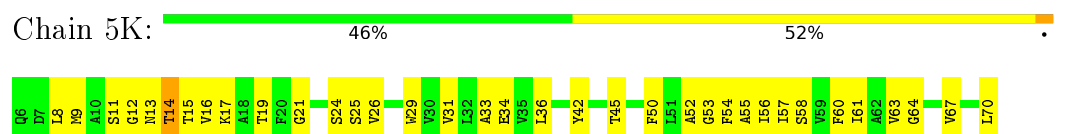
- Molecule 1: Pilin



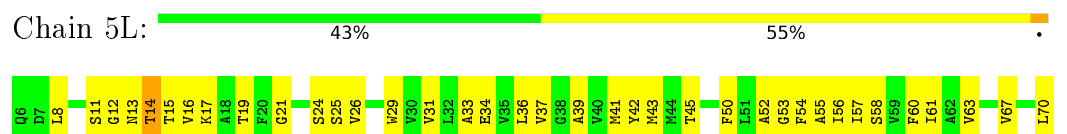
- Molecule 1: Pilin



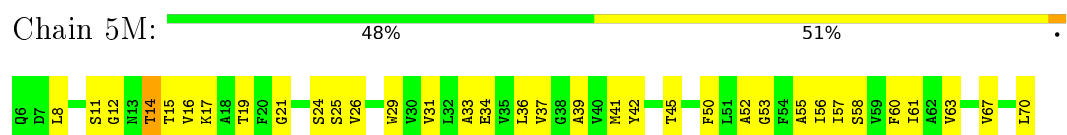
- Molecule 1: Pilin



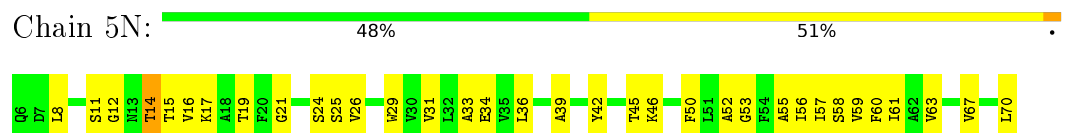
- Molecule 1: Pilin



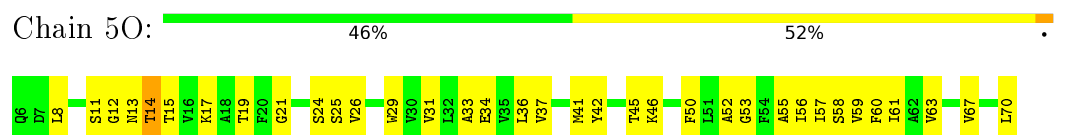
- Molecule 1: Pilin



- Molecule 1: Pilin



- Molecule 1: Pilin



## 4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of segments used	16426	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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	0.51	0/482	0.63	0/651
1	1B	0.51	0/482	0.63	0/651
1	1C	0.51	0/482	0.63	0/651
1	1D	0.51	0/482	0.63	0/651
1	1E	0.51	0/482	0.63	0/651
1	1F	0.51	0/482	0.63	0/651
1	1G	0.51	0/482	0.63	0/651
1	1H	0.51	0/482	0.63	0/651
1	1I	0.51	0/482	0.63	0/651
1	1J	0.51	0/482	0.63	0/651
1	1K	0.51	0/482	0.63	0/651
1	1L	0.51	0/482	0.63	0/651
1	1M	0.51	0/482	0.63	0/651
1	1N	0.51	0/482	0.63	0/651
1	1O	0.51	0/482	0.63	0/651
1	2A	0.51	0/482	0.63	0/651
1	2B	0.51	0/482	0.63	0/651
1	2C	0.51	0/482	0.63	0/651
1	2D	0.51	0/482	0.63	0/651
1	2E	0.51	0/482	0.63	0/651
1	2F	0.51	0/482	0.63	0/651
1	2G	0.51	0/482	0.63	0/651
1	2H	0.51	0/482	0.63	0/651
1	2I	0.51	0/482	0.63	0/651
1	2J	0.51	0/482	0.63	0/651
1	2K	0.51	0/482	0.63	0/651
1	2L	0.51	0/482	0.63	0/651
1	2M	0.51	0/482	0.63	0/651
1	2N	0.51	0/482	0.63	0/651
1	2O	0.51	0/482	0.63	0/651
1	3A	0.51	0/482	0.63	0/651
1	3B	0.51	0/482	0.63	0/651

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	3C	0.51	0/482	0.63	0/651
1	3D	0.51	0/482	0.63	0/651
1	3E	0.51	0/482	0.63	0/651
1	3F	0.51	0/482	0.63	0/651
1	3G	0.51	0/482	0.63	0/651
1	3H	0.51	0/482	0.63	0/651
1	3I	0.51	0/482	0.63	0/651
1	3J	0.51	0/482	0.63	0/651
1	3K	0.51	0/482	0.63	0/651
1	3L	0.51	0/482	0.63	0/651
1	3M	0.51	0/482	0.63	0/651
1	3N	0.51	0/482	0.63	0/651
1	3O	0.51	0/482	0.63	0/651
1	4A	0.51	0/482	0.63	0/651
1	4B	0.51	0/482	0.63	0/651
1	4C	0.51	0/482	0.63	0/651
1	4D	0.51	0/482	0.63	0/651
1	4E	0.51	0/482	0.63	0/651
1	4F	0.51	0/482	0.63	0/651
1	4G	0.51	0/482	0.63	0/651
1	4H	0.51	0/482	0.63	0/651
1	4I	0.51	0/482	0.63	0/651
1	4J	0.51	0/482	0.63	0/651
1	4K	0.51	0/482	0.63	0/651
1	4L	0.51	0/482	0.63	0/651
1	4M	0.51	0/482	0.63	0/651
1	4N	0.51	0/482	0.63	0/651
1	4O	0.51	0/482	0.63	0/651
1	5A	0.51	0/482	0.63	0/651
1	5B	0.51	0/482	0.63	0/651
1	5C	0.51	0/482	0.63	0/651
1	5D	0.51	0/482	0.63	0/651
1	5E	0.51	0/482	0.63	0/651
1	5F	0.51	0/482	0.63	0/651
1	5G	0.51	0/482	0.63	0/651
1	5H	0.51	0/482	0.63	0/651
1	5I	0.51	0/482	0.63	0/651
1	5J	0.51	0/482	0.63	0/651
1	5K	0.51	0/482	0.63	0/651
1	5L	0.51	0/482	0.63	0/651
1	5M	0.51	0/482	0.63	0/651
1	5N	0.51	0/482	0.63	0/651
1	5O	0.51	0/482	0.63	0/651

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
All	All	0.51	0/36150	0.63	0/48825

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	476	0	509	48	0
1	1B	476	0	509	60	0
1	1C	476	0	507	72	0
1	1D	476	0	509	70	0
1	1E	476	0	509	59	0
1	1F	476	0	509	70	0
1	1G	476	0	509	62	0
1	1H	476	0	509	63	0
1	1I	476	0	507	46	0
1	1J	476	0	507	56	0
1	1K	476	0	507	79	0
1	1L	476	0	509	83	0
1	1M	476	0	507	62	0
1	1N	476	0	509	44	0
1	1O	476	0	509	33	0
1	2A	476	0	509	46	0
1	2B	476	0	509	58	0
1	2C	476	0	509	79	0
1	2D	476	0	509	70	0
1	2E	476	0	509	66	0
1	2F	476	0	507	59	0
1	2G	476	0	507	62	0
1	2H	476	0	507	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2I	476	0	507	69	0
1	2J	476	0	507	64	0
1	2K	476	0	507	53	0
1	2L	476	0	509	70	0
1	2M	476	0	509	63	0
1	2N	476	0	509	58	0
1	2O	476	0	509	41	0
1	3A	476	0	509	42	0
1	3B	476	0	509	56	0
1	3C	476	0	509	75	0
1	3D	476	0	509	67	0
1	3E	476	0	509	68	0
1	3F	476	0	507	61	0
1	3G	476	0	507	62	0
1	3H	476	0	507	61	0
1	3I	476	0	507	58	0
1	3J	476	0	507	54	0
1	3K	476	0	507	60	0
1	3L	476	0	509	66	0
1	3M	476	0	509	53	0
1	3N	476	0	509	63	0
1	3O	476	0	509	48	0
1	4A	476	0	509	44	0
1	4B	476	0	509	57	0
1	4C	476	0	509	77	0
1	4D	476	0	509	64	0
1	4E	476	0	509	70	0
1	4F	476	0	507	63	0
1	4G	476	0	507	60	0
1	4H	476	0	507	59	0
1	4I	476	0	507	61	0
1	4J	476	0	507	53	0
1	4K	476	0	507	59	0
1	4L	476	0	509	64	0
1	4M	476	0	509	52	0
1	4N	476	0	509	62	0
1	4O	476	0	509	49	0
1	5A	476	0	509	47	0
1	5B	476	0	509	61	0
1	5C	476	0	508	67	0
1	5D	476	0	509	70	0
1	5E	476	0	507	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5F	476	0	507	57	0
1	5G	476	0	507	60	0
1	5H	476	0	507	58	0
1	5I	476	0	509	69	0
1	5J	476	0	509	68	0
1	5K	476	0	509	58	0
1	5L	476	0	509	45	0
1	5M	476	0	509	45	0
1	5N	476	0	509	63	0
1	5O	476	0	509	48	0
2	1A	12	0	0	0	0
2	1B	12	0	0	0	0
2	1C	12	0	0	0	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	1	0
2	1H	12	0	0	1	0
2	1I	12	0	0	2	0
2	1J	12	0	0	0	0
2	1K	12	0	0	0	0
2	1L	12	0	0	0	0
2	1M	12	0	0	0	0
2	1N	12	0	0	0	0
2	1O	12	0	0	0	0
2	2A	12	0	0	0	0
2	2B	12	0	0	0	0
2	2C	12	0	0	0	0
2	2D	12	0	0	0	0
2	2E	12	0	0	0	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	2	0
2	2K	12	0	0	2	0
2	2L	12	0	0	2	0
2	2M	12	0	0	2	0
2	2N	12	0	0	1	0
2	2O	12	0	0	1	0
2	3A	12	0	0	0	0
2	3B	12	0	0	0	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	5O	12	0	0	0	0
All	All	36600	0	38120	3319	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 44.

The worst 5 of 3319 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)
1:1G:9:MET:CE	1:2I:67:VAL:HG13	1.25	1.63
1:1L:13:ASN:HD21	1:2N:63:VAL:CB	1.12	1.62
1:1H:9:MET:HE2	1:2J:67:VAL:CG1	1.26	1.60
1:1J:9:MET:CE	1:2L:67:VAL:CG1	1.76	1.55
1:1H:9:MET:CE	1:2J:67:VAL:HG13	1.13	1.55

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%)	51 (81%)	12 (19%)	0	100	100
1	1B	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1C	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1D	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1E	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1F	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1G	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1H	63/65 (97%)	51 (81%)	12 (19%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1I	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1J	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1K	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1L	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1M	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1N	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	1O	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2A	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2B	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2C	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2D	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2E	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2F	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2G	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2H	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2I	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2J	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2K	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2L	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2M	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2N	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	2O	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3A	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3B	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3C	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3D	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3E	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3F	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3G	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3H	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3I	63/65 (97%)	51 (81%)	12 (19%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3J	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3K	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3L	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3M	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3N	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	3O	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4A	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4B	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4C	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4D	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4E	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4F	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4G	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4H	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4I	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4J	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4K	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4L	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4M	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4N	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	4O	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5A	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5B	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5C	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5D	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5E	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5F	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5G	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5H	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5I	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5J	63/65 (97%)	51 (81%)	12 (19%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5K	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5L	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5M	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5N	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
1	5O	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
All	All	4725/4875 (97%)	3825 (81%)	900 (19%)	0	100	100

There are no Ramachandran outliers to report.

### 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	51/51 (100%)	51 (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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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	3825/3825 (100%)	3825 (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. 5 of 36 such

sidechains are listed below:

Mol	Chain	Res	Type
1	3B	13	ASN
1	3L	13	ASN
1	5J	13	ASN
1	3D	13	ASN
1	3M	13	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

75 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	0.55	0	11,14,54	0.52	0
2	6V6	1B	101	-	11,11,48	0.54	0	11,14,54	0.51	0
2	6V6	1C	101	-	11,11,48	0.55	0	11,14,54	0.53	0
2	6V6	1D	101	-	11,11,48	0.55	0	11,14,54	0.51	0
2	6V6	1E	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	1F	101	-	11,11,48	0.55	0	11,14,54	0.53	0
2	6V6	1G	101	-	11,11,48	0.54	0	11,14,54	0.52	0
2	6V6	1H	101	-	11,11,48	0.55	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	1I	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	1J	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	1K	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	1L	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	1M	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	1N	101	-	11,11,48	0.54	0	11,14,54	0.52	0
2	6V6	1O	101	-	11,11,48	0.56	0	11,14,54	0.53	0
2	6V6	2A	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	2B	101	-	11,11,48	0.54	0	11,14,54	0.51	0
2	6V6	2C	101	-	11,11,48	0.55	0	11,14,54	0.53	0
2	6V6	2D	101	-	11,11,48	0.56	0	11,14,54	0.51	0
2	6V6	2E	101	-	11,11,48	0.55	0	11,14,54	0.53	0
2	6V6	2F	101	-	11,11,48	0.55	0	11,14,54	0.53	0
2	6V6	2G	101	-	11,11,48	0.54	0	11,14,54	0.52	0
2	6V6	2H	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	2I	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	2J	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	2K	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	2L	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	2M	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	2N	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	2O	101	-	11,11,48	0.56	0	11,14,54	0.53	0
2	6V6	3A	101	-	11,11,48	0.55	0	11,14,54	0.53	0
2	6V6	3B	101	-	11,11,48	0.54	0	11,14,54	0.52	0
2	6V6	3C	101	-	11,11,48	0.55	0	11,14,54	0.53	0
2	6V6	3D	101	-	11,11,48	0.56	0	11,14,54	0.51	0
2	6V6	3E	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	3F	101	-	11,11,48	0.55	0	11,14,54	0.53	0
2	6V6	3G	101	-	11,11,48	0.54	0	11,14,54	0.52	0
2	6V6	3H	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	3I	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	3J	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	3K	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	3L	101	-	11,11,48	0.54	0	11,14,54	0.52	0
2	6V6	3M	101	-	11,11,48	0.54	0	11,14,54	0.52	0
2	6V6	3N	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	3O	101	-	11,11,48	0.56	0	11,14,54	0.53	0
2	6V6	4A	101	-	11,11,48	0.56	0	11,14,54	0.52	0
2	6V6	4B	101	-	11,11,48	0.54	0	11,14,54	0.51	0
2	6V6	4C	101	-	11,11,48	0.55	0	11,14,54	0.53	0
2	6V6	4D	101	-	11,11,48	0.55	0	11,14,54	0.51	0
2	6V6	4E	101	-	11,11,48	0.54	0	11,14,54	0.52	0
2	6V6	4F	101	-	11,11,48	0.55	0	11,14,54	0.53	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	6V6	4G	101	-	11,11,48	0.54	0	11,14,54	0.52	0
2	6V6	4H	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	4I	101	-	11,11,48	0.55	0	11,14,54	0.53	0
2	6V6	4J	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	4K	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	4L	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	4M	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	4N	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	4O	101	-	11,11,48	0.56	0	11,14,54	0.53	0
2	6V6	5A	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	5B	101	-	11,11,48	0.54	0	11,14,54	0.51	0
2	6V6	5C	101	-	11,11,48	0.55	0	11,14,54	0.53	0
2	6V6	5D	101	-	11,11,48	0.55	0	11,14,54	0.51	0
2	6V6	5E	101	-	11,11,48	0.55	0	11,14,54	0.53	0
2	6V6	5F	101	-	11,11,48	0.55	0	11,14,54	0.53	0
2	6V6	5G	101	-	11,11,48	0.54	0	11,14,54	0.52	0
2	6V6	5H	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	5I	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	5J	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	5K	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	5L	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	5M	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	5N	101	-	11,11,48	0.55	0	11,14,54	0.52	0
2	6V6	5O	101	-	11,11,48	0.56	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1O	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
2	6V6	2N	101	-	-	0/12/12/53	0/0/0/0
2	6V6	2O	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	3O	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	4O	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
2	6V6	5N	101	-	-	0/12/12/53	0/0/0/0
2	6V6	5O	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.

37 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1D	101	6V6	1	0
2	1E	101	6V6	1	0
2	1F	101	6V6	1	0
2	1G	101	6V6	1	0
2	1H	101	6V6	1	0
2	1I	101	6V6	2	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

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

## 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.