



## wwPDB EM Map/Model Validation Report ⓘ

Sep 19, 2016 – 03:19 PM EDT

PDB ID : 5LEG  
EMDB ID: : EMD-4042  
Title : Structure of the bacterial sex F pilus (pED208)  
Authors : Costa, T.R.D.; Ilangoan, I.; Ukleja, M.; Redzej, A.; Santini, J.M.; Smith, T.K.; Egelman, E.H.; Waksman, G.  
Deposited on : 2016-06-29  
Resolution : 3.60 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

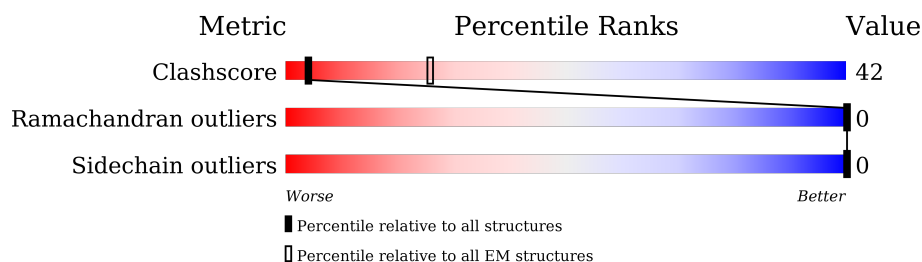
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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.















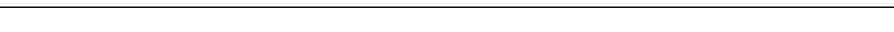

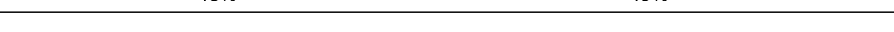

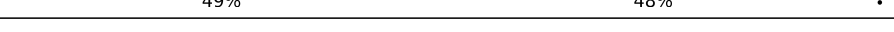








Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	63	52% 44% .
1	1B	63	49% 48% .
1	1C	63	48% 49% .
1	1D	63	48% 49% .
1	1E	63	46% 51% .
1	1F	63	46% 51% .
1	1G	63	48% 49% .
1	1H	63	48% 49% .
1	1I	63	48% 49% .




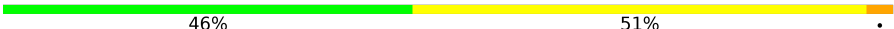
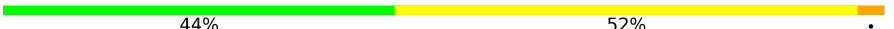
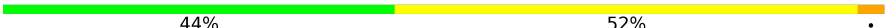
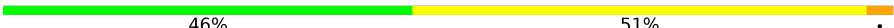









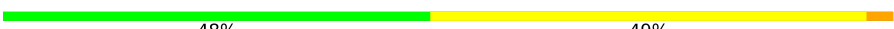


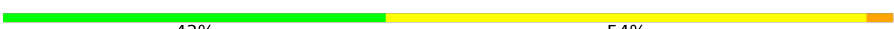
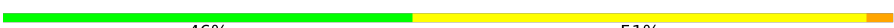




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Mol	Chain	Length	Quality of chain
1	1J	63	 46% 51% .
1	1K	63	 48% 49% .
1	1L	63	 51% 46% .
1	1M	63	 51% 46% .
1	1N	63	 51% 46% .
1	1O	63	 52% 44% .
1	1P	63	 56% 43% .
1	2A	63	 51% 46% .
1	2B	63	 46% 51% .
1	2C	63	 48% 49% .
1	2D	63	 48% 49% .
1	2E	63	 48% 49% .
1	2F	63	 46% 51% .
1	2G	63	 48% 49% .
1	2H	63	 48% 49% .
1	2I	63	 49% 48% .
1	2J	63	 51% 46% .
1	2K	63	 51% 46% .
1	2L	63	 51% 46% .
1	2M	63	 51% 46% .
1	2N	63	 51% 46% .
1	2O	63	 52% 44% .
1	2P	63	 59% 40% .
1	3A	63	 51% 46% .
1	3B	63	 48% 49% .

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Mol	Chain	Length	Quality of chain
1	3C	63	 48% 49% .
1	3D	63	 48% 49% .
1	3E	63	 48% 49% .
1	3F	63	 46% 51% .
1	3G	63	 44% 52% .
1	3H	63	 44% 52% .
1	3I	63	 46% 51% .
1	3J	63	 48% 49% .
1	3K	63	 48% 49% .
1	3L	63	 49% 48% .
1	3M	63	 49% 48% .
1	3N	63	 51% 46% .
1	3O	63	 51% 46% .
1	3P	63	 59% 40% .
1	4A	63	 52% 44% .
1	4B	63	 49% 48% .
1	4C	63	 48% 49% .
1	4D	63	 51% 46% .
1	4E	63	 46% 51% .
1	4F	63	 43% 54% .
1	4G	63	 46% 51% .
1	4H	63	 48% 49% .
1	4I	63	 49% 48% .
1	4J	63	 51% 46% .
1	4K	63	 51% 46% .

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Mol	Chain	Length	Quality of chain	
1	4L	63	<div><div></div></div> 51%	<div><div></div></div> 46%
1	4M	63	<div><div></div></div> 51%	<div><div></div></div> 46%
1	4N	63	<div><div></div></div> 51%	<div><div></div></div> 46%
1	4O	63	<div><div></div></div> 52%	<div><div></div></div> 44%
1	4P	63	<div><div></div></div> 62%	<div><div></div></div> 37%
1	5A	63	<div><div></div></div> 52%	<div><div></div></div> 44%
1	5B	63	<div><div></div></div> 48%	<div><div></div></div> 49%
1	5C	63	<div><div></div></div> 48%	<div><div></div></div> 49%
1	5D	63	<div><div></div></div> 48%	<div><div></div></div> 49%
1	5E	63	<div><div></div></div> 46%	<div><div></div></div> 51%
1	5F	63	<div><div></div></div> 48%	<div><div></div></div> 49%
1	5G	63	<div><div></div></div> 49%	<div><div></div></div> 48%
1	5H	63	<div><div></div></div> 49%	<div><div></div></div> 48%
1	5I	63	<div><div></div></div> 48%	<div><div></div></div> 49%
1	5J	63	<div><div></div></div> 49%	<div><div></div></div> 48%
1	5K	63	<div><div></div></div> 49%	<div><div></div></div> 48%
1	5L	63	<div><div></div></div> 48%	<div><div></div></div> 49%
1	5M	63	<div><div></div></div> 48%	<div><div></div></div> 49%
1	5N	63	<div><div></div></div> 49%	<div><div></div></div> 48%
1	5O	63	<div><div></div></div> 49%	<div><div></div></div> 48%
1	5P	63	<div><div></div></div> 59%	<div><div></div></div> 40%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LHG	1A	101	-	-	X	-
2	LHG	1B	101	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LHG	1C	101	-	-	X	-
2	LHG	1D	101	-	-	X	-
2	LHG	1E	101	-	-	X	-
2	LHG	1F	101	-	-	X	-
2	LHG	1G	101	-	-	X	-
2	LHG	1H	101	-	-	X	-
2	LHG	1I	101	-	-	X	-
2	LHG	1J	101	-	-	X	-
2	LHG	1K	101	-	-	X	-
2	LHG	1L	101	-	-	X	-
2	LHG	1M	101	-	-	X	-
2	LHG	1N	101	-	-	X	-
2	LHG	1O	101	-	-	X	-
2	LHG	2A	101	-	-	X	-
2	LHG	2B	101	-	-	X	-
2	LHG	2C	101	-	-	X	-
2	LHG	2D	101	-	-	X	-
2	LHG	2E	101	-	-	X	-
2	LHG	2F	101	-	-	X	-
2	LHG	2G	101	-	-	X	-
2	LHG	2H	101	-	-	X	-
2	LHG	2I	101	-	-	X	-
2	LHG	2J	101	-	-	X	-
2	LHG	2K	101	-	-	X	-
2	LHG	2L	101	-	-	X	-
2	LHG	2M	101	-	-	X	-
2	LHG	2N	101	-	-	X	-
2	LHG	2O	101	-	-	X	-
2	LHG	3A	101	-	-	X	-
2	LHG	3B	101	-	-	X	-
2	LHG	3C	101	-	-	X	-
2	LHG	3D	101	-	-	X	-
2	LHG	3E	101	-	-	X	-
2	LHG	3F	101	-	-	X	-
2	LHG	3G	101	-	-	X	-
2	LHG	3H	101	-	-	X	-
2	LHG	3I	101	-	-	X	-
2	LHG	3J	101	-	-	X	-
2	LHG	3K	101	-	-	X	-
2	LHG	3L	101	-	-	X	-
2	LHG	3M	101	-	-	X	-
2	LHG	3N	101	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LHG	3O	101	-	-	X	-
2	LHG	4A	101	-	-	X	-
2	LHG	4B	101	-	-	X	-
2	LHG	4C	101	-	-	X	-
2	LHG	4D	101	-	-	X	-
2	LHG	4E	101	-	-	X	-
2	LHG	4F	101	-	-	X	-
2	LHG	4G	101	-	-	X	-
2	LHG	4H	101	-	-	X	-
2	LHG	4I	101	-	-	X	-
2	LHG	4J	101	-	-	X	-
2	LHG	4K	101	-	-	X	-
2	LHG	4L	101	-	-	X	-
2	LHG	4M	101	-	-	X	-
2	LHG	4N	101	-	-	X	-
2	LHG	4O	101	-	-	X	-
2	LHG	5A	101	-	-	X	-
2	LHG	5B	101	-	-	X	-
2	LHG	5C	101	-	-	X	-
2	LHG	5D	101	-	-	X	-
2	LHG	5E	101	-	-	X	-
2	LHG	5F	101	-	-	X	-
2	LHG	5G	101	-	-	X	-
2	LHG	5H	101	-	-	X	-
2	LHG	5I	101	-	-	X	-
2	LHG	5J	101	-	-	X	-
2	LHG	5K	101	-	-	X	-
2	LHG	5L	101	-	-	X	-
2	LHG	5M	101	-	-	X	-
2	LHG	5N	101	-	-	X	-
2	LHG	5O	101	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 41355 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	63	Total	C	N	O	S	0	0
			471	315	71	81	4		
1	1B	63	Total	C	N	O	S	0	0
			471	315	71	81	4		
1	1C	63	Total	C	N	O	S	0	0
			471	315	71	81	4		
1	1D	63	Total	C	N	O	S	0	0
			471	315	71	81	4		
1	1E	63	Total	C	N	O	S	0	0
			471	315	71	81	4		
1	1F	63	Total	C	N	O	S	0	0
			471	315	71	81	4		
1	1G	63	Total	C	N	O	S	0	0
			471	315	71	81	4		
1	1H	63	Total	C	N	O	S	0	0
			471	315	71	81	4		
1	1I	63	Total	C	N	O	S	0	0
			471	315	71	81	4		
1	1J	63	Total	C	N	O	S	0	0
			471	315	71	81	4		
1	1K	63	Total	C	N	O	S	0	0
			471	315	71	81	4		
1	1L	63	Total	C	N	O	S	0	0
			471	315	71	81	4		
1	1M	63	Total	C	N	O	S	0	0
			471	315	71	81	4		
1	1N	63	Total	C	N	O	S	0	0
			471	315	71	81	4		
1	1O	63	Total	C	N	O	S	0	0
			471	315	71	81	4		
1	1P	63	Total	C	N	O	S	0	0
			471	315	71	81	4		
1	2A	63	Total	C	N	O	S	0	0
			471	315	71	81	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	2B	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	2C	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	2D	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	2E	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	2F	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	2G	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	2H	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	2I	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	2J	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	2K	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	2L	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	2M	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	2N	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	2O	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	2P	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	3A	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	3B	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	3C	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	3D	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	3E	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	3F	63	Total 471	C 315	N 71	O 81	S 4	0	0

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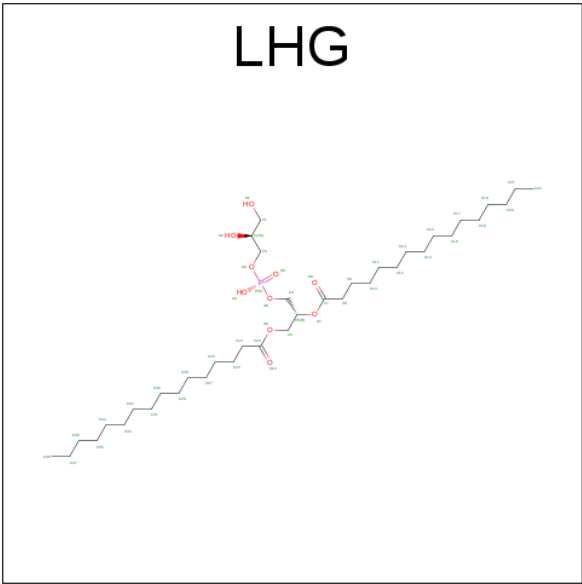
Mol	Chain	Residues	Atoms					AltConf	Trace
1	3G	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	3H	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	3I	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	3J	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	3K	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	3L	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	3M	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	3N	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	3O	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	3P	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	4A	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	4B	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	4C	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	4D	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	4E	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	4F	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	4G	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	4H	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	4I	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	4J	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	4K	63	Total 471	C 315	N 71	O 81	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	4L	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	4M	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	4N	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	4O	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	4P	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	5A	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	5B	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	5C	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	5D	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	5E	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	5F	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	5G	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	5H	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	5I	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	5J	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	5K	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	5L	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	5M	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	5N	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	5O	63	Total 471	C 315	N 71	O 81	S 4	0	0
1	5P	63	Total 471	C 315	N 71	O 81	S 4	0	0

- Molecule 2 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms				AltConf
2	1A	1	Total	C	O	P	0
			49	38	10	1	
2	1B	1	Total	C	O	P	0
			49	38	10	1	
2	1C	1	Total	C	O	P	0
			49	38	10	1	
2	1D	1	Total	C	O	P	0
			49	38	10	1	
2	1E	1	Total	C	O	P	0
			49	38	10	1	
2	1F	1	Total	C	O	P	0
			49	38	10	1	
2	1G	1	Total	C	O	P	0
			49	38	10	1	
2	1H	1	Total	C	O	P	0
			49	38	10	1	
2	1I	1	Total	C	O	P	0
			49	38	10	1	
2	1J	1	Total	C	O	P	0
			49	38	10	1	
2	1K	1	Total	C	O	P	0
			49	38	10	1	
2	1L	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
2	1M	1	Total 49	C 38	O 10	P 1	0
2	1N	1	Total 49	C 38	O 10	P 1	0
2	1O	1	Total 49	C 38	O 10	P 1	0
2	2A	1	Total 49	C 38	O 10	P 1	0
2	2B	1	Total 49	C 38	O 10	P 1	0
2	2C	1	Total 49	C 38	O 10	P 1	0
2	2D	1	Total 49	C 38	O 10	P 1	0
2	2E	1	Total 49	C 38	O 10	P 1	0
2	2F	1	Total 49	C 38	O 10	P 1	0
2	2G	1	Total 49	C 38	O 10	P 1	0
2	2H	1	Total 49	C 38	O 10	P 1	0
2	2I	1	Total 49	C 38	O 10	P 1	0
2	2J	1	Total 49	C 38	O 10	P 1	0
2	2K	1	Total 49	C 38	O 10	P 1	0
2	2L	1	Total 49	C 38	O 10	P 1	0
2	2M	1	Total 49	C 38	O 10	P 1	0
2	2N	1	Total 49	C 38	O 10	P 1	0
2	2O	1	Total 49	C 38	O 10	P 1	0
2	3A	1	Total 49	C 38	O 10	P 1	0
2	3B	1	Total 49	C 38	O 10	P 1	0
2	3C	1	Total 49	C 38	O 10	P 1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf
2	3D	1	Total 49	C 38	O 10	P 1	0
2	3E	1	Total 49	C 38	O 10	P 1	0
2	3F	1	Total 49	C 38	O 10	P 1	0
2	3G	1	Total 49	C 38	O 10	P 1	0
2	3H	1	Total 49	C 38	O 10	P 1	0
2	3I	1	Total 49	C 38	O 10	P 1	0
2	3J	1	Total 49	C 38	O 10	P 1	0
2	3K	1	Total 49	C 38	O 10	P 1	0
2	3L	1	Total 49	C 38	O 10	P 1	0
2	3M	1	Total 49	C 38	O 10	P 1	0
2	3N	1	Total 49	C 38	O 10	P 1	0
2	3O	1	Total 49	C 38	O 10	P 1	0
2	4A	1	Total 49	C 38	O 10	P 1	0
2	4B	1	Total 49	C 38	O 10	P 1	0
2	4C	1	Total 49	C 38	O 10	P 1	0
2	4D	1	Total 49	C 38	O 10	P 1	0
2	4E	1	Total 49	C 38	O 10	P 1	0
2	4F	1	Total 49	C 38	O 10	P 1	0
2	4G	1	Total 49	C 38	O 10	P 1	0
2	4H	1	Total 49	C 38	O 10	P 1	0
2	4I	1	Total 49	C 38	O 10	P 1	0

*Continued on next page...*

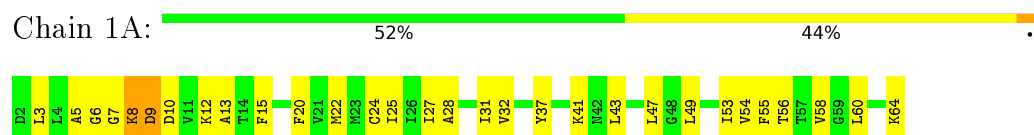
*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf
2	4J	1	Total	C	O	P	0
			49	38	10	1	
2	4K	1	Total	C	O	P	0
			49	38	10	1	
2	4L	1	Total	C	O	P	0
			49	38	10	1	
2	4M	1	Total	C	O	P	0
			49	38	10	1	
2	4N	1	Total	C	O	P	0
			49	38	10	1	
2	4O	1	Total	C	O	P	0
			49	38	10	1	
2	5A	1	Total	C	O	P	0
			49	38	10	1	
2	5B	1	Total	C	O	P	0
			49	38	10	1	
2	5C	1	Total	C	O	P	0
			49	38	10	1	
2	5D	1	Total	C	O	P	0
			49	38	10	1	
2	5E	1	Total	C	O	P	0
			49	38	10	1	
2	5F	1	Total	C	O	P	0
			49	38	10	1	
2	5G	1	Total	C	O	P	0
			49	38	10	1	
2	5H	1	Total	C	O	P	0
			49	38	10	1	
2	5I	1	Total	C	O	P	0
			49	38	10	1	
2	5J	1	Total	C	O	P	0
			49	38	10	1	
2	5K	1	Total	C	O	P	0
			49	38	10	1	
2	5L	1	Total	C	O	P	0
			49	38	10	1	
2	5M	1	Total	C	O	P	0
			49	38	10	1	
2	5N	1	Total	C	O	P	0
			49	38	10	1	
2	5O	1	Total	C	O	P	0
			49	38	10	1	

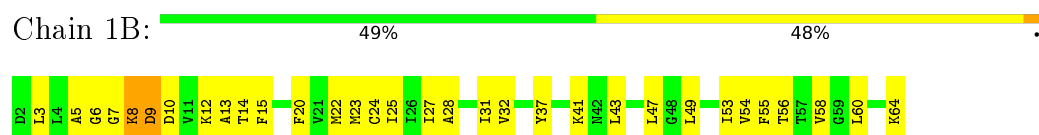
### 3 Residue-property plots

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.

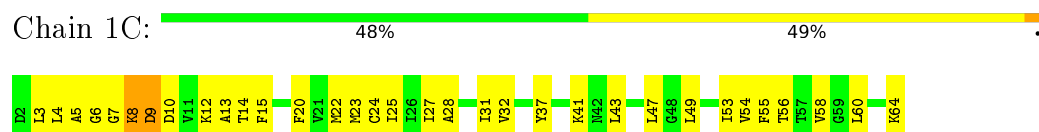
- Molecule 1: Pilin



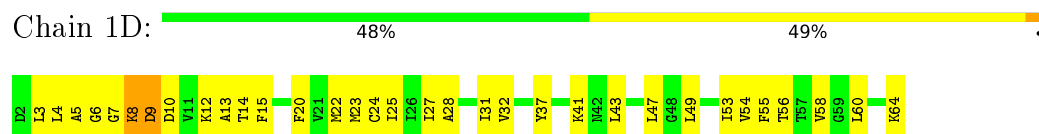
- Molecule 1: Pilin



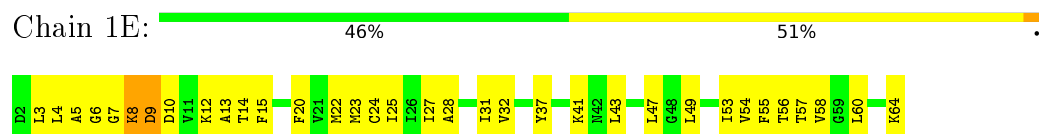
- Molecule 1: Pilin



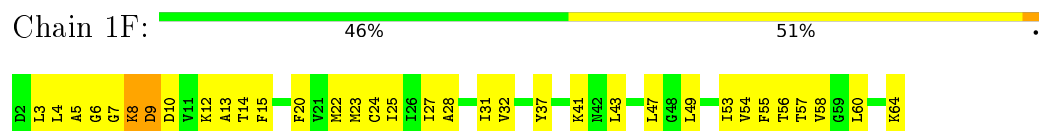
- Molecule 1: Pilin



- Molecule 1: Pilin



- Molecule 1: Pilin





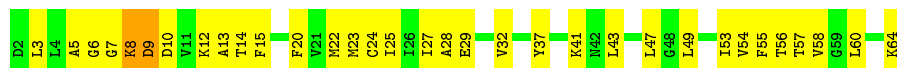
## ● Molecule 1: Pilin

Chain 1G:  .

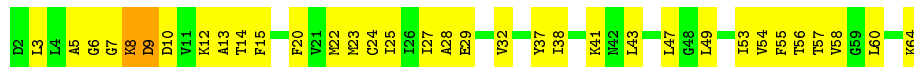
## ● Molecule 1: Pilin

Chain 1H:  .

## ● Molecule 1: Pilin

Chain 1I:  .

## ● Molecule 1: Pilin

Chain 1J:  .

## ● Molecule 1: Pilin

Chain 1K:  .

## ● Molecule 1: Pilin

Chain 1L:  .

## ● Molecule 1: Pilin

Chain 1M:  .

## ● Molecule 1: Pilin

Chain 1N:  .



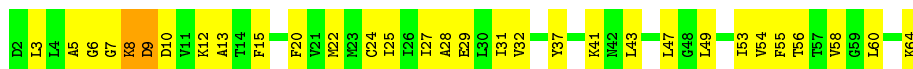
- Molecule 1: Pilin



- Molecule 1: Pilin



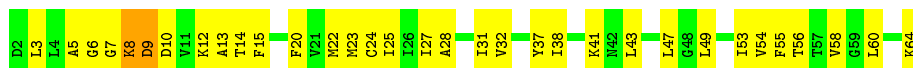
- Molecule 1: Pilin



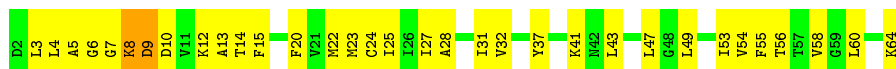
- Molecule 1: Pilin



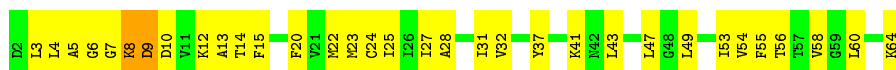
- Molecule 1: Pilin



- Molecule 1: Pilin

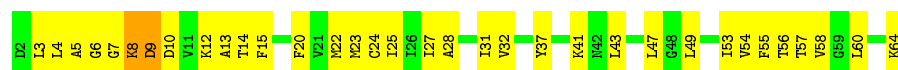


- Molecule 1: Pilin



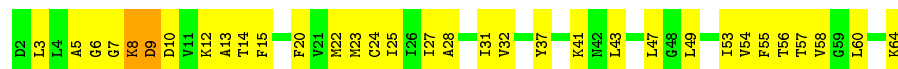
- Molecule 1: Pilin

Chain 2F:  .



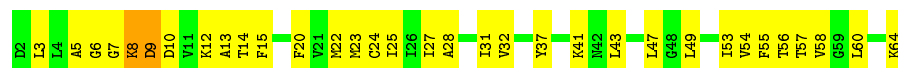
• Molecule 1: Pilin

Chain 2G:  .



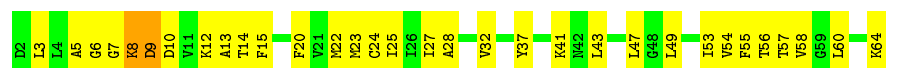
• Molecule 1: Pilin

Chain 2H:  .



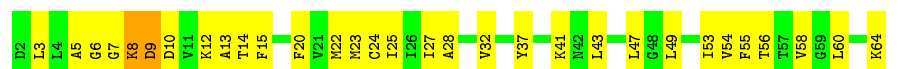
• Molecule 1: Pilin

Chain 2I:  .



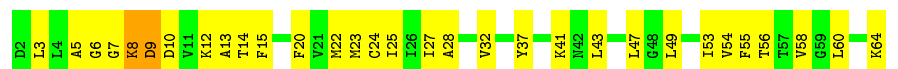
• Molecule 1: Pilin

Chain 2J:  .



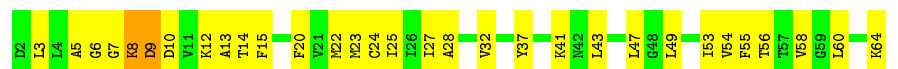
• Molecule 1: Pilin

Chain 2K:  .



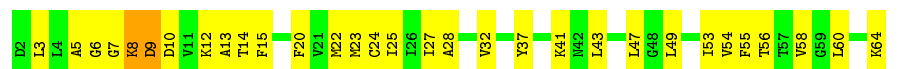
• Molecule 1: Pilin

Chain 2L:  .



• Molecule 1: Pilin

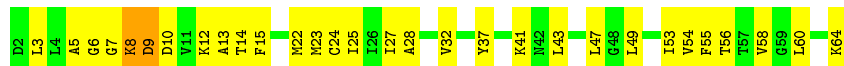
Chain 2M:  .



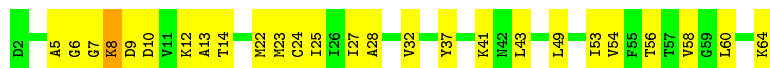
## • Molecule 1: Pilin

Chain 2N:  51% 46%

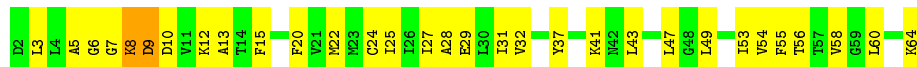
## • Molecule 1: Pilin

Chain 2O:  52% 44%

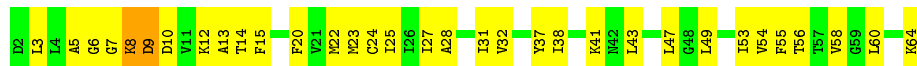
## • Molecule 1: Pilin

Chain 2P:  59% 40%

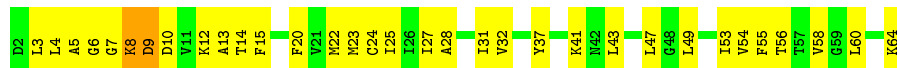
## • Molecule 1: Pilin

Chain 3A:  51% 46%

## • Molecule 1: Pilin

Chain 3B:  48% 49%

## • Molecule 1: Pilin

Chain 3C:  48% 49%

## • Molecule 1: Pilin

Chain 3D:  48% 49%

## • Molecule 1: Pilin

Chain 3E:  48% 49%



- Molecule 1: Pilin

Chain 3F: 46% 51%



- Molecule 1: Pilin

Chain 3G: 44% 52%



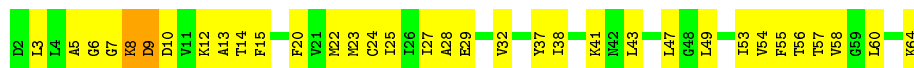
- Molecule 1: Pilin

Chain 3H: 44% 52%



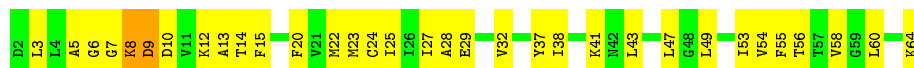
- Molecule 1: Pilin

Chain 3I: 46% 51%



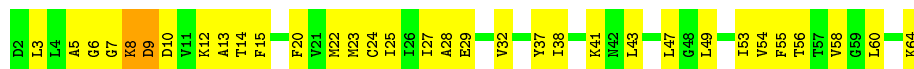
- Molecule 1: Pilin

Chain 3J: 48% 49%



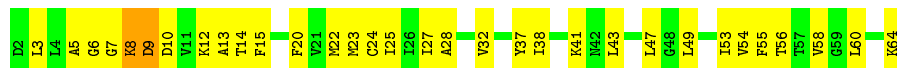
- Molecule 1: Pilin

Chain 3K: 48% 49%



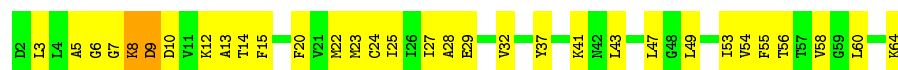
- Molecule 1: Pilin

Chain 3L: 49% 48%



- Molecule 1: Pilin

Chain 3M:  49% 48%



• Molecule 1: Pilin

Chain 3N:  51% 46%



• Molecule 1: Pilin

Chain 3O:  51% 46%



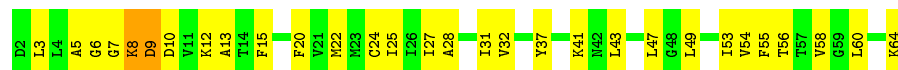
• Molecule 1: Pilin

Chain 3P:  59% 40%



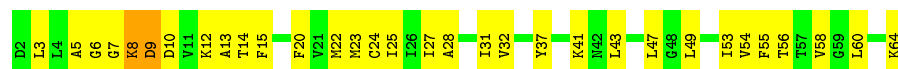
• Molecule 1: Pilin

Chain 4A:  52% 44%



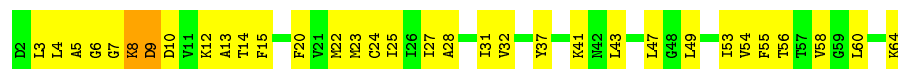
• Molecule 1: Pilin

Chain 4B:  49% 48%



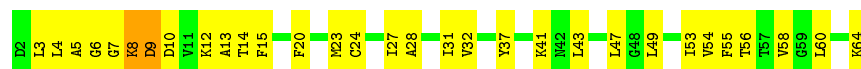
• Molecule 1: Pilin

Chain 4C:  48% 49%

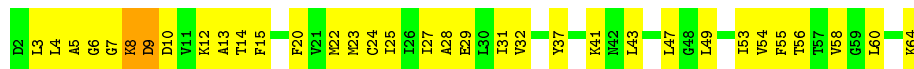


• Molecule 1: Pilin

Chain 4D:  51% 46%



## • Molecule 1: Pilin

Chain 4E:  46% 51%

## • Molecule 1: Pilin

Chain 4F:  43% 54%

## • Molecule 1: Pilin

Chain 4G:  46% 51%

## • Molecule 1: Pilin

Chain 4H:  48% 49%

## • Molecule 1: Pilin

Chain 4I:  49% 48%

## • Molecule 1: Pilin

Chain 4J:  51% 46%

## • Molecule 1: Pilin

Chain 4K:  51% 46%

## • Molecule 1: Pilin

Chain 4L:  51% 46%



- Molecule 1: Pilin

Chain 4M: 51% 46%



- Molecule 1: Pilin

Chain 4N: 51% 46%



- Molecule 1: Pilin

Chain 4O: 52% 44%



- Molecule 1: Pilin

Chain 4P: 62% 37%



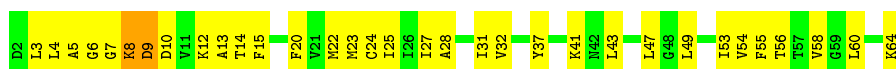
- Molecule 1: Pilin

Chain 5A: 52% 44%



- Molecule 1: Pilin

Chain 5B: 48% 49%



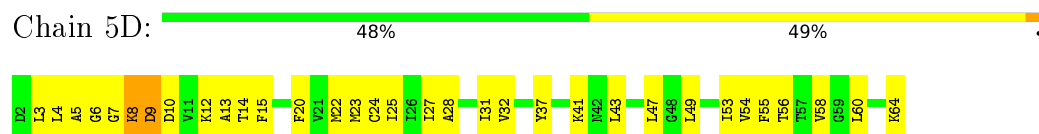
- Molecule 1: Pilin

Chain 5C: 48% 49%

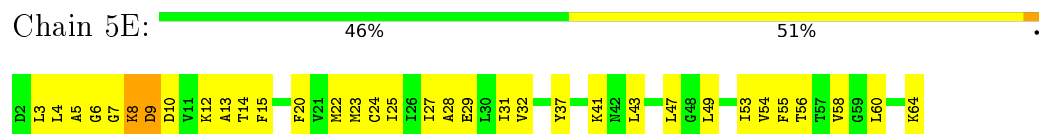


- Molecule 1: Pilin

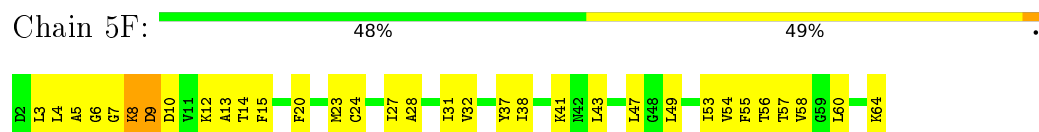




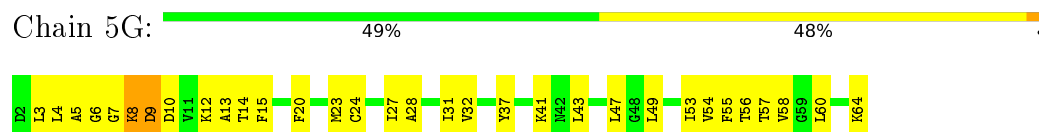
- Molecule 1: Pilin



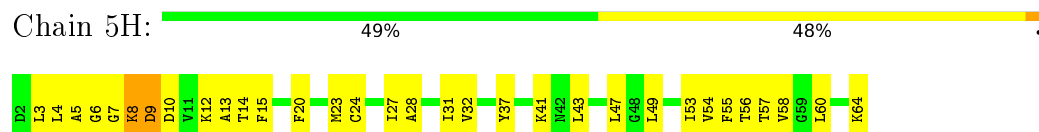
- Molecule 1: Pilin



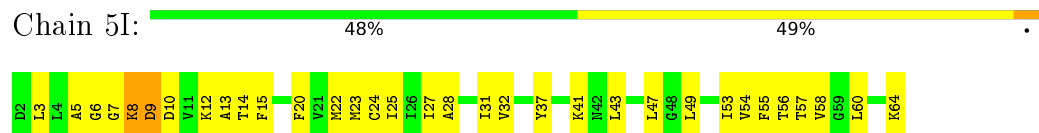
- Molecule 1: Pilin



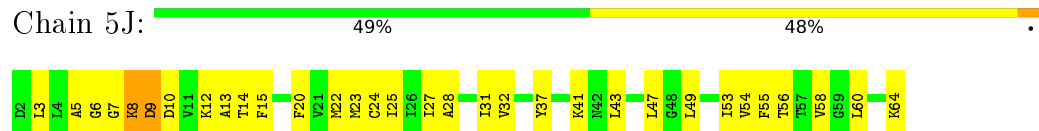
- Molecule 1: Pilin



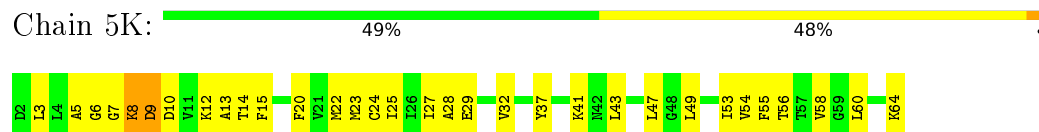
- Molecule 1: Pilin



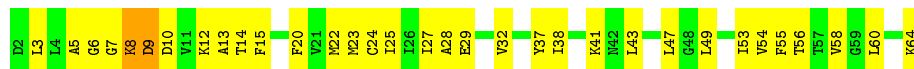
- Molecule 1: Pilin



- Molecule 1: Pilin



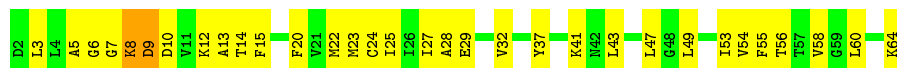
## ● Molecule 1: Pilin

Chain 5L:  48% 49%

## ● Molecule 1: Pilin

Chain 5M:  48% 49%

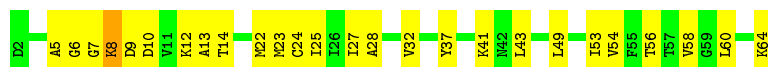
## ● Molecule 1: Pilin

Chain 5N:  49% 48%

## ● Molecule 1: Pilin

Chain 5O:  49% 48%

## ● Molecule 1: Pilin

Chain 5P:  59% 40%

## 4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of segments used	43952	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: LHG

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	0.40	0/475	0.52	0/642
1	1B	0.40	0/475	0.52	0/642
1	1C	0.40	0/475	0.52	0/642
1	1D	0.40	0/475	0.52	0/642
1	1E	0.40	0/475	0.52	0/642
1	1F	0.40	0/475	0.52	0/642
1	1G	0.40	0/475	0.52	0/642
1	1H	0.40	0/475	0.52	0/642
1	1I	0.40	0/475	0.52	0/642
1	1J	0.40	0/475	0.52	0/642
1	1K	0.40	0/475	0.52	0/642
1	1L	0.40	0/475	0.52	0/642
1	1M	0.40	0/475	0.52	0/642
1	1N	0.40	0/475	0.52	0/642
1	1O	0.40	0/475	0.52	0/642
1	1P	0.40	0/475	0.52	0/642
1	2A	0.40	0/475	0.52	0/642
1	2B	0.40	0/475	0.52	0/642
1	2C	0.40	0/475	0.52	0/642
1	2D	0.40	0/475	0.52	0/642
1	2E	0.40	0/475	0.52	0/642
1	2F	0.40	0/475	0.52	0/642
1	2G	0.40	0/475	0.52	0/642
1	2H	0.40	0/475	0.52	0/642
1	2I	0.40	0/475	0.52	0/642
1	2J	0.40	0/475	0.52	0/642
1	2K	0.40	0/475	0.52	0/642
1	2L	0.40	0/475	0.52	0/642
1	2M	0.40	0/475	0.52	0/642
1	2N	0.40	0/475	0.52	0/642
1	2O	0.40	0/475	0.52	0/642
1	2P	0.40	0/475	0.52	0/642

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	3A	0.40	0/475	0.52	0/642
1	3B	0.40	0/475	0.52	0/642
1	3C	0.40	0/475	0.52	0/642
1	3D	0.40	0/475	0.52	0/642
1	3E	0.40	0/475	0.52	0/642
1	3F	0.40	0/475	0.52	0/642
1	3G	0.40	0/475	0.52	0/642
1	3H	0.40	0/475	0.52	0/642
1	3I	0.40	0/475	0.52	0/642
1	3J	0.40	0/475	0.52	0/642
1	3K	0.40	0/475	0.52	0/642
1	3L	0.40	0/475	0.52	0/642
1	3M	0.40	0/475	0.52	0/642
1	3N	0.41	0/475	0.52	0/642
1	3O	0.40	0/475	0.52	0/642
1	3P	0.41	0/475	0.52	0/642
1	4A	0.40	0/475	0.52	0/642
1	4B	0.40	0/475	0.52	0/642
1	4C	0.40	0/475	0.52	0/642
1	4D	0.40	0/475	0.52	0/642
1	4E	0.40	0/475	0.52	0/642
1	4F	0.40	0/475	0.52	0/642
1	4G	0.40	0/475	0.52	0/642
1	4H	0.40	0/475	0.52	0/642
1	4I	0.40	0/475	0.52	0/642
1	4J	0.40	0/475	0.52	0/642
1	4K	0.40	0/475	0.52	0/642
1	4L	0.40	0/475	0.52	0/642
1	4M	0.40	0/475	0.52	0/642
1	4N	0.41	0/475	0.52	0/642
1	4O	0.41	0/475	0.52	0/642
1	4P	0.41	0/475	0.52	0/642
1	5A	0.40	0/475	0.52	0/642
1	5B	0.40	0/475	0.52	0/642
1	5C	0.40	0/475	0.52	0/642
1	5D	0.40	0/475	0.52	0/642
1	5E	0.40	0/475	0.52	0/642
1	5F	0.40	0/475	0.52	0/642
1	5G	0.40	0/475	0.52	0/642
1	5H	0.40	0/475	0.52	0/642
1	5I	0.40	0/475	0.52	0/642
1	5J	0.40	0/475	0.52	0/642
1	5K	0.40	0/475	0.52	0/642

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	5L	0.40	0/475	0.52	0/642
1	5M	0.40	0/475	0.52	0/642
1	5N	0.41	0/475	0.52	0/642
1	5O	0.40	0/475	0.52	0/642
1	5P	0.41	0/475	0.52	0/642
All	All	0.40	0/38000	0.52	0/51360

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	2N	0	6
1	2O	0	6
1	2P	0	6
1	3A	0	6
1	3B	0	6
1	3C	0	6
1	3D	0	6
1	3E	0	6
1	3F	0	6
1	3G	0	6
1	3H	0	6
1	3I	0	6
1	3J	0	6
1	3K	0	6
1	3L	0	6
1	3M	0	6
1	3N	0	6
1	3O	0	6
1	3P	0	6
1	4A	0	6
1	4B	0	6
1	4C	0	6
1	4D	0	6
1	4E	0	6
1	4F	0	6
1	4G	0	6
1	4H	0	6
1	4I	0	6
1	4J	0	6
1	4K	0	6
1	4L	0	6
1	4M	0	6
1	4N	0	6
1	4O	0	6
1	4P	0	6
1	5A	0	6
1	5B	0	6
1	5C	0	6
1	5D	0	6
1	5E	0	6
1	5F	0	6
1	5G	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	5H	0	6
1	5I	0	6
1	5J	0	6
1	5K	0	6
1	5L	0	6
1	5M	0	6
1	5N	0	6
1	5O	0	6
1	5P	0	6
All	All	0	480

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (480) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1A	43	LEU	Peptide
1	1A	5	ALA	Peptide
1	1A	6	GLY	Peptide
1	1A	7	GLY	Peptide
1	1A	8	LYS	Peptide
1	1A	9	ASP	Peptide
1	1B	43	LEU	Peptide
1	1B	5	ALA	Peptide
1	1B	6	GLY	Peptide
1	1B	7	GLY	Peptide
1	1B	8	LYS	Peptide
1	1B	9	ASP	Peptide
1	1C	43	LEU	Peptide
1	1C	5	ALA	Peptide
1	1C	6	GLY	Peptide
1	1C	7	GLY	Peptide
1	1C	8	LYS	Peptide
1	1C	9	ASP	Peptide
1	1D	43	LEU	Peptide
1	1D	5	ALA	Peptide
1	1D	6	GLY	Peptide
1	1D	7	GLY	Peptide
1	1D	8	LYS	Peptide
1	1D	9	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	1E	43	LEU	Peptide
1	1E	5	ALA	Peptide
1	1E	6	GLY	Peptide
1	1E	7	GLY	Peptide
1	1E	8	LYS	Peptide
1	1E	9	ASP	Peptide
1	1F	43	LEU	Peptide
1	1F	5	ALA	Peptide
1	1F	6	GLY	Peptide
1	1F	7	GLY	Peptide
1	1F	8	LYS	Peptide
1	1F	9	ASP	Peptide
1	1G	43	LEU	Peptide
1	1G	5	ALA	Peptide
1	1G	6	GLY	Peptide
1	1G	7	GLY	Peptide
1	1G	8	LYS	Peptide
1	1G	9	ASP	Peptide
1	1H	43	LEU	Peptide
1	1H	5	ALA	Peptide
1	1H	6	GLY	Peptide
1	1H	7	GLY	Peptide
1	1H	8	LYS	Peptide
1	1H	9	ASP	Peptide
1	1I	43	LEU	Peptide
1	1I	5	ALA	Peptide
1	1I	6	GLY	Peptide
1	1I	7	GLY	Peptide
1	1I	8	LYS	Peptide
1	1I	9	ASP	Peptide
1	1J	43	LEU	Peptide
1	1J	5	ALA	Peptide
1	1J	6	GLY	Peptide
1	1J	7	GLY	Peptide
1	1J	8	LYS	Peptide
1	1J	9	ASP	Peptide
1	1K	43	LEU	Peptide
1	1K	5	ALA	Peptide
1	1K	6	GLY	Peptide
1	1K	7	GLY	Peptide
1	1K	8	LYS	Peptide
1	1K	9	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	1L	43	LEU	Peptide
1	1L	5	ALA	Peptide
1	1L	6	GLY	Peptide
1	1L	7	GLY	Peptide
1	1L	8	LYS	Peptide
1	1L	9	ASP	Peptide
1	1M	43	LEU	Peptide
1	1M	5	ALA	Peptide
1	1M	6	GLY	Peptide
1	1M	7	GLY	Peptide
1	1M	8	LYS	Peptide
1	1M	9	ASP	Peptide
1	1N	43	LEU	Peptide
1	1N	5	ALA	Peptide
1	1N	6	GLY	Peptide
1	1N	7	GLY	Peptide
1	1N	8	LYS	Peptide
1	1N	9	ASP	Peptide
1	1O	43	LEU	Peptide
1	1O	5	ALA	Peptide
1	1O	6	GLY	Peptide
1	1O	7	GLY	Peptide
1	1O	8	LYS	Peptide
1	1O	9	ASP	Peptide
1	1P	43	LEU	Peptide
1	1P	5	ALA	Peptide
1	1P	6	GLY	Peptide
1	1P	7	GLY	Peptide
1	1P	8	LYS	Peptide
1	1P	9	ASP	Peptide
1	2A	43	LEU	Peptide
1	2A	5	ALA	Peptide
1	2A	6	GLY	Peptide
1	2A	7	GLY	Peptide
1	2A	8	LYS	Peptide
1	2A	9	ASP	Peptide
1	2B	43	LEU	Peptide
1	2B	5	ALA	Peptide
1	2B	6	GLY	Peptide
1	2B	7	GLY	Peptide
1	2B	8	LYS	Peptide
1	2B	9	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	2C	43	LEU	Peptide
1	2C	5	ALA	Peptide
1	2C	6	GLY	Peptide
1	2C	7	GLY	Peptide
1	2C	8	LYS	Peptide
1	2C	9	ASP	Peptide
1	2D	43	LEU	Peptide
1	2D	5	ALA	Peptide
1	2D	6	GLY	Peptide
1	2D	7	GLY	Peptide
1	2D	8	LYS	Peptide
1	2D	9	ASP	Peptide
1	2E	43	LEU	Peptide
1	2E	5	ALA	Peptide
1	2E	6	GLY	Peptide
1	2E	7	GLY	Peptide
1	2E	8	LYS	Peptide
1	2E	9	ASP	Peptide
1	2F	43	LEU	Peptide
1	2F	5	ALA	Peptide
1	2F	6	GLY	Peptide
1	2F	7	GLY	Peptide
1	2F	8	LYS	Peptide
1	2F	9	ASP	Peptide
1	2G	43	LEU	Peptide
1	2G	5	ALA	Peptide
1	2G	6	GLY	Peptide
1	2G	7	GLY	Peptide
1	2G	8	LYS	Peptide
1	2G	9	ASP	Peptide
1	2H	43	LEU	Peptide
1	2H	5	ALA	Peptide
1	2H	6	GLY	Peptide
1	2H	7	GLY	Peptide
1	2H	8	LYS	Peptide
1	2H	9	ASP	Peptide
1	2I	43	LEU	Peptide
1	2I	5	ALA	Peptide
1	2I	6	GLY	Peptide
1	2I	7	GLY	Peptide
1	2I	8	LYS	Peptide
1	2I	9	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	2J	43	LEU	Peptide
1	2J	5	ALA	Peptide
1	2J	6	GLY	Peptide
1	2J	7	GLY	Peptide
1	2J	8	LYS	Peptide
1	2J	9	ASP	Peptide
1	2K	43	LEU	Peptide
1	2K	5	ALA	Peptide
1	2K	6	GLY	Peptide
1	2K	7	GLY	Peptide
1	2K	8	LYS	Peptide
1	2K	9	ASP	Peptide
1	2L	43	LEU	Peptide
1	2L	5	ALA	Peptide
1	2L	6	GLY	Peptide
1	2L	7	GLY	Peptide
1	2L	8	LYS	Peptide
1	2L	9	ASP	Peptide
1	2M	43	LEU	Peptide
1	2M	5	ALA	Peptide
1	2M	6	GLY	Peptide
1	2M	7	GLY	Peptide
1	2M	8	LYS	Peptide
1	2M	9	ASP	Peptide
1	2N	43	LEU	Peptide
1	2N	5	ALA	Peptide
1	2N	6	GLY	Peptide
1	2N	7	GLY	Peptide
1	2N	8	LYS	Peptide
1	2N	9	ASP	Peptide
1	2O	43	LEU	Peptide
1	2O	5	ALA	Peptide
1	2O	6	GLY	Peptide
1	2O	7	GLY	Peptide
1	2O	8	LYS	Peptide
1	2O	9	ASP	Peptide
1	2P	43	LEU	Peptide
1	2P	5	ALA	Peptide
1	2P	6	GLY	Peptide
1	2P	7	GLY	Peptide
1	2P	8	LYS	Peptide
1	2P	9	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	3A	43	LEU	Peptide
1	3A	5	ALA	Peptide
1	3A	6	GLY	Peptide
1	3A	7	GLY	Peptide
1	3A	8	LYS	Peptide
1	3A	9	ASP	Peptide
1	3B	43	LEU	Peptide
1	3B	5	ALA	Peptide
1	3B	6	GLY	Peptide
1	3B	7	GLY	Peptide
1	3B	8	LYS	Peptide
1	3B	9	ASP	Peptide
1	3C	43	LEU	Peptide
1	3C	5	ALA	Peptide
1	3C	6	GLY	Peptide
1	3C	7	GLY	Peptide
1	3C	8	LYS	Peptide
1	3C	9	ASP	Peptide
1	3D	43	LEU	Peptide
1	3D	5	ALA	Peptide
1	3D	6	GLY	Peptide
1	3D	7	GLY	Peptide
1	3D	8	LYS	Peptide
1	3D	9	ASP	Peptide
1	3E	43	LEU	Peptide
1	3E	5	ALA	Peptide
1	3E	6	GLY	Peptide
1	3E	7	GLY	Peptide
1	3E	8	LYS	Peptide
1	3E	9	ASP	Peptide
1	3F	43	LEU	Peptide
1	3F	5	ALA	Peptide
1	3F	6	GLY	Peptide
1	3F	7	GLY	Peptide
1	3F	8	LYS	Peptide
1	3F	9	ASP	Peptide
1	3G	43	LEU	Peptide
1	3G	5	ALA	Peptide
1	3G	6	GLY	Peptide
1	3G	7	GLY	Peptide
1	3G	8	LYS	Peptide
1	3G	9	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	3H	43	LEU	Peptide
1	3H	5	ALA	Peptide
1	3H	6	GLY	Peptide
1	3H	7	GLY	Peptide
1	3H	8	LYS	Peptide
1	3H	9	ASP	Peptide
1	3I	43	LEU	Peptide
1	3I	5	ALA	Peptide
1	3I	6	GLY	Peptide
1	3I	7	GLY	Peptide
1	3I	8	LYS	Peptide
1	3I	9	ASP	Peptide
1	3J	43	LEU	Peptide
1	3J	5	ALA	Peptide
1	3J	6	GLY	Peptide
1	3J	7	GLY	Peptide
1	3J	8	LYS	Peptide
1	3J	9	ASP	Peptide
1	3K	43	LEU	Peptide
1	3K	5	ALA	Peptide
1	3K	6	GLY	Peptide
1	3K	7	GLY	Peptide
1	3K	8	LYS	Peptide
1	3K	9	ASP	Peptide
1	3L	43	LEU	Peptide
1	3L	5	ALA	Peptide
1	3L	6	GLY	Peptide
1	3L	7	GLY	Peptide
1	3L	8	LYS	Peptide
1	3L	9	ASP	Peptide
1	3M	43	LEU	Peptide
1	3M	5	ALA	Peptide
1	3M	6	GLY	Peptide
1	3M	7	GLY	Peptide
1	3M	8	LYS	Peptide
1	3M	9	ASP	Peptide
1	3N	43	LEU	Peptide
1	3N	5	ALA	Peptide
1	3N	6	GLY	Peptide
1	3N	7	GLY	Peptide
1	3N	8	LYS	Peptide
1	3N	9	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	3O	43	LEU	Peptide
1	3O	5	ALA	Peptide
1	3O	6	GLY	Peptide
1	3O	7	GLY	Peptide
1	3O	8	LYS	Peptide
1	3O	9	ASP	Peptide
1	3P	43	LEU	Peptide
1	3P	5	ALA	Peptide
1	3P	6	GLY	Peptide
1	3P	7	GLY	Peptide
1	3P	8	LYS	Peptide
1	3P	9	ASP	Peptide
1	4A	43	LEU	Peptide
1	4A	5	ALA	Peptide
1	4A	6	GLY	Peptide
1	4A	7	GLY	Peptide
1	4A	8	LYS	Peptide
1	4A	9	ASP	Peptide
1	4B	43	LEU	Peptide
1	4B	5	ALA	Peptide
1	4B	6	GLY	Peptide
1	4B	7	GLY	Peptide
1	4B	8	LYS	Peptide
1	4B	9	ASP	Peptide
1	4C	43	LEU	Peptide
1	4C	5	ALA	Peptide
1	4C	6	GLY	Peptide
1	4C	7	GLY	Peptide
1	4C	8	LYS	Peptide
1	4C	9	ASP	Peptide
1	4D	43	LEU	Peptide
1	4D	5	ALA	Peptide
1	4D	6	GLY	Peptide
1	4D	7	GLY	Peptide
1	4D	8	LYS	Peptide
1	4D	9	ASP	Peptide
1	4E	43	LEU	Peptide
1	4E	5	ALA	Peptide
1	4E	6	GLY	Peptide
1	4E	7	GLY	Peptide
1	4E	8	LYS	Peptide
1	4E	9	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	4F	43	LEU	Peptide
1	4F	5	ALA	Peptide
1	4F	6	GLY	Peptide
1	4F	7	GLY	Peptide
1	4F	8	LYS	Peptide
1	4F	9	ASP	Peptide
1	4G	43	LEU	Peptide
1	4G	5	ALA	Peptide
1	4G	6	GLY	Peptide
1	4G	7	GLY	Peptide
1	4G	8	LYS	Peptide
1	4G	9	ASP	Peptide
1	4H	43	LEU	Peptide
1	4H	5	ALA	Peptide
1	4H	6	GLY	Peptide
1	4H	7	GLY	Peptide
1	4H	8	LYS	Peptide
1	4H	9	ASP	Peptide
1	4I	43	LEU	Peptide
1	4I	5	ALA	Peptide
1	4I	6	GLY	Peptide
1	4I	7	GLY	Peptide
1	4I	8	LYS	Peptide
1	4I	9	ASP	Peptide
1	4J	43	LEU	Peptide
1	4J	5	ALA	Peptide
1	4J	6	GLY	Peptide
1	4J	7	GLY	Peptide
1	4J	8	LYS	Peptide
1	4J	9	ASP	Peptide
1	4K	43	LEU	Peptide
1	4K	5	ALA	Peptide
1	4K	6	GLY	Peptide
1	4K	7	GLY	Peptide
1	4K	8	LYS	Peptide
1	4K	9	ASP	Peptide
1	4L	43	LEU	Peptide
1	4L	5	ALA	Peptide
1	4L	6	GLY	Peptide
1	4L	7	GLY	Peptide
1	4L	8	LYS	Peptide
1	4L	9	ASP	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
1	4M	43	LEU	Peptide
1	4M	5	ALA	Peptide
1	4M	6	GLY	Peptide
1	4M	7	GLY	Peptide
1	4M	8	LYS	Peptide
1	4M	9	ASP	Peptide
1	4N	43	LEU	Peptide
1	4N	5	ALA	Peptide
1	4N	6	GLY	Peptide
1	4N	7	GLY	Peptide
1	4N	8	LYS	Peptide
1	4N	9	ASP	Peptide
1	4O	43	LEU	Peptide
1	4O	5	ALA	Peptide
1	4O	6	GLY	Peptide
1	4O	7	GLY	Peptide
1	4O	8	LYS	Peptide
1	4O	9	ASP	Peptide
1	4P	43	LEU	Peptide
1	4P	5	ALA	Peptide
1	4P	6	GLY	Peptide
1	4P	7	GLY	Peptide
1	4P	8	LYS	Peptide
1	4P	9	ASP	Peptide
1	5A	43	LEU	Peptide
1	5A	5	ALA	Peptide
1	5A	6	GLY	Peptide
1	5A	7	GLY	Peptide
1	5A	8	LYS	Peptide
1	5A	9	ASP	Peptide
1	5B	43	LEU	Peptide
1	5B	5	ALA	Peptide
1	5B	6	GLY	Peptide
1	5B	7	GLY	Peptide
1	5B	8	LYS	Peptide
1	5B	9	ASP	Peptide
1	5C	43	LEU	Peptide
1	5C	5	ALA	Peptide
1	5C	6	GLY	Peptide
1	5C	7	GLY	Peptide
1	5C	8	LYS	Peptide
1	5C	9	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	5D	43	LEU	Peptide
1	5D	5	ALA	Peptide
1	5D	6	GLY	Peptide
1	5D	7	GLY	Peptide
1	5D	8	LYS	Peptide
1	5D	9	ASP	Peptide
1	5E	43	LEU	Peptide
1	5E	5	ALA	Peptide
1	5E	6	GLY	Peptide
1	5E	7	GLY	Peptide
1	5E	8	LYS	Peptide
1	5E	9	ASP	Peptide
1	5F	43	LEU	Peptide
1	5F	5	ALA	Peptide
1	5F	6	GLY	Peptide
1	5F	7	GLY	Peptide
1	5F	8	LYS	Peptide
1	5F	9	ASP	Peptide
1	5G	43	LEU	Peptide
1	5G	5	ALA	Peptide
1	5G	6	GLY	Peptide
1	5G	7	GLY	Peptide
1	5G	8	LYS	Peptide
1	5G	9	ASP	Peptide
1	5H	43	LEU	Peptide
1	5H	5	ALA	Peptide
1	5H	6	GLY	Peptide
1	5H	7	GLY	Peptide
1	5H	8	LYS	Peptide
1	5H	9	ASP	Peptide
1	5I	43	LEU	Peptide
1	5I	5	ALA	Peptide
1	5I	6	GLY	Peptide
1	5I	7	GLY	Peptide
1	5I	8	LYS	Peptide
1	5I	9	ASP	Peptide
1	5J	43	LEU	Peptide
1	5J	5	ALA	Peptide
1	5J	6	GLY	Peptide
1	5J	7	GLY	Peptide
1	5J	8	LYS	Peptide
1	5J	9	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	5K	43	LEU	Peptide
1	5K	5	ALA	Peptide
1	5K	6	GLY	Peptide
1	5K	7	GLY	Peptide
1	5K	8	LYS	Peptide
1	5K	9	ASP	Peptide
1	5L	43	LEU	Peptide
1	5L	5	ALA	Peptide
1	5L	6	GLY	Peptide
1	5L	7	GLY	Peptide
1	5L	8	LYS	Peptide
1	5L	9	ASP	Peptide
1	5M	43	LEU	Peptide
1	5M	5	ALA	Peptide
1	5M	6	GLY	Peptide
1	5M	7	GLY	Peptide
1	5M	8	LYS	Peptide
1	5M	9	ASP	Peptide
1	5N	43	LEU	Peptide
1	5N	5	ALA	Peptide
1	5N	6	GLY	Peptide
1	5N	7	GLY	Peptide
1	5N	8	LYS	Peptide
1	5N	9	ASP	Peptide
1	5O	43	LEU	Peptide
1	5O	5	ALA	Peptide
1	5O	6	GLY	Peptide
1	5O	7	GLY	Peptide
1	5O	8	LYS	Peptide
1	5O	9	ASP	Peptide
1	5P	43	LEU	Peptide
1	5P	5	ALA	Peptide
1	5P	6	GLY	Peptide
1	5P	7	GLY	Peptide
1	5P	8	LYS	Peptide
1	5P	9	ASP	Peptide

## 5.2 Too-close contacts ⓘ

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	471	0	520	42	0
1	1B	471	0	520	49	0
1	1C	471	0	520	49	0
1	1D	471	0	520	50	0
1	1E	471	0	520	52	0
1	1F	471	0	520	53	0
1	1G	471	0	520	53	0
1	1H	471	0	520	51	0
1	1I	471	0	520	51	0
1	1J	471	0	520	48	0
1	1K	471	0	520	47	0
1	1L	471	0	520	43	0
1	1M	471	0	520	42	0
1	1N	471	0	520	43	0
1	1O	471	0	520	41	0
1	1P	471	0	520	22	0
1	2A	471	0	520	42	0
1	2B	471	0	520	50	0
1	2C	471	0	520	51	0
1	2D	471	0	520	49	0
1	2E	471	0	520	50	0
1	2F	471	0	520	51	0
1	2G	471	0	520	52	0
1	2H	471	0	520	51	0
1	2I	471	0	520	50	0
1	2J	471	0	520	45	0
1	2K	471	0	520	44	0
1	2L	471	0	520	43	0
1	2M	471	0	520	43	0
1	2N	471	0	520	43	0
1	2O	471	0	520	40	0
1	2P	471	0	520	20	0
1	3A	471	0	520	42	0
1	3B	471	0	520	49	0
1	3C	471	0	520	49	0
1	3D	471	0	520	51	0
1	3E	471	0	520	51	0
1	3F	471	0	520	52	0
1	3G	471	0	520	53	0
1	3H	471	0	520	54	0
1	3I	471	0	520	49	0
1	3J	471	0	520	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3K	471	0	520	46	0
1	3L	471	0	520	44	0
1	3M	471	0	520	44	0
1	3N	471	0	520	44	0
1	3O	471	0	520	42	0
1	3P	471	0	520	20	0
1	4A	471	0	520	41	0
1	4B	471	0	520	48	0
1	4C	471	0	520	50	0
1	4D	471	0	520	49	0
1	4E	471	0	520	53	0
1	4F	471	0	520	54	0
1	4G	471	0	520	53	0
1	4H	471	0	520	52	0
1	4I	471	0	520	51	0
1	4J	471	0	520	46	0
1	4K	471	0	520	45	0
1	4L	471	0	520	43	0
1	4M	471	0	520	42	0
1	4N	471	0	520	43	0
1	4O	471	0	520	41	0
1	4P	471	0	520	19	0
1	5A	471	0	520	40	0
1	5B	471	0	520	48	0
1	5C	471	0	520	51	0
1	5D	471	0	520	52	0
1	5E	471	0	520	53	0
1	5F	471	0	520	54	0
1	5G	471	0	520	54	0
1	5H	471	0	520	53	0
1	5I	471	0	520	52	0
1	5J	471	0	520	47	0
1	5K	471	0	520	46	0
1	5L	471	0	520	45	0
1	5M	471	0	520	45	0
1	5N	471	0	520	43	0
1	5O	471	0	520	42	0
1	5P	471	0	520	20	0
2	1A	49	0	74	23	0
2	1B	49	0	74	28	0
2	1C	49	0	74	28	0
2	1D	49	0	74	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1E	49	0	74	30	0
2	1F	49	0	74	31	0
2	1G	49	0	74	31	0
2	1H	49	0	74	30	0
2	1I	49	0	74	30	0
2	1J	49	0	74	29	0
2	1K	49	0	74	29	0
2	1L	49	0	74	27	0
2	1M	49	0	74	24	0
2	1N	49	0	74	25	0
2	1O	49	0	74	25	0
2	2A	49	0	74	22	0
2	2B	49	0	74	28	0
2	2C	49	0	74	29	0
2	2D	49	0	74	28	0
2	2E	49	0	74	29	0
2	2F	49	0	74	29	0
2	2G	49	0	74	29	0
2	2H	49	0	74	30	0
2	2I	49	0	74	29	0
2	2J	49	0	74	29	0
2	2K	49	0	74	28	0
2	2L	49	0	74	27	0
2	2M	49	0	74	26	0
2	2N	49	0	74	25	0
2	2O	49	0	74	24	0
2	3A	49	0	74	22	0
2	3B	49	0	74	27	0
2	3C	49	0	74	29	0
2	3D	49	0	74	30	0
2	3E	49	0	74	29	0
2	3F	49	0	74	29	0
2	3G	49	0	74	29	0
2	3H	49	0	74	30	0
2	3I	49	0	74	29	0
2	3J	49	0	74	28	0
2	3K	49	0	74	28	0
2	3L	49	0	74	27	0
2	3M	49	0	74	26	0
2	3N	49	0	74	26	0
2	3O	49	0	74	26	0
2	4A	49	0	74	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	4B	49	0	74	28	0
2	4C	49	0	74	28	0
2	4D	49	0	74	28	0
2	4E	49	0	74	30	0
2	4F	49	0	74	31	0
2	4G	49	0	74	30	0
2	4H	49	0	74	29	0
2	4I	49	0	74	30	0
2	4J	49	0	74	28	0
2	4K	49	0	74	28	0
2	4L	49	0	74	27	0
2	4M	49	0	74	26	0
2	4N	49	0	74	26	0
2	4O	49	0	74	26	0
2	5A	49	0	74	22	0
2	5B	49	0	74	28	0
2	5C	49	0	74	29	0
2	5D	49	0	74	30	0
2	5E	49	0	74	30	0
2	5F	49	0	74	30	0
2	5G	49	0	74	30	0
2	5H	49	0	74	30	0
2	5I	49	0	74	29	0
2	5J	49	0	74	29	0
2	5K	49	0	74	28	0
2	5L	49	0	74	27	0
2	5M	49	0	74	25	0
2	5N	49	0	74	26	0
2	5O	49	0	74	25	0
All	All	41355	0	47150	3731	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 42.

All (3731) 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)
1:2J:47:LEU:HD22	2:2J:101:LHG:H102	1.34	1.10
1:1O:47:LEU:HD22	2:1O:101:LHG:H102	1.34	1.09
1:2F:47:LEU:HD22	2:2F:101:LHG:H102	1.34	1.09
1:2I:47:LEU:HD22	2:2I:101:LHG:H102	1.34	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2G:47:LEU:HD22	2:2G:101:LHG:H102	1.34	1.09
1:2H:47:LEU:HD22	2:2H:101:LHG:H102	1.34	1.09
1:5M:47:LEU:HD22	2:5M:101:LHG:H102	1.34	1.09
1:2E:47:LEU:HD22	2:2E:101:LHG:H102	1.35	1.09
1:3G:47:LEU:HD22	2:3G:101:LHG:H102	1.34	1.09
1:5N:47:LEU:HD22	2:5N:101:LHG:H102	1.34	1.09
1:3H:47:LEU:HD22	2:3H:101:LHG:H102	1.34	1.09
1:3K:47:LEU:HD22	2:3K:101:LHG:H102	1.34	1.09
1:3L:47:LEU:HD22	2:3L:101:LHG:H102	1.34	1.09
1:1G:47:LEU:HD22	2:1G:101:LHG:H102	1.34	1.09
1:3I:47:LEU:HD22	2:3I:101:LHG:H102	1.34	1.09
1:5O:47:LEU:HD22	2:5O:101:LHG:H102	1.34	1.09
1:3J:47:LEU:HD22	2:3J:101:LHG:H102	1.34	1.09
1:1F:47:LEU:HD22	2:1F:101:LHG:H102	1.34	1.09
1:1H:47:LEU:HD22	2:1H:101:LHG:H102	1.34	1.09
1:1E:47:LEU:HD22	2:1E:101:LHG:H102	1.34	1.09
1:1C:47:LEU:HD22	2:1C:101:LHG:H102	1.35	1.09
1:1N:47:LEU:HD22	2:1N:101:LHG:H102	1.34	1.09
1:2D:47:LEU:HD22	2:2D:101:LHG:H102	1.34	1.09
1:2K:47:LEU:HD22	2:2K:101:LHG:H102	1.34	1.09
1:1D:47:LEU:HD22	2:1D:101:LHG:H102	1.35	1.09
1:3M:47:LEU:HD22	2:3M:101:LHG:H102	1.34	1.09
1:4A:47:LEU:HD22	2:4A:101:LHG:H102	1.35	1.09
1:5L:47:LEU:HD22	2:5L:101:LHG:H102	1.34	1.09
1:4B:47:LEU:HD22	2:4B:101:LHG:H102	1.35	1.08
1:4O:47:LEU:HD22	2:4O:101:LHG:H102	1.34	1.08
1:3F:47:LEU:HD22	2:3F:101:LHG:H102	1.34	1.08
1:1B:47:LEU:HD22	2:1B:101:LHG:H102	1.35	1.08
1:1I:47:LEU:HD22	2:1I:101:LHG:H102	1.34	1.08
1:4J:47:LEU:HD22	2:4J:101:LHG:H102	1.34	1.08
1:3A:47:LEU:HD22	2:3A:101:LHG:H102	1.35	1.08
1:4I:47:LEU:HD22	2:4I:101:LHG:H102	1.34	1.08
1:4K:47:LEU:HD22	2:4K:101:LHG:H102	1.34	1.08
1:4N:47:LEU:HD22	2:4N:101:LHG:H102	1.34	1.08
1:4L:47:LEU:HD22	2:4L:101:LHG:H102	1.34	1.08
1:4M:47:LEU:HD22	2:4M:101:LHG:H102	1.34	1.08
1:5E:47:LEU:HD22	2:5E:101:LHG:H102	1.34	1.08
1:5F:47:LEU:HD22	2:5F:101:LHG:H102	1.34	1.08
1:4C:47:LEU:HD22	2:4C:101:LHG:H102	1.35	1.08
1:4H:47:LEU:HD22	2:4H:101:LHG:H102	1.34	1.08
1:5D:47:LEU:HD22	2:5D:101:LHG:H102	1.34	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1M:47:LEU:HD22	2:1M:101:LHG:H102	1.34	1.07
1:2L:47:LEU:HD22	2:2L:101:LHG:H102	1.34	1.07
1:5A:47:LEU:HD22	2:5A:101:LHG:H102	1.35	1.07
1:5C:47:LEU:HD22	2:5C:101:LHG:H102	1.35	1.07
1:5G:47:LEU:HD22	2:5G:101:LHG:H102	1.34	1.07
1:1J:47:LEU:HD22	2:1J:101:LHG:H102	1.34	1.07
1:2C:47:LEU:HD22	2:2C:101:LHG:H102	1.35	1.07
1:2O:47:LEU:HD22	2:2O:101:LHG:H102	1.34	1.07
1:3E:47:LEU:HD22	2:3E:101:LHG:H102	1.34	1.07
1:5B:47:LEU:HD22	2:5B:101:LHG:H102	1.35	1.07
1:5K:47:LEU:HD22	2:5K:101:LHG:H102	1.34	1.07
1:3N:47:LEU:HD22	2:3N:101:LHG:H102	1.34	1.07
1:1A:47:LEU:HD22	2:1A:101:LHG:H102	1.35	1.07
1:4G:47:LEU:HD22	2:4G:101:LHG:H102	1.34	1.07
1:5H:47:LEU:HD22	2:5H:101:LHG:H102	1.34	1.07
1:3O:47:LEU:HD22	2:3O:101:LHG:H102	1.34	1.07
1:5I:47:LEU:HD22	2:5I:101:LHG:H102	1.34	1.07
1:5J:47:LEU:HD22	2:5J:101:LHG:H102	1.34	1.07
1:3B:47:LEU:HD22	2:3B:101:LHG:H102	1.35	1.06
1:4F:47:LEU:HD22	2:4F:101:LHG:H102	1.34	1.06
1:1K:47:LEU:HD22	2:1K:101:LHG:H102	1.34	1.06
1:2N:47:LEU:HD22	2:2N:101:LHG:H102	1.34	1.06
1:4E:47:LEU:HD22	2:4E:101:LHG:H102	1.34	1.06
1:4D:47:LEU:HD22	2:4D:101:LHG:H102	1.34	1.06
1:3D:47:LEU:HD22	2:3D:101:LHG:H102	1.34	1.06
1:1L:47:LEU:HD22	2:1L:101:LHG:H102	1.34	1.06
1:2M:47:LEU:HD22	2:2M:101:LHG:H102	1.34	1.06
1:2A:47:LEU:HD22	2:2A:101:LHG:H102	1.35	1.06
1:2B:47:LEU:HD22	2:2B:101:LHG:H102	1.35	1.06
1:3C:47:LEU:HD22	2:3C:101:LHG:H102	1.34	1.05
2:2I:101:LHG:H372	2:2I:101:LHG:H212	1.40	1.04
2:1H:101:LHG:H372	2:1H:101:LHG:H212	1.40	1.04
2:4B:101:LHG:H372	2:4B:101:LHG:H212	1.40	1.04
2:4L:101:LHG:H212	2:4L:101:LHG:H372	1.40	1.04
2:5E:101:LHG:H372	2:5E:101:LHG:H212	1.40	1.04
2:2K:101:LHG:H212	2:2K:101:LHG:H372	1.40	1.04
2:3I:101:LHG:H212	2:3I:101:LHG:H372	1.40	1.04
2:5O:101:LHG:H372	2:5O:101:LHG:H212	1.40	1.04
2:2G:101:LHG:H212	2:2G:101:LHG:H372	1.40	1.04
2:3A:101:LHG:H212	2:3A:101:LHG:H372	1.40	1.04
2:3J:101:LHG:H212	2:3J:101:LHG:H372	1.40	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1F:101:LHG:H372	2:1F:101:LHG:H212	1.40	1.04
2:3L:101:LHG:H212	2:3L:101:LHG:H372	1.40	1.04
2:1D:101:LHG:H372	2:1D:101:LHG:H212	1.40	1.04
2:2F:101:LHG:H372	2:2F:101:LHG:H212	1.40	1.04
2:2H:101:LHG:H212	2:2H:101:LHG:H372	1.40	1.04
2:2J:101:LHG:H372	2:2J:101:LHG:H212	1.40	1.04
2:3K:101:LHG:H372	2:3K:101:LHG:H212	1.40	1.04
2:4M:101:LHG:H372	2:4M:101:LHG:H212	1.40	1.04
2:1C:101:LHG:H372	2:1C:101:LHG:H212	1.40	1.03
2:4O:101:LHG:H212	2:4O:101:LHG:H372	1.40	1.03
2:5M:101:LHG:H372	2:5M:101:LHG:H212	1.40	1.03
2:1G:101:LHG:H212	2:1G:101:LHG:H372	1.40	1.03
2:3M:101:LHG:H212	2:3M:101:LHG:H372	1.40	1.03
2:3N:101:LHG:H372	2:3N:101:LHG:H212	1.40	1.03
2:4J:101:LHG:H372	2:4J:101:LHG:H212	1.40	1.03
2:4N:101:LHG:H212	2:4N:101:LHG:H372	1.40	1.03
2:5A:101:LHG:H212	2:5A:101:LHG:H372	1.40	1.03
2:5B:101:LHG:H212	2:5B:101:LHG:H372	1.40	1.03
2:5C:101:LHG:H372	2:5C:101:LHG:H212	1.40	1.03
2:1E:101:LHG:H372	2:1E:101:LHG:H212	1.40	1.03
2:4D:101:LHG:H212	2:4D:101:LHG:H372	1.40	1.03
2:5D:101:LHG:H212	2:5D:101:LHG:H372	1.40	1.03
2:4A:101:LHG:H212	2:4A:101:LHG:H372	1.40	1.03
2:4K:101:LHG:H212	2:4K:101:LHG:H372	1.40	1.03
2:3H:101:LHG:H372	2:3H:101:LHG:H212	1.40	1.03
2:5N:101:LHG:H212	2:5N:101:LHG:H372	1.40	1.03
2:3G:101:LHG:H372	2:3G:101:LHG:H212	1.40	1.03
2:5G:101:LHG:H212	2:5G:101:LHG:H372	1.40	1.03
2:1J:101:LHG:H372	2:1J:101:LHG:H212	1.40	1.03
2:2E:101:LHG:H212	2:2E:101:LHG:H372	1.40	1.03
2:4C:101:LHG:H212	2:4C:101:LHG:H372	1.40	1.03
2:1B:101:LHG:H372	2:1B:101:LHG:H212	1.40	1.02
2:2D:101:LHG:H212	2:2D:101:LHG:H372	1.40	1.02
2:5F:101:LHG:H372	2:5F:101:LHG:H212	1.40	1.02
2:1N:101:LHG:H212	2:1N:101:LHG:H372	1.40	1.02
2:1I:101:LHG:H212	2:1I:101:LHG:H372	1.40	1.02
2:1O:101:LHG:H372	2:1O:101:LHG:H212	1.40	1.02
2:2M:101:LHG:H212	2:2M:101:LHG:H372	1.40	1.02
2:1A:101:LHG:H372	2:1A:101:LHG:H212	1.40	1.02
2:2L:101:LHG:H212	2:2L:101:LHG:H372	1.40	1.02
2:4I:101:LHG:H372	2:4I:101:LHG:H212	1.40	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5K:101:LHG:H212	2:5K:101:LHG:H372	1.40	1.02
2:3B:101:LHG:H212	2:3B:101:LHG:H372	1.40	1.02
2:3C:101:LHG:H372	2:3C:101:LHG:H212	1.40	1.02
2:5L:101:LHG:H212	2:5L:101:LHG:H372	1.40	1.02
2:3O:101:LHG:H372	2:3O:101:LHG:H212	1.40	1.02
2:4H:101:LHG:H372	2:4H:101:LHG:H212	1.40	1.02
2:4F:101:LHG:H372	2:4F:101:LHG:H212	1.40	1.02
2:2B:101:LHG:H372	2:2B:101:LHG:H212	1.40	1.01
2:5I:101:LHG:H372	2:5I:101:LHG:H212	1.40	1.01
2:1L:101:LHG:H212	2:1L:101:LHG:H372	1.40	1.01
2:2O:101:LHG:H372	2:2O:101:LHG:H212	1.40	1.01
2:3E:101:LHG:H372	2:3E:101:LHG:H212	1.40	1.01
2:3F:101:LHG:H212	2:3F:101:LHG:H372	1.40	1.01
2:4E:101:LHG:H372	2:4E:101:LHG:H212	1.40	1.01
2:2C:101:LHG:H372	2:2C:101:LHG:H212	1.40	1.01
2:5H:101:LHG:H212	2:5H:101:LHG:H372	1.40	1.01
2:1K:101:LHG:H212	2:1K:101:LHG:H372	1.40	1.01
2:2A:101:LHG:H372	2:2A:101:LHG:H212	1.40	1.01
2:2N:101:LHG:H212	2:2N:101:LHG:H372	1.40	1.01
2:1M:101:LHG:H212	2:1M:101:LHG:H372	1.40	1.01
2:3D:101:LHG:H372	2:3D:101:LHG:H212	1.40	1.00
2:4G:101:LHG:H212	2:4G:101:LHG:H372	1.40	1.00
2:5J:101:LHG:H212	2:5J:101:LHG:H372	1.40	1.00
1:2G:55:PHE:HA	2:2G:101:LHG:H223	1.46	0.98
1:2H:55:PHE:HA	2:2H:101:LHG:H223	1.46	0.98
1:2I:55:PHE:HA	2:2I:101:LHG:H223	1.46	0.98
1:1E:55:PHE:HA	2:1E:101:LHG:H223	1.46	0.98
1:1F:55:PHE:HA	2:1F:101:LHG:H223	1.46	0.98
1:1G:55:PHE:HA	2:1G:101:LHG:H223	1.46	0.98
1:3J:55:PHE:HA	2:3J:101:LHG:H223	1.46	0.98
1:2J:55:PHE:HA	2:2J:101:LHG:H223	1.46	0.98
1:5N:55:PHE:HA	2:5N:101:LHG:H223	1.46	0.98
1:2F:55:PHE:HA	2:2F:101:LHG:H223	1.46	0.97
1:3I:55:PHE:HA	2:3I:101:LHG:H223	1.46	0.97
1:3K:55:PHE:HA	2:3K:101:LHG:H223	1.46	0.97
1:5O:55:PHE:HA	2:5O:101:LHG:H223	1.46	0.97
1:1D:55:PHE:HA	2:1D:101:LHG:H223	1.46	0.97
1:4L:55:PHE:HA	2:4L:101:LHG:H223	1.46	0.97
1:3L:55:PHE:HA	2:3L:101:LHG:H223	1.46	0.97
1:4A:55:PHE:HA	2:4A:101:LHG:H223	1.46	0.97
1:1C:55:PHE:HA	2:1C:101:LHG:H223	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1H:55:PHE:HA	2:1H:101:LHG:H223	1.46	0.97
1:4K:55:PHE:HA	2:4K:101:LHG:H223	1.46	0.97
1:4M:55:PHE:HA	2:4M:101:LHG:H223	1.46	0.97
1:4N:55:PHE:HA	2:4N:101:LHG:H223	1.46	0.97
1:5M:55:PHE:HA	2:5M:101:LHG:H223	1.46	0.97
1:3H:55:PHE:HA	2:3H:101:LHG:H223	1.46	0.97
1:5E:55:PHE:HA	2:5E:101:LHG:H223	1.46	0.97
1:2E:55:PHE:HA	2:2E:101:LHG:H223	1.46	0.97
1:2K:55:PHE:HA	2:2K:101:LHG:H223	1.46	0.97
1:4O:55:PHE:HA	2:4O:101:LHG:H223	1.46	0.97
1:5B:55:PHE:HA	2:5B:101:LHG:H223	1.46	0.97
1:1O:55:PHE:HA	2:1O:101:LHG:H223	1.46	0.97
1:4B:55:PHE:HA	2:4B:101:LHG:H223	1.46	0.97
1:5A:55:PHE:HA	2:5A:101:LHG:H223	1.46	0.97
1:5C:55:PHE:HA	2:5C:101:LHG:H223	1.46	0.97
1:5D:55:PHE:HA	2:5D:101:LHG:H223	1.46	0.97
1:3M:55:PHE:HA	2:3M:101:LHG:H223	1.46	0.97
1:5F:55:PHE:HA	2:5F:101:LHG:H223	1.46	0.97
1:1I:55:PHE:HA	2:1I:101:LHG:H223	1.46	0.96
1:3A:55:PHE:HA	2:3A:101:LHG:H223	1.46	0.96
1:3G:55:PHE:HA	2:3G:101:LHG:H223	1.46	0.96
1:4J:55:PHE:HA	2:4J:101:LHG:H223	1.46	0.96
1:1B:55:PHE:HA	2:1B:101:LHG:H223	1.46	0.96
1:5L:55:PHE:HA	2:5L:101:LHG:H223	1.46	0.96
1:4C:55:PHE:HA	2:4C:101:LHG:H223	1.46	0.96
1:2D:55:PHE:HA	2:2D:101:LHG:H223	1.46	0.96
1:1N:55:PHE:HA	2:1N:101:LHG:H223	1.46	0.96
1:2L:55:PHE:HA	2:2L:101:LHG:H223	1.46	0.96
1:3N:55:PHE:HA	2:3N:101:LHG:H223	1.46	0.96
1:5G:55:PHE:HA	2:5G:101:LHG:H223	1.46	0.96
1:1J:55:PHE:HA	2:1J:101:LHG:H223	1.46	0.96
1:3F:55:PHE:HA	2:3F:101:LHG:H223	1.46	0.96
1:4I:55:PHE:HA	2:4I:101:LHG:H223	1.46	0.95
1:3O:55:PHE:HA	2:3O:101:LHG:H223	1.46	0.95
1:4D:55:PHE:HA	2:4D:101:LHG:H223	1.46	0.95
1:3B:55:PHE:HA	2:3B:101:LHG:H223	1.46	0.95
1:5H:55:PHE:HA	2:5H:101:LHG:H223	1.46	0.95
1:5K:55:PHE:HA	2:5K:101:LHG:H223	1.46	0.95
1:4H:55:PHE:HA	2:4H:101:LHG:H223	1.46	0.95
1:1A:55:PHE:HA	2:1A:101:LHG:H223	1.46	0.95
1:2C:55:PHE:HA	2:2C:101:LHG:H223	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1M:55:PHE:HA	2:1M:101:LHG:H223	1.46	0.95
1:4E:55:PHE:HA	2:4E:101:LHG:H223	1.46	0.95
1:2O:55:PHE:HA	2:2O:101:LHG:H223	1.46	0.95
1:3E:55:PHE:HA	2:3E:101:LHG:H223	1.46	0.95
1:4F:55:PHE:HA	2:4F:101:LHG:H223	1.46	0.95
1:1K:55:PHE:HA	2:1K:101:LHG:H223	1.46	0.95
1:4G:55:PHE:HA	2:4G:101:LHG:H223	1.46	0.95
1:5I:55:PHE:HA	2:5I:101:LHG:H223	1.46	0.95
1:5J:55:PHE:HA	2:5J:101:LHG:H223	1.46	0.94
1:2N:55:PHE:HA	2:2N:101:LHG:H223	1.46	0.94
1:3D:55:PHE:HA	2:3D:101:LHG:H223	1.46	0.94
1:2M:55:PHE:HA	2:2M:101:LHG:H223	1.46	0.94
1:1L:55:PHE:HA	2:1L:101:LHG:H223	1.46	0.94
1:2A:55:PHE:HA	2:2A:101:LHG:H223	1.46	0.94
1:3C:55:PHE:HA	2:3C:101:LHG:H223	1.46	0.94
1:2B:55:PHE:HA	2:2B:101:LHG:H223	1.46	0.94
1:1N:55:PHE:CD1	2:1N:101:LHG:H223	2.05	0.92
1:2M:55:PHE:CD1	2:2M:101:LHG:H223	2.05	0.92
1:4L:55:PHE:CD1	2:4L:101:LHG:H223	2.05	0.92
1:5O:55:PHE:CD1	2:5O:101:LHG:H223	2.05	0.92
1:1C:55:PHE:CD1	2:1C:101:LHG:H223	2.05	0.92
1:1O:55:PHE:CD1	2:1O:101:LHG:H223	2.05	0.92
1:2F:55:PHE:CD1	2:2F:101:LHG:H223	2.05	0.92
1:3N:55:PHE:CD1	2:3N:101:LHG:H223	2.05	0.92
1:4E:55:PHE:CD1	2:4E:101:LHG:H223	2.05	0.92
1:4M:55:PHE:CD1	2:4M:101:LHG:H223	2.05	0.92
1:5F:55:PHE:CD1	2:5F:101:LHG:H223	2.05	0.92
1:2G:55:PHE:CD1	2:2G:101:LHG:H223	2.05	0.92
1:3I:55:PHE:CD1	2:3I:101:LHG:H223	2.05	0.92
1:3M:55:PHE:CD1	2:3M:101:LHG:H223	2.05	0.92
1:5K:55:PHE:CD1	2:5K:101:LHG:H223	2.05	0.92
1:2L:55:PHE:CD1	2:2L:101:LHG:H223	2.05	0.92
1:3J:55:PHE:CD1	2:3J:101:LHG:H223	2.05	0.92
1:4A:55:PHE:CD1	2:4A:101:LHG:H223	2.05	0.92
1:5A:55:PHE:CD1	2:5A:101:LHG:H223	2.05	0.92
1:5L:55:PHE:CD1	2:5L:101:LHG:H223	2.05	0.92
1:1B:55:PHE:CD1	2:1B:101:LHG:H223	2.05	0.92
1:1D:55:PHE:CD1	2:1D:101:LHG:H223	2.05	0.92
1:1M:55:PHE:CD1	2:1M:101:LHG:H223	2.05	0.92
1:3E:55:PHE:CD1	2:3E:101:LHG:H223	2.05	0.92
1:4D:55:PHE:CD1	2:4D:101:LHG:H223	2.05	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4H:55:PHE:CD1	2:4H:101:LHG:H223	2.05	0.92
1:4O:55:PHE:CD1	2:4O:101:LHG:H223	2.05	0.92
1:2E:55:PHE:CD1	2:2E:101:LHG:H223	2.05	0.92
1:3C:55:PHE:CD1	2:3C:101:LHG:H223	2.05	0.92
1:4F:55:PHE:CD1	2:4F:101:LHG:H223	2.05	0.92
1:5E:55:PHE:CD1	2:5E:101:LHG:H223	2.05	0.92
1:5J:55:PHE:CD1	2:5J:101:LHG:H223	2.05	0.92
1:2A:55:PHE:CD1	2:2A:101:LHG:H223	2.05	0.91
1:2B:55:PHE:CD1	2:2B:101:LHG:H223	2.05	0.91
1:2N:55:PHE:CD1	2:2N:101:LHG:H223	2.05	0.91
1:3F:55:PHE:CD1	2:3F:101:LHG:H223	2.05	0.91
1:3O:55:PHE:CD1	2:3O:101:LHG:H223	2.05	0.91
1:4G:55:PHE:CD1	2:4G:101:LHG:H223	2.05	0.91
1:4I:55:PHE:CD1	2:4I:101:LHG:H223	2.05	0.91
1:1G:55:PHE:CD1	2:1G:101:LHG:H223	2.05	0.91
1:3D:55:PHE:CD1	2:3D:101:LHG:H223	2.05	0.91
1:3H:55:PHE:CD1	2:3H:101:LHG:H223	2.05	0.91
1:5G:55:PHE:CD1	2:5G:101:LHG:H223	2.05	0.91
1:1K:55:PHE:CD1	2:1K:101:LHG:H223	2.05	0.91
1:1L:55:PHE:CD1	2:1L:101:LHG:H223	2.05	0.91
1:4B:55:PHE:CD1	2:4B:101:LHG:H223	2.05	0.91
1:4N:55:PHE:CD1	2:4N:101:LHG:H223	2.05	0.91
1:5D:55:PHE:CD1	2:5D:101:LHG:H223	2.05	0.91
1:5N:55:PHE:CD1	2:5N:101:LHG:H223	2.05	0.91
1:2C:55:PHE:CD1	2:2C:101:LHG:H223	2.05	0.91
1:3K:55:PHE:CD1	2:3K:101:LHG:H223	2.05	0.91
1:1H:55:PHE:CD1	2:1H:101:LHG:H223	2.05	0.91
1:4K:55:PHE:CD1	2:4K:101:LHG:H223	2.05	0.91
1:5C:55:PHE:CD1	2:5C:101:LHG:H223	2.05	0.91
1:2K:55:PHE:CD1	2:2K:101:LHG:H223	2.05	0.91
1:2H:55:PHE:CD1	2:2H:101:LHG:H223	2.05	0.91
1:2J:55:PHE:CD1	2:2J:101:LHG:H223	2.05	0.91
1:5M:55:PHE:CD1	2:5M:101:LHG:H223	2.05	0.91
1:1A:55:PHE:CD1	2:1A:101:LHG:H223	2.05	0.91
1:1E:55:PHE:CD1	2:1E:101:LHG:H223	2.05	0.91
1:1I:55:PHE:CD1	2:1I:101:LHG:H223	2.05	0.91
1:4C:55:PHE:CD1	2:4C:101:LHG:H223	2.05	0.91
1:5B:55:PHE:CD1	2:5B:101:LHG:H223	2.05	0.91
1:1F:55:PHE:CD1	2:1F:101:LHG:H223	2.05	0.91
1:1J:55:PHE:CD1	2:1J:101:LHG:H223	2.05	0.90
1:2O:55:PHE:CD1	2:2O:101:LHG:H223	2.05	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3G:55:PHE:CD1	2:3G:101:LHG:H223	2.05	0.90
1:4J:55:PHE:CD1	2:4J:101:LHG:H223	2.05	0.90
1:5I:55:PHE:CD1	2:5I:101:LHG:H223	2.05	0.90
1:2D:55:PHE:CD1	2:2D:101:LHG:H223	2.05	0.90
1:3B:55:PHE:CD1	2:3B:101:LHG:H223	2.05	0.90
1:2I:55:PHE:CD1	2:2I:101:LHG:H223	2.05	0.90
1:3L:55:PHE:CD1	2:3L:101:LHG:H223	2.05	0.90
1:5H:55:PHE:CD1	2:5H:101:LHG:H223	2.05	0.90
1:3A:55:PHE:CD1	2:3A:101:LHG:H223	2.05	0.90
1:1D:58:VAL:CG2	2:1D:101:LHG:H222	2.03	0.89
1:3F:58:VAL:CG2	2:3F:101:LHG:H222	2.03	0.89
1:3J:58:VAL:CG2	2:3J:101:LHG:H222	2.03	0.89
1:4I:58:VAL:CG2	2:4I:101:LHG:H222	2.03	0.89
1:2C:58:VAL:CG2	2:2C:101:LHG:H222	2.04	0.88
1:2G:58:VAL:CG2	2:2G:101:LHG:H222	2.04	0.88
1:3E:58:VAL:CG2	2:3E:101:LHG:H222	2.03	0.88
1:5A:58:VAL:CG2	2:5A:101:LHG:H222	2.04	0.88
1:1G:58:VAL:CG2	2:1G:101:LHG:H222	2.04	0.88
1:1M:58:VAL:CG2	2:1M:101:LHG:H222	2.04	0.88
1:2I:58:VAL:CG2	2:2I:101:LHG:H222	2.03	0.88
1:4M:58:VAL:CG2	2:4M:101:LHG:H222	2.04	0.88
1:5D:58:VAL:CG2	2:5D:101:LHG:H222	2.03	0.88
1:1O:58:VAL:CG2	2:1O:101:LHG:H222	2.04	0.88
1:2D:58:VAL:CG2	2:2D:101:LHG:H222	2.03	0.88
1:4A:58:VAL:CG2	2:4A:101:LHG:H222	2.04	0.88
1:5L:58:VAL:CG2	2:5L:101:LHG:H222	2.04	0.88
1:1A:58:VAL:CG2	2:1A:101:LHG:H222	2.03	0.88
1:1C:58:VAL:CG2	2:1C:101:LHG:H222	2.04	0.88
1:2F:58:VAL:CG2	2:2F:101:LHG:H222	2.04	0.88
1:2H:58:VAL:CG2	2:2H:101:LHG:H222	2.04	0.88
1:3D:58:VAL:CG2	2:3D:101:LHG:H222	2.03	0.88
1:3I:58:VAL:CG2	2:3I:101:LHG:H222	2.03	0.88
1:4B:58:VAL:CG2	2:4B:101:LHG:H222	2.03	0.88
1:4J:58:VAL:CG2	2:4J:101:LHG:H222	2.04	0.88
1:4O:58:VAL:CG2	2:4O:101:LHG:H222	2.04	0.88
1:1L:58:VAL:CG2	2:1L:101:LHG:H222	2.04	0.88
1:3G:58:VAL:CG2	2:3G:101:LHG:H222	2.04	0.88
1:5E:58:VAL:CG2	2:5E:101:LHG:H222	2.03	0.88
1:5M:58:VAL:CG2	2:5M:101:LHG:H222	2.04	0.88
1:2J:58:VAL:CG2	2:2J:101:LHG:H222	2.04	0.88
1:2O:58:VAL:CG2	2:2O:101:LHG:H222	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4L:58:VAL:CG2	2:4L:101:LHG:H222	2.04	0.88
1:5I:58:VAL:CG2	2:5I:101:LHG:H222	2.04	0.88
1:5K:58:VAL:CG2	2:5K:101:LHG:H222	2.04	0.88
1:1H:58:VAL:CG2	2:1H:101:LHG:H222	2.04	0.88
1:2N:58:VAL:CG2	2:2N:101:LHG:H222	2.04	0.88
1:4E:58:VAL:CG2	2:4E:101:LHG:H222	2.03	0.88
1:4F:58:VAL:CG2	2:4F:101:LHG:H222	2.04	0.88
1:5B:58:VAL:CG2	2:5B:101:LHG:H222	2.03	0.88
1:5O:58:VAL:CG2	2:5O:101:LHG:H222	2.04	0.88
1:1E:58:VAL:CG2	2:1E:101:LHG:H222	2.04	0.88
1:1K:58:VAL:CG2	2:1K:101:LHG:H222	2.04	0.88
1:2K:58:VAL:CG2	2:2K:101:LHG:H222	2.04	0.88
1:3B:58:VAL:CG2	2:3B:101:LHG:H222	2.03	0.88
1:3K:58:VAL:CG2	2:3K:101:LHG:H222	2.04	0.88
1:3M:58:VAL:CG2	2:3M:101:LHG:H222	2.04	0.88
1:4H:58:VAL:CG2	2:4H:101:LHG:H222	2.03	0.88
1:5H:58:VAL:CG2	2:5H:101:LHG:H222	2.04	0.88
1:1B:58:VAL:CG2	2:1B:101:LHG:H222	2.04	0.88
1:1F:58:VAL:CG2	2:1F:101:LHG:H222	2.04	0.88
1:2B:58:VAL:CG2	2:2B:101:LHG:H222	2.04	0.88
1:3C:58:VAL:CG2	2:3C:101:LHG:H222	2.03	0.88
1:5F:58:VAL:CG2	2:5F:101:LHG:H222	2.04	0.88
1:1N:58:VAL:CG2	2:1N:101:LHG:H222	2.04	0.88
1:2M:58:VAL:CG2	2:2M:101:LHG:H222	2.04	0.88
1:3N:58:VAL:CG2	2:3N:101:LHG:H222	2.04	0.88
1:4G:58:VAL:CG2	2:4G:101:LHG:H222	2.04	0.88
1:4N:58:VAL:CG2	2:4N:101:LHG:H222	2.04	0.88
1:5G:58:VAL:CG2	2:5G:101:LHG:H222	2.04	0.87
1:3O:58:VAL:CG2	2:3O:101:LHG:H222	2.04	0.87
1:4K:58:VAL:CG2	2:4K:101:LHG:H222	2.04	0.87
1:5C:58:VAL:CG2	2:5C:101:LHG:H222	2.04	0.87
1:5J:58:VAL:CG2	2:5J:101:LHG:H222	2.04	0.87
1:3A:58:VAL:CG2	2:3A:101:LHG:H222	2.04	0.87
1:4C:58:VAL:CG2	2:4C:101:LHG:H222	2.03	0.87
1:1I:58:VAL:CG2	2:1I:101:LHG:H222	2.04	0.87
1:3L:58:VAL:CG2	2:3L:101:LHG:H222	2.04	0.87
1:4D:58:VAL:CG2	2:4D:101:LHG:H222	2.04	0.87
1:1J:58:VAL:CG2	2:1J:101:LHG:H222	2.04	0.87
1:2E:58:VAL:CG2	2:2E:101:LHG:H222	2.04	0.87
1:3H:58:VAL:CG2	2:3H:101:LHG:H222	2.04	0.87
1:2A:58:VAL:CG2	2:2A:101:LHG:H222	2.03	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2L:58:VAL:CG2	2:2L:101:LHG:H222	2.04	0.87
1:5N:58:VAL:CG2	2:5N:101:LHG:H222	2.04	0.87
1:4M:55:PHE:CD1	2:4M:101:LHG:C22	2.59	0.86
1:1E:55:PHE:CD1	2:1E:101:LHG:C22	2.59	0.86
1:2A:55:PHE:CD1	2:2A:101:LHG:C22	2.59	0.86
1:2B:55:PHE:CD1	2:2B:101:LHG:C22	2.59	0.86
1:2H:55:PHE:CD1	2:2H:101:LHG:C22	2.59	0.86
1:5J:55:PHE:CD1	2:5J:101:LHG:C22	2.59	0.86
1:5N:55:PHE:CD1	2:5N:101:LHG:C22	2.59	0.86
1:1A:55:PHE:CD1	2:1A:101:LHG:C22	2.59	0.86
1:1O:55:PHE:CD1	2:1O:101:LHG:C22	2.59	0.86
1:2G:55:PHE:CD1	2:2G:101:LHG:C22	2.59	0.86
1:3I:55:PHE:CD1	2:3I:101:LHG:C22	2.59	0.86
1:4A:55:PHE:CD1	2:4A:101:LHG:C22	2.59	0.86
1:4H:55:PHE:CD1	2:4H:101:LHG:C22	2.59	0.86
1:4L:55:PHE:CD1	2:4L:101:LHG:C22	2.59	0.86
1:5A:55:PHE:CD1	2:5A:101:LHG:C22	2.59	0.86
1:5I:55:PHE:CD1	2:5I:101:LHG:C22	2.59	0.86
1:5O:55:PHE:CD1	2:5O:101:LHG:C22	2.59	0.86
1:1D:55:PHE:CD1	2:1D:101:LHG:C22	2.59	0.86
1:1K:55:PHE:CD1	2:1K:101:LHG:C22	2.59	0.86
1:2F:55:PHE:CD1	2:2F:101:LHG:C22	2.59	0.86
1:3K:55:PHE:CD1	2:3K:101:LHG:C22	2.59	0.86
1:5B:55:PHE:CD1	2:5B:101:LHG:C22	2.59	0.86
1:5C:55:PHE:CD1	2:5C:101:LHG:C22	2.59	0.86
1:1B:55:PHE:CD1	2:1B:101:LHG:C22	2.59	0.86
1:2C:55:PHE:CD1	2:2C:101:LHG:C22	2.59	0.86
1:2I:55:PHE:CD1	2:2I:101:LHG:C22	2.59	0.86
1:2O:55:PHE:CD1	2:2O:101:LHG:C22	2.59	0.86
1:3G:55:PHE:CD1	2:3G:101:LHG:C22	2.59	0.86
1:3H:55:PHE:CD1	2:3H:101:LHG:C22	2.59	0.86
1:3J:55:PHE:CD1	2:3J:101:LHG:C22	2.59	0.86
1:3L:55:PHE:CD1	2:3L:101:LHG:C22	2.59	0.86
1:4I:55:PHE:CD1	2:4I:101:LHG:C22	2.59	0.86
1:5D:55:PHE:CD1	2:5D:101:LHG:C22	2.59	0.86
1:5K:55:PHE:CD1	2:5K:101:LHG:C22	2.59	0.86
1:1F:55:PHE:CD1	2:1F:101:LHG:C22	2.59	0.85
1:1N:55:PHE:CD1	2:1N:101:LHG:C22	2.59	0.85
1:3C:55:PHE:CD1	2:3C:101:LHG:C22	2.59	0.85
1:4J:55:PHE:CD1	2:4J:101:LHG:C22	2.59	0.85
1:4N:55:PHE:CD1	2:4N:101:LHG:C22	2.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5M:55:PHE:CD1	2:5M:101:LHG:C22	2.59	0.85
1:1G:55:PHE:CD1	2:1G:101:LHG:C22	2.59	0.85
1:1J:55:PHE:CD1	2:1J:101:LHG:C22	2.59	0.85
1:1L:55:PHE:CD1	2:1L:101:LHG:C22	2.59	0.85
1:2E:55:PHE:CD1	2:2E:101:LHG:C22	2.59	0.85
1:3F:55:PHE:CD1	2:3F:101:LHG:C22	2.59	0.85
1:4G:55:PHE:CD1	2:4G:101:LHG:C22	2.59	0.85
1:5H:55:PHE:CD1	2:5H:101:LHG:C22	2.59	0.85
1:1H:55:PHE:CD1	2:1H:101:LHG:C22	2.59	0.85
1:1I:55:PHE:CD1	2:1I:101:LHG:C22	2.59	0.85
1:2J:55:PHE:CD1	2:2J:101:LHG:C22	2.59	0.85
1:3B:55:PHE:CD1	2:3B:101:LHG:C22	2.59	0.85
1:3D:55:PHE:CD1	2:3D:101:LHG:C22	2.59	0.85
1:4O:55:PHE:CD1	2:4O:101:LHG:C22	2.59	0.85
1:2K:55:PHE:CD1	2:2K:101:LHG:C22	2.59	0.85
1:2L:55:PHE:CD1	2:2L:101:LHG:C22	2.59	0.85
1:3A:55:PHE:CD1	2:3A:101:LHG:C22	2.59	0.85
1:4B:55:PHE:CD1	2:4B:101:LHG:C22	2.59	0.85
1:4K:55:PHE:CD1	2:4K:101:LHG:C22	2.59	0.85
1:1C:55:PHE:CD1	2:1C:101:LHG:C22	2.59	0.85
1:3M:55:PHE:CD1	2:3M:101:LHG:C22	2.59	0.85
1:3O:55:PHE:CD1	2:3O:101:LHG:C22	2.59	0.85
1:4C:55:PHE:CD1	2:4C:101:LHG:C22	2.59	0.85
1:5E:55:PHE:CD1	2:5E:101:LHG:C22	2.59	0.85
1:2M:55:PHE:CD1	2:2M:101:LHG:C22	2.59	0.85
1:4D:55:PHE:CD1	2:4D:101:LHG:C22	2.59	0.85
1:5G:55:PHE:CD1	2:5G:101:LHG:C22	2.59	0.85
1:2D:55:PHE:CD1	2:2D:101:LHG:C22	2.59	0.85
1:5L:55:PHE:CD1	2:5L:101:LHG:C22	2.59	0.85
1:1K:47:LEU:CD2	2:1K:101:LHG:H102	2.07	0.85
1:2N:47:LEU:CD2	2:2N:101:LHG:H102	2.07	0.85
1:5H:47:LEU:CD2	2:5H:101:LHG:H102	2.07	0.85
2:1H:101:LHG:C37	1:5G:20:PHE:HE2	1.90	0.85
1:1M:55:PHE:CD1	2:1M:101:LHG:C22	2.59	0.85
1:4E:55:PHE:CD1	2:4E:101:LHG:C22	2.59	0.85
1:1J:47:LEU:CD2	2:1J:101:LHG:H102	2.07	0.85
1:2N:55:PHE:CD1	2:2N:101:LHG:C22	2.59	0.85
1:3E:55:PHE:CD1	2:3E:101:LHG:C22	2.59	0.85
1:3M:47:LEU:CD2	2:3M:101:LHG:H102	2.07	0.85
1:4E:47:LEU:CD2	2:4E:101:LHG:H102	2.07	0.85
1:4H:47:LEU:CD2	2:4H:101:LHG:H102	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2B:47:LEU:CD2	2:2B:101:LHG:H102	2.07	0.84
1:2J:47:LEU:CD2	2:2J:101:LHG:H102	2.07	0.84
1:2M:47:LEU:CD2	2:2M:101:LHG:H102	2.07	0.84
1:3B:47:LEU:CD2	2:3B:101:LHG:H102	2.07	0.84
1:3E:47:LEU:CD2	2:3E:101:LHG:H102	2.07	0.84
1:3N:55:PHE:CD1	2:3N:101:LHG:C22	2.59	0.84
1:5G:47:LEU:CD2	2:5G:101:LHG:H102	2.07	0.84
1:5K:47:LEU:CD2	2:5K:101:LHG:H102	2.07	0.84
1:2C:47:LEU:CD2	2:2C:101:LHG:H102	2.07	0.84
1:3A:47:LEU:CD2	2:3A:101:LHG:H102	2.07	0.84
1:3F:47:LEU:CD2	2:3F:101:LHG:H102	2.07	0.84
1:4D:47:LEU:CD2	2:4D:101:LHG:H102	2.07	0.84
1:4I:47:LEU:CD2	2:4I:101:LHG:H102	2.07	0.84
1:1N:47:LEU:CD2	2:1N:101:LHG:H102	2.07	0.84
1:4F:55:PHE:CD1	2:4F:101:LHG:C22	2.59	0.84
1:5F:55:PHE:CD1	2:5F:101:LHG:C22	2.59	0.84
1:1G:47:LEU:CD2	2:1G:101:LHG:H102	2.07	0.84
1:5L:47:LEU:CD2	2:5L:101:LHG:H102	2.07	0.84
1:1O:47:LEU:CD2	2:1O:101:LHG:H102	2.07	0.84
1:2O:47:LEU:CD2	2:2O:101:LHG:H102	2.07	0.84
1:3N:47:LEU:CD2	2:3N:101:LHG:H102	2.07	0.84
1:5I:47:LEU:CD2	2:5I:101:LHG:H102	2.07	0.84
1:1L:47:LEU:CD2	2:1L:101:LHG:H102	2.07	0.84
1:2K:47:LEU:CD2	2:2K:101:LHG:H102	2.07	0.84
1:4O:47:LEU:CD2	2:4O:101:LHG:H102	2.07	0.84
1:5D:47:LEU:CD2	2:5D:101:LHG:H102	2.07	0.84
1:1H:47:LEU:CD2	2:1H:101:LHG:H102	2.07	0.84
1:3L:47:LEU:CD2	2:3L:101:LHG:H102	2.07	0.84
1:4F:47:LEU:CD2	2:4F:101:LHG:H102	2.07	0.84
1:1H:20:PHE:HE2	2:2I:101:LHG:H371	1.43	0.84
1:3C:47:LEU:CD2	2:3C:101:LHG:H102	2.07	0.84
1:3D:47:LEU:CD2	2:3D:101:LHG:H102	2.07	0.84
1:4G:20:PHE:HE2	2:5H:101:LHG:H371	1.43	0.84
1:1C:47:LEU:CD2	2:1C:101:LHG:H102	2.07	0.84
1:2F:47:LEU:CD2	2:2F:101:LHG:H102	2.07	0.84
1:2I:47:LEU:CD2	2:2I:101:LHG:H102	2.07	0.84
1:3I:47:LEU:CD2	2:3I:101:LHG:H102	2.07	0.84
1:2H:20:PHE:HE2	2:3I:101:LHG:H371	1.43	0.84
1:4A:47:LEU:CD2	2:4A:101:LHG:H102	2.07	0.84
1:4G:47:LEU:CD2	2:4G:101:LHG:H102	2.07	0.84
1:5E:47:LEU:CD2	2:5E:101:LHG:H102	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1F:47:LEU:CD2	2:1F:101:LHG:H102	2.07	0.84
1:2A:47:LEU:CD2	2:2A:101:LHG:H102	2.07	0.84
1:5J:47:LEU:CD2	2:5J:101:LHG:H102	2.07	0.84
1:5O:47:LEU:CD2	2:5O:101:LHG:H102	2.07	0.84
1:1I:47:LEU:CD2	2:1I:101:LHG:H102	2.07	0.83
1:1M:47:LEU:CD2	2:1M:101:LHG:H102	2.07	0.83
1:4L:47:LEU:CD2	2:4L:101:LHG:H102	2.07	0.83
1:1B:47:LEU:CD2	2:1B:101:LHG:H102	2.07	0.83
1:4M:47:LEU:CD2	2:4M:101:LHG:H102	2.07	0.83
1:5F:47:LEU:CD2	2:5F:101:LHG:H102	2.07	0.83
1:2D:47:LEU:CD2	2:2D:101:LHG:H102	2.07	0.83
1:2G:47:LEU:CD2	2:2G:101:LHG:H102	2.07	0.83
1:1G:20:PHE:HE2	2:2H:101:LHG:H371	1.43	0.83
1:2L:47:LEU:CD2	2:2L:101:LHG:H102	2.07	0.83
1:3G:47:LEU:CD2	2:3G:101:LHG:H102	2.07	0.83
1:3J:47:LEU:CD2	2:3J:101:LHG:H102	2.07	0.83
1:3O:47:LEU:CD2	2:3O:101:LHG:H102	2.07	0.83
1:4B:47:LEU:CD2	2:4B:101:LHG:H102	2.07	0.83
1:4C:47:LEU:CD2	2:4C:101:LHG:H102	2.07	0.83
1:5C:47:LEU:CD2	2:5C:101:LHG:H102	2.07	0.83
1:1A:47:LEU:CD2	2:1A:101:LHG:H102	2.07	0.83
1:1D:47:LEU:CD2	2:1D:101:LHG:H102	2.07	0.83
1:2E:47:LEU:CD2	2:2E:101:LHG:H102	2.07	0.83
1:4J:47:LEU:CD2	2:4J:101:LHG:H102	2.07	0.83
1:3G:20:PHE:HE2	2:4H:101:LHG:H371	1.43	0.83
1:3H:47:LEU:CD2	2:3H:101:LHG:H102	2.07	0.83
1:5A:47:LEU:CD2	2:5A:101:LHG:H102	2.07	0.83
2:1G:101:LHG:C37	1:5F:20:PHE:HE2	1.91	0.83
1:5M:47:LEU:CD2	2:5M:101:LHG:H102	2.07	0.83
1:4K:47:LEU:CD2	2:4K:101:LHG:H102	2.07	0.83
1:5N:47:LEU:CD2	2:5N:101:LHG:H102	2.07	0.83
2:1I:101:LHG:H371	1:5H:20:PHE:HE2	1.44	0.83
1:3H:20:PHE:HE2	2:4I:101:LHG:H371	1.43	0.83
1:4H:20:PHE:HE2	2:5I:101:LHG:H371	1.43	0.83
1:2G:20:PHE:HE2	2:3H:101:LHG:H371	1.43	0.82
1:3K:47:LEU:CD2	2:3K:101:LHG:H102	2.07	0.82
1:4N:47:LEU:CD2	2:4N:101:LHG:H102	2.07	0.82
1:1E:47:LEU:CD2	2:1E:101:LHG:H102	2.07	0.82
1:2H:47:LEU:CD2	2:2H:101:LHG:H102	2.07	0.82
2:1I:101:LHG:C37	1:5H:20:PHE:HE2	1.92	0.82
1:5B:47:LEU:CD2	2:5B:101:LHG:H102	2.07	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3A:3:LEU:HD12	1:3B:14:THR:HA	1.63	0.81
1:1J:3:LEU:HD12	1:1K:14:THR:HA	1.63	0.81
1:2B:3:LEU:HD12	1:2C:14:THR:HA	1.63	0.81
1:3C:3:LEU:HD12	1:3D:14:THR:HA	1.63	0.81
1:5I:3:LEU:HD12	1:5J:14:THR:HA	1.63	0.81
1:1L:3:LEU:HD12	1:1M:14:THR:HA	1.63	0.81
1:2K:3:LEU:HD12	1:2L:14:THR:HA	1.63	0.81
1:2M:3:LEU:HD12	1:2N:14:THR:HA	1.63	0.81
1:4D:3:LEU:HD12	1:4E:14:THR:HA	1.63	0.81
1:4F:3:LEU:HD12	1:4G:14:THR:HA	1.63	0.81
1:3F:20:PHE:HE2	2:4G:101:LHG:H371	1.46	0.81
1:5G:3:LEU:HD12	1:5H:14:THR:HA	1.63	0.81
1:1H:3:LEU:HD12	1:1I:14:THR:HA	1.63	0.81
1:2O:3:LEU:HD12	1:2P:14:THR:HA	1.63	0.81
1:3C:3:LEU:CD1	1:3D:14:THR:HA	2.11	0.81
1:3E:3:LEU:HD12	1:3F:14:THR:HA	1.63	0.81
1:4C:3:LEU:CD1	1:4D:14:THR:HA	2.11	0.81
1:4H:3:LEU:HD12	1:4I:14:THR:HA	1.63	0.81
1:5K:3:LEU:HD12	1:5L:14:THR:HA	1.63	0.81
1:2C:3:LEU:HD12	1:2D:14:THR:HA	1.63	0.81
1:2J:3:LEU:CD1	1:2K:14:THR:HA	2.11	0.81
1:3B:3:LEU:CD1	1:3C:14:THR:HA	2.11	0.81
1:2F:20:PHE:HE2	2:3G:101:LHG:H371	1.46	0.81
1:3N:3:LEU:HD12	1:3O:14:THR:HA	1.63	0.81
1:4B:3:LEU:HD12	1:4C:14:THR:HA	1.63	0.81
1:4F:3:LEU:CD1	1:4G:14:THR:HA	2.11	0.81
1:5E:3:LEU:HD12	1:5F:14:THR:HA	1.63	0.81
1:1A:3:LEU:HD12	1:1B:14:THR:HA	1.63	0.81
1:1I:3:LEU:HD12	1:1J:14:THR:HA	1.63	0.81
1:2J:3:LEU:HD12	1:2K:14:THR:HA	1.63	0.81
1:2K:3:LEU:CD1	1:2L:14:THR:HA	2.11	0.81
1:3B:3:LEU:HD12	1:3C:14:THR:HA	1.63	0.81
1:3O:3:LEU:HD12	1:3P:14:THR:HA	1.63	0.81
1:4B:3:LEU:CD1	1:4C:14:THR:HA	2.11	0.81
1:1N:3:LEU:HD12	1:1O:14:THR:HA	1.63	0.80
1:2A:3:LEU:HD12	1:2B:14:THR:HA	1.63	0.80
1:2L:3:LEU:HD12	1:2M:14:THR:HA	1.63	0.80
1:3I:20:PHE:HE2	2:4J:101:LHG:H371	1.47	0.80
1:3M:3:LEU:HD12	1:3N:14:THR:HA	1.63	0.80
1:4C:3:LEU:HD12	1:4D:14:THR:HA	1.63	0.80
1:4E:3:LEU:CD1	1:4F:14:THR:HA	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5I:3:LEU:CD1	1:5J:14:THR:HA	2.11	0.80
2:1H:101:LHG:H371	1:5G:20:PHE:HE2	1.45	0.80
1:1L:3:LEU:CD1	1:1M:14:THR:HA	2.11	0.80
1:2D:3:LEU:HD12	1:2E:14:THR:HA	1.63	0.80
1:1F:20:PHE:HE2	2:2G:101:LHG:H371	1.46	0.80
1:2L:3:LEU:CD1	1:2M:14:THR:HA	2.11	0.80
1:2O:3:LEU:CD1	1:2P:14:THR:HA	2.12	0.80
1:3D:3:LEU:HD12	1:3E:14:THR:HA	1.63	0.80
1:3D:3:LEU:CD1	1:3E:14:THR:HA	2.11	0.80
1:3F:3:LEU:HD12	1:3G:14:THR:HA	1.63	0.80
1:3F:3:LEU:CD1	1:3G:14:THR:HA	2.11	0.80
1:4D:3:LEU:CD1	1:4E:14:THR:HA	2.11	0.80
1:4H:3:LEU:CD1	1:4I:14:THR:HA	2.12	0.80
1:4I:3:LEU:CD1	1:4J:14:THR:HA	2.11	0.80
1:5F:3:LEU:HD12	1:5G:14:THR:HA	1.63	0.80
1:1A:3:LEU:CD1	1:1B:14:THR:HA	2.11	0.80
1:1G:3:LEU:HD12	1:1H:14:THR:HA	1.63	0.80
1:1K:3:LEU:HD12	1:1L:14:THR:HA	1.63	0.80
1:2N:3:LEU:HD12	1:2O:14:THR:HA	1.63	0.80
1:3G:3:LEU:CD1	1:3H:14:THR:HA	2.11	0.80
1:4E:3:LEU:HD12	1:4F:14:THR:HA	1.63	0.80
1:4G:3:LEU:CD1	1:4H:14:THR:HA	2.12	0.80
1:4G:3:LEU:HD12	1:4H:14:THR:HA	1.63	0.80
1:4I:3:LEU:HD12	1:4J:14:THR:HA	1.63	0.80
1:4O:3:LEU:HD12	1:4P:14:THR:HA	1.63	0.80
1:5H:3:LEU:HD12	1:5I:14:THR:HA	1.63	0.80
1:4I:20:PHE:HE2	2:5J:101:LHG:H371	1.46	0.80
1:5J:3:LEU:HD12	1:5K:14:THR:HA	1.63	0.80
1:1M:3:LEU:CD1	1:1N:14:THR:HA	2.11	0.80
1:2A:3:LEU:CD1	1:2B:14:THR:HA	2.11	0.80
1:2I:3:LEU:HD12	1:2J:14:THR:HA	1.63	0.80
1:2I:3:LEU:CD1	1:2J:14:THR:HA	2.11	0.80
1:2M:3:LEU:CD1	1:2N:14:THR:HA	2.11	0.80
1:3A:3:LEU:CD1	1:3B:14:THR:HA	2.11	0.80
1:3E:3:LEU:CD1	1:3F:14:THR:HA	2.11	0.80
1:3G:3:LEU:HD12	1:3H:14:THR:HA	1.63	0.80
1:3L:3:LEU:HD12	1:3M:14:THR:HA	1.63	0.80
1:3N:3:LEU:CD1	1:3O:14:THR:HA	2.12	0.80
1:4A:3:LEU:CD1	1:4B:14:THR:HA	2.11	0.80
1:5D:3:LEU:HD12	1:5E:14:THR:HA	1.63	0.80
1:5J:3:LEU:CD1	1:5K:14:THR:HA	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1B:3:LEU:HD12	1:1C:14:THR:HA	1.63	0.80
1:1K:3:LEU:CD1	1:1L:14:THR:HA	2.11	0.80
1:1M:3:LEU:HD12	1:1N:14:THR:HA	1.63	0.80
1:1N:3:LEU:CD1	1:1O:14:THR:HA	2.11	0.80
1:2N:3:LEU:CD1	1:2O:14:THR:HA	2.12	0.80
1:3M:3:LEU:CD1	1:3N:14:THR:HA	2.11	0.80
1:5H:3:LEU:CD1	1:5I:14:THR:HA	2.12	0.80
1:1F:3:LEU:HD12	1:1G:14:THR:HA	1.63	0.80
1:1O:3:LEU:CD1	1:1P:14:THR:HA	2.11	0.80
1:1G:20:PHE:HE2	2:2H:101:LHG:C37	1.95	0.80
1:2I:20:PHE:HE2	2:3J:101:LHG:H371	1.46	0.80
1:4A:3:LEU:HD12	1:4B:14:THR:HA	1.63	0.80
1:4J:3:LEU:HD12	1:4K:14:THR:HA	1.63	0.80
1:4F:20:PHE:HE2	2:5G:101:LHG:H371	1.46	0.80
1:1H:3:LEU:CD1	1:1I:14:THR:HA	2.11	0.80
1:1I:3:LEU:CD1	1:1J:14:THR:HA	2.11	0.80
1:3O:3:LEU:CD1	1:3P:14:THR:HA	2.11	0.80
1:4N:3:LEU:HD12	1:4O:14:THR:HA	1.63	0.80
1:5C:3:LEU:HD12	1:5D:14:THR:HA	1.63	0.80
1:1B:3:LEU:CD1	1:1C:14:THR:HA	2.11	0.80
1:1C:3:LEU:HD12	1:1D:14:THR:HA	1.63	0.80
1:1G:3:LEU:CD1	1:1H:14:THR:HA	2.11	0.80
1:2G:20:PHE:HE2	2:3H:101:LHG:C37	1.95	0.80
1:3H:3:LEU:CD1	1:3I:14:THR:HA	2.12	0.80
1:5L:3:LEU:HD12	1:5M:14:THR:HA	1.63	0.80
1:1O:3:LEU:HD12	1:1P:14:THR:HA	1.63	0.80
1:2E:3:LEU:HD12	1:2F:14:THR:HA	1.63	0.80
1:3K:3:LEU:HD12	1:3L:14:THR:HA	1.63	0.80
1:5M:3:LEU:HD12	1:5N:14:THR:HA	1.63	0.80
1:1D:3:LEU:HD12	1:1E:14:THR:HA	1.63	0.80
1:1J:3:LEU:CD1	1:1K:14:THR:HA	2.11	0.80
1:2D:3:LEU:CD1	1:2E:14:THR:HA	2.11	0.80
1:2F:3:LEU:HD12	1:2G:14:THR:HA	1.63	0.80
1:3L:3:LEU:CD1	1:3M:14:THR:HA	2.11	0.80
1:4J:3:LEU:CD1	1:4K:14:THR:HA	2.12	0.80
1:5A:3:LEU:CD1	1:5B:14:THR:HA	2.11	0.80
1:5A:3:LEU:HD12	1:5B:14:THR:HA	1.63	0.80
1:5D:3:LEU:CD1	1:5E:14:THR:HA	2.11	0.80
1:5E:3:LEU:CD1	1:5F:14:THR:HA	2.11	0.80
1:5G:3:LEU:CD1	1:5H:14:THR:HA	2.11	0.80
1:5K:3:LEU:CD1	1:5L:14:THR:HA	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2E:3:LEU:CD1	1:2F:14:THR:HA	2.11	0.79
1:2H:3:LEU:CD1	1:2I:14:THR:HA	2.12	0.79
1:3H:3:LEU:HD12	1:3I:14:THR:HA	1.63	0.79
1:5C:3:LEU:CD1	1:5D:14:THR:HA	2.11	0.79
1:1E:3:LEU:HD12	1:1F:14:THR:HA	1.63	0.79
1:2C:3:LEU:CD1	1:2D:14:THR:HA	2.11	0.79
1:2G:3:LEU:HD12	1:2H:14:THR:HA	1.63	0.79
1:2H:3:LEU:HD12	1:2I:14:THR:HA	1.63	0.79
1:3I:3:LEU:CD1	1:3J:14:THR:HA	2.12	0.79
1:3I:3:LEU:HD12	1:3J:14:THR:HA	1.63	0.79
1:3J:3:LEU:HD12	1:3K:14:THR:HA	1.63	0.79
1:4K:3:LEU:HD12	1:4L:14:THR:HA	1.63	0.79
1:4L:3:LEU:HD12	1:4M:14:THR:HA	1.63	0.79
1:4M:3:LEU:HD12	1:4N:14:THR:HA	1.63	0.79
1:4O:3:LEU:CD1	1:4P:14:THR:HA	2.12	0.79
1:5B:3:LEU:HD12	1:5C:14:THR:HA	1.63	0.79
1:4G:20:PHE:HE2	2:5H:101:LHG:C37	1.95	0.79
1:1F:3:LEU:CD1	1:1G:14:THR:HA	2.11	0.79
1:2B:3:LEU:CD1	1:2C:14:THR:HA	2.11	0.79
1:3K:3:LEU:CD1	1:3L:14:THR:HA	2.12	0.79
1:5B:3:LEU:CD1	1:5C:14:THR:HA	2.11	0.79
1:5O:3:LEU:HD12	1:5P:14:THR:HA	1.63	0.79
1:3J:3:LEU:CD1	1:3K:14:THR:HA	2.12	0.79
2:1J:101:LHG:H371	1:5I:20:PHE:HE2	1.47	0.79
1:2G:3:LEU:CD1	1:2H:14:THR:HA	2.11	0.79
2:1F:101:LHG:C37	1:5E:20:PHE:HE2	1.95	0.79
1:1C:3:LEU:CD1	1:1D:14:THR:HA	2.11	0.79
1:4K:3:LEU:CD1	1:4L:14:THR:HA	2.11	0.79
2:1G:101:LHG:H371	1:5F:20:PHE:HE2	1.48	0.79
1:5F:3:LEU:CD1	1:5G:14:THR:HA	2.11	0.79
1:5N:3:LEU:CD1	1:5O:14:THR:HA	2.11	0.79
1:2F:3:LEU:CD1	1:2G:14:THR:HA	2.11	0.79
1:1D:3:LEU:CD1	1:1E:14:THR:HA	2.11	0.79
1:2F:20:PHE:HE2	2:3G:101:LHG:C37	1.96	0.79
1:5O:3:LEU:CD1	1:5P:14:THR:HA	2.12	0.79
1:3F:20:PHE:HE2	2:4G:101:LHG:C37	1.96	0.79
1:4L:3:LEU:CD1	1:4M:14:THR:HA	2.11	0.79
1:1E:3:LEU:CD1	1:1F:14:THR:HA	2.11	0.79
1:5M:3:LEU:CD1	1:5N:14:THR:HA	2.11	0.79
1:3G:20:PHE:HE2	2:4H:101:LHG:C37	1.95	0.78
1:4N:3:LEU:CD1	1:4O:14:THR:HA	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1I:20:PHE:HE2	2:2J:101:LHG:H371	1.46	0.78
1:4M:3:LEU:CD1	1:4N:14:THR:HA	2.12	0.78
1:5N:3:LEU:HD12	1:5O:14:THR:HA	1.63	0.78
1:5L:3:LEU:CD1	1:5M:14:THR:HA	2.12	0.78
1:1F:20:PHE:HE2	2:2G:101:LHG:C37	1.96	0.78
1:4F:20:PHE:HE2	2:5G:101:LHG:C37	1.96	0.78
1:4H:20:PHE:HE2	2:5I:101:LHG:C37	1.97	0.78
1:1H:20:PHE:HE2	2:2I:101:LHG:C37	1.98	0.77
1:1E:20:PHE:HE2	2:2F:101:LHG:H371	1.50	0.77
2:1E:101:LHG:C37	1:5D:20:PHE:HE2	1.98	0.77
1:3H:20:PHE:HE2	2:4I:101:LHG:C37	1.98	0.77
2:2B:101:LHG:C37	2:2B:101:LHG:H212	2.15	0.77
1:2H:20:PHE:HE2	2:3I:101:LHG:C37	1.98	0.77
2:4H:101:LHG:H212	2:4H:101:LHG:C37	2.15	0.77
2:3E:101:LHG:C37	2:3E:101:LHG:H212	2.15	0.76
1:2E:20:PHE:HE2	2:3F:101:LHG:H371	1.50	0.76
2:1J:101:LHG:C37	1:5I:20:PHE:HE2	1.98	0.76
2:5K:101:LHG:C37	2:5K:101:LHG:H212	2.15	0.76
2:2A:101:LHG:C37	2:2A:101:LHG:H212	2.15	0.76
2:3D:101:LHG:C37	2:3D:101:LHG:H212	2.15	0.76
2:3O:101:LHG:C37	2:3O:101:LHG:H212	2.15	0.76
2:4G:101:LHG:H212	2:4G:101:LHG:C37	2.15	0.76
1:3E:20:PHE:HE2	2:4F:101:LHG:C37	1.99	0.76
2:1N:101:LHG:H212	2:1N:101:LHG:C37	2.15	0.76
1:4E:20:PHE:HE2	2:5F:101:LHG:C37	1.99	0.76
2:5J:101:LHG:H212	2:5J:101:LHG:C37	2.15	0.76
2:1M:101:LHG:H212	2:1M:101:LHG:C37	2.15	0.76
2:3C:101:LHG:C37	2:3C:101:LHG:H212	2.16	0.76
2:3N:101:LHG:H212	2:3N:101:LHG:C37	2.15	0.76
1:2E:20:PHE:HE2	2:3F:101:LHG:C37	1.99	0.75
2:2H:101:LHG:H212	2:2H:101:LHG:C37	2.15	0.75
2:4F:101:LHG:C37	2:4F:101:LHG:H212	2.15	0.75
1:4E:20:PHE:HE2	2:5F:101:LHG:H371	1.50	0.75
2:1E:101:LHG:C37	2:1E:101:LHG:H212	2.15	0.75
2:2I:101:LHG:C37	2:2I:101:LHG:H212	2.15	0.75
1:3E:20:PHE:HE2	2:4F:101:LHG:H371	1.50	0.75
2:1F:101:LHG:H212	2:1F:101:LHG:C37	2.15	0.75
2:5I:101:LHG:C37	2:5I:101:LHG:H212	2.15	0.75
2:1D:101:LHG:C37	2:1D:101:LHG:H212	2.15	0.75
1:1E:20:PHE:HE2	2:2F:101:LHG:C37	1.99	0.75
2:2G:101:LHG:H212	2:2G:101:LHG:C37	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3J:101:LHG:H212	2:3J:101:LHG:C37	2.15	0.75
2:3K:101:LHG:C37	2:3K:101:LHG:H212	2.15	0.75
2:5B:101:LHG:H212	2:5B:101:LHG:C37	2.15	0.75
2:5C:101:LHG:H212	2:5C:101:LHG:C37	2.15	0.75
2:1G:101:LHG:H212	2:1G:101:LHG:C37	2.15	0.75
2:5D:101:LHG:H212	2:5D:101:LHG:C37	2.15	0.75
2:1L:101:LHG:C37	2:1L:101:LHG:H212	2.15	0.75
2:3I:101:LHG:H212	2:3I:101:LHG:C37	2.15	0.75
2:4A:101:LHG:H212	2:4A:101:LHG:C37	2.15	0.75
2:2F:101:LHG:H212	2:2F:101:LHG:C37	2.15	0.75
2:2J:101:LHG:C37	2:2J:101:LHG:H212	2.15	0.75
2:3L:101:LHG:H212	2:3L:101:LHG:C37	2.15	0.75
2:4B:101:LHG:C37	2:4B:101:LHG:H212	2.15	0.75
2:5A:101:LHG:H212	2:5A:101:LHG:C37	2.15	0.75
2:1B:101:LHG:C37	2:1B:101:LHG:H212	2.15	0.75
2:3B:101:LHG:H212	2:3B:101:LHG:C37	2.15	0.75
2:4M:101:LHG:C37	2:4M:101:LHG:H212	2.15	0.75
2:5E:101:LHG:C37	2:5E:101:LHG:H212	2.15	0.75
2:1C:101:LHG:C37	2:1C:101:LHG:H212	2.15	0.74
2:1H:101:LHG:H212	2:1H:101:LHG:C37	2.15	0.74
2:4L:101:LHG:H212	2:4L:101:LHG:C37	2.15	0.74
2:2O:101:LHG:C37	2:2O:101:LHG:H212	2.15	0.74
2:3H:101:LHG:H212	2:3H:101:LHG:C37	2.15	0.74
2:3M:101:LHG:C37	2:3M:101:LHG:H212	2.15	0.74
2:4E:101:LHG:C37	2:4E:101:LHG:H212	2.15	0.74
2:4N:101:LHG:H212	2:4N:101:LHG:C37	2.15	0.74
2:2E:101:LHG:H212	2:2E:101:LHG:C37	2.15	0.74
2:4K:101:LHG:H212	2:4K:101:LHG:C37	2.15	0.74
1:2J:55:PHE:HA	2:2J:101:LHG:C22	2.18	0.74
1:3B:55:PHE:HA	2:3B:101:LHG:C22	2.18	0.74
1:3H:55:PHE:HA	2:3H:101:LHG:C22	2.18	0.74
1:1B:55:PHE:HA	2:1B:101:LHG:C22	2.18	0.74
1:1G:55:PHE:HA	2:1G:101:LHG:C22	2.18	0.74
1:2E:55:PHE:HA	2:2E:101:LHG:C22	2.18	0.74
2:2K:101:LHG:H212	2:2K:101:LHG:C37	2.15	0.74
1:3I:55:PHE:HA	2:3I:101:LHG:C22	2.18	0.74
1:3M:55:PHE:HA	2:3M:101:LHG:C22	2.18	0.74
2:4C:101:LHG:C37	2:4C:101:LHG:H212	2.15	0.74
1:4K:55:PHE:HA	2:4K:101:LHG:C22	2.18	0.74
1:4L:55:PHE:HA	2:4L:101:LHG:C22	2.18	0.74
2:5H:101:LHG:H212	2:5H:101:LHG:C37	2.15	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:55:PHE:HA	2:1A:101:LHG:C22	2.18	0.74
1:2K:55:PHE:HA	2:2K:101:LHG:C22	2.18	0.74
1:3C:55:PHE:HA	2:3C:101:LHG:C22	2.18	0.74
1:4A:55:PHE:HA	2:4A:101:LHG:C22	2.18	0.74
1:4E:55:PHE:HA	2:4E:101:LHG:C22	2.18	0.74
1:4F:55:PHE:HA	2:4F:101:LHG:C22	2.18	0.74
2:5F:101:LHG:C37	2:5F:101:LHG:H212	2.15	0.74
2:5O:101:LHG:H212	2:5O:101:LHG:C37	2.15	0.74
2:1A:101:LHG:C37	2:1A:101:LHG:H212	2.15	0.74
1:1F:55:PHE:HA	2:1F:101:LHG:C22	2.18	0.74
1:1L:55:PHE:HA	2:1L:101:LHG:C22	2.18	0.74
1:2F:55:PHE:HA	2:2F:101:LHG:C22	2.18	0.74
1:3A:55:PHE:HA	2:3A:101:LHG:C22	2.18	0.74
1:3N:55:PHE:HA	2:3N:101:LHG:C22	2.18	0.74
2:4O:101:LHG:H212	2:4O:101:LHG:C37	2.15	0.74
1:5I:55:PHE:HA	2:5I:101:LHG:C22	2.18	0.74
1:5N:55:PHE:HA	2:5N:101:LHG:C22	2.18	0.74
1:5O:55:PHE:HA	2:5O:101:LHG:C22	2.18	0.74
1:1C:55:PHE:HA	2:1C:101:LHG:C22	2.18	0.74
2:1I:101:LHG:H212	2:1I:101:LHG:C37	2.15	0.74
2:1K:101:LHG:C37	2:1K:101:LHG:H212	2.15	0.74
1:2D:55:PHE:HA	2:2D:101:LHG:C22	2.18	0.74
2:4J:101:LHG:C37	2:4J:101:LHG:H212	2.15	0.74
1:5C:55:PHE:HA	2:5C:101:LHG:C22	2.18	0.74
1:5H:55:PHE:HA	2:5H:101:LHG:C22	2.18	0.74
1:1M:55:PHE:HA	2:1M:101:LHG:C22	2.18	0.74
1:2I:55:PHE:HA	2:2I:101:LHG:C22	2.18	0.74
1:2O:55:PHE:HA	2:2O:101:LHG:C22	2.18	0.74
2:3G:101:LHG:H212	2:3G:101:LHG:C37	2.15	0.74
1:3L:55:PHE:HA	2:3L:101:LHG:C22	2.18	0.74
1:5D:55:PHE:HA	2:5D:101:LHG:C22	2.18	0.74
1:5E:55:PHE:HA	2:5E:101:LHG:C22	2.18	0.74
1:5J:55:PHE:HA	2:5J:101:LHG:C22	2.18	0.74
2:5N:101:LHG:H212	2:5N:101:LHG:C37	2.15	0.74
1:1H:55:PHE:HA	2:1H:101:LHG:C22	2.18	0.73
1:3J:20:PHE:HE2	2:4K:101:LHG:H371	1.53	0.73
1:4O:55:PHE:HA	2:4O:101:LHG:C22	2.18	0.73
2:2D:101:LHG:C37	2:2D:101:LHG:H212	2.15	0.73
1:1J:20:PHE:HE2	2:2K:101:LHG:H371	1.53	0.73
2:3A:101:LHG:H212	2:3A:101:LHG:C37	2.15	0.73
1:3J:55:PHE:HA	2:3J:101:LHG:C22	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4D:101:LHG:H212	2:4D:101:LHG:C37	2.15	0.73
1:1N:55:PHE:HA	2:1N:101:LHG:C22	2.18	0.73
1:4B:55:PHE:HA	2:4B:101:LHG:C22	2.18	0.73
1:4G:55:PHE:HA	2:4G:101:LHG:C22	2.18	0.73
2:1F:101:LHG:H371	1:5E:20:PHE:HE2	1.52	0.73
1:2G:55:PHE:HA	2:2G:101:LHG:C22	2.18	0.73
2:2N:101:LHG:H212	2:2N:101:LHG:C37	2.15	0.73
1:3D:55:PHE:HA	2:3D:101:LHG:C22	2.18	0.73
2:4I:101:LHG:C37	2:4I:101:LHG:H212	2.15	0.73
1:4M:55:PHE:HA	2:4M:101:LHG:C22	2.18	0.73
1:5B:55:PHE:HA	2:5B:101:LHG:C22	2.18	0.73
2:1D:101:LHG:C37	1:5C:20:PHE:HE2	2.01	0.73
1:5K:55:PHE:HA	2:5K:101:LHG:C22	2.18	0.73
2:5M:101:LHG:C37	2:5M:101:LHG:H212	2.15	0.73
1:1E:55:PHE:HA	2:1E:101:LHG:C22	2.18	0.73
1:3O:55:PHE:HA	2:3O:101:LHG:C22	2.18	0.73
2:5G:101:LHG:C37	2:5G:101:LHG:H212	2.15	0.73
2:1K:101:LHG:H371	1:5J:20:PHE:HE2	1.53	0.73
1:2A:55:PHE:HA	2:2A:101:LHG:C22	2.18	0.73
2:2L:101:LHG:H212	2:2L:101:LHG:C37	2.15	0.73
1:2L:55:PHE:HA	2:2L:101:LHG:C22	2.18	0.73
1:4J:20:PHE:HE2	2:5K:101:LHG:H371	1.53	0.73
1:5A:55:PHE:HA	2:5A:101:LHG:C22	2.18	0.73
1:4D:20:PHE:HE2	2:5E:101:LHG:H371	1.54	0.73
1:1D:55:PHE:HA	2:1D:101:LHG:C22	2.18	0.73
2:1J:101:LHG:C37	2:1J:101:LHG:H212	2.15	0.73
2:3F:101:LHG:H212	2:3F:101:LHG:C37	2.15	0.73
1:4H:55:PHE:HA	2:4H:101:LHG:C22	2.18	0.73
1:1I:55:PHE:HA	2:1I:101:LHG:C22	2.18	0.73
1:1O:55:PHE:HA	2:1O:101:LHG:C22	2.18	0.73
2:5L:101:LHG:H212	2:5L:101:LHG:C37	2.15	0.73
2:2C:101:LHG:H212	2:2C:101:LHG:C37	2.15	0.73
1:5F:55:PHE:HA	2:5F:101:LHG:C22	2.18	0.73
2:1C:101:LHG:C37	1:5B:20:PHE:HE2	2.02	0.72
1:5L:55:PHE:HA	2:5L:101:LHG:C22	2.18	0.72
1:3E:55:PHE:HA	2:3E:101:LHG:C22	2.18	0.72
2:1O:101:LHG:H212	2:1O:101:LHG:C37	2.15	0.72
1:1D:20:PHE:HE2	2:2E:101:LHG:C37	2.02	0.72
1:4C:55:PHE:HA	2:4C:101:LHG:C22	2.18	0.72
1:2B:55:PHE:HA	2:2B:101:LHG:C22	2.18	0.72
1:3K:55:PHE:HA	2:3K:101:LHG:C22	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4N:55:PHE:HA	2:4N:101:LHG:C22	2.18	0.72
2:2M:101:LHG:C37	2:2M:101:LHG:H212	2.15	0.72
1:2J:20:PHE:HE2	2:3K:101:LHG:H371	1.53	0.72
1:1F:55:PHE:CA	2:1F:101:LHG:H223	2.20	0.72
1:2I:55:PHE:CA	2:2I:101:LHG:H223	2.20	0.72
1:3A:55:PHE:CA	2:3A:101:LHG:H223	2.20	0.72
1:3L:55:PHE:CA	2:3L:101:LHG:H223	2.20	0.72
2:1B:101:LHG:C37	1:5A:20:PHE:HE2	2.02	0.72
1:2D:20:PHE:HE2	2:3E:101:LHG:H371	1.54	0.72
1:1D:20:PHE:HE2	2:2E:101:LHG:H371	1.54	0.72
1:4I:55:PHE:HA	2:4I:101:LHG:C22	2.18	0.72
1:4O:55:PHE:CA	2:4O:101:LHG:H223	2.20	0.72
1:4D:20:PHE:HE2	2:5E:101:LHG:C37	2.02	0.72
1:2H:55:PHE:HA	2:2H:101:LHG:C22	2.18	0.72
1:2M:55:PHE:HA	2:2M:101:LHG:C22	2.18	0.72
1:3D:20:PHE:HE2	2:4E:101:LHG:H371	1.54	0.72
1:5C:55:PHE:CA	2:5C:101:LHG:H223	2.20	0.72
1:2D:20:PHE:HE2	2:3E:101:LHG:C37	2.02	0.72
1:4K:55:PHE:CA	2:4K:101:LHG:H223	2.20	0.72
1:5N:55:PHE:CA	2:5N:101:LHG:H223	2.20	0.72
1:1J:55:PHE:HA	2:1J:101:LHG:C22	2.18	0.71
1:2J:55:PHE:CA	2:2J:101:LHG:H223	2.20	0.71
1:3F:55:PHE:HA	2:3F:101:LHG:C22	2.18	0.71
1:3D:20:PHE:HE2	2:4E:101:LHG:C37	2.02	0.71
1:1G:55:PHE:CA	2:1G:101:LHG:H223	2.20	0.71
1:3H:55:PHE:CA	2:3H:101:LHG:H223	2.20	0.71
1:3M:55:PHE:CA	2:3M:101:LHG:H223	2.20	0.71
1:3I:20:PHE:HE2	2:4J:101:LHG:C37	2.03	0.71
1:4I:20:PHE:HE2	2:5J:101:LHG:C37	2.03	0.71
1:3B:55:PHE:CA	2:3B:101:LHG:H223	2.20	0.71
1:5M:55:PHE:HA	2:5M:101:LHG:C22	2.18	0.71
1:2I:8:LYS:HD2	1:2I:8:LYS:N	2.06	0.71
1:4A:55:PHE:CA	2:4A:101:LHG:H223	2.20	0.71
1:5C:8:LYS:HD2	1:5C:8:LYS:N	2.06	0.71
1:5D:55:PHE:CA	2:5D:101:LHG:H223	2.20	0.71
1:5G:55:PHE:HA	2:5G:101:LHG:C22	2.18	0.71
1:1F:8:LYS:N	1:1F:8:LYS:HD2	2.06	0.71
1:2H:8:LYS:HD2	1:2H:8:LYS:N	2.06	0.71
1:4E:55:PHE:CA	2:4E:101:LHG:H223	2.20	0.71
1:5B:8:LYS:N	1:5B:8:LYS:HD2	2.06	0.71
1:5O:55:PHE:CA	2:5O:101:LHG:H223	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1E:8:LYS:N	1:1E:8:LYS:HD2	2.06	0.71
1:1P:8:LYS:N	1:1P:8:LYS:HD2	2.06	0.71
1:2A:8:LYS:N	1:2A:8:LYS:HD2	2.06	0.71
1:2C:55:PHE:HA	2:2C:101:LHG:C22	2.18	0.71
1:2E:55:PHE:CA	2:2E:101:LHG:H223	2.20	0.71
1:3L:8:LYS:HD2	1:3L:8:LYS:N	2.06	0.71
1:4J:8:LYS:HD2	1:4J:8:LYS:N	2.06	0.71
1:4L:55:PHE:CA	2:4L:101:LHG:H223	2.20	0.71
1:5H:8:LYS:HD2	1:5H:8:LYS:N	2.06	0.71
1:1L:8:LYS:N	1:1L:8:LYS:HD2	2.06	0.71
1:2J:8:LYS:N	1:2J:8:LYS:HD2	2.06	0.71
1:3D:8:LYS:N	1:3D:8:LYS:HD2	2.06	0.71
1:3G:8:LYS:HD2	1:3G:8:LYS:N	2.06	0.71
1:4H:8:LYS:HD2	1:4H:8:LYS:N	2.06	0.71
1:4J:55:PHE:HA	2:4J:101:LHG:C22	2.18	0.71
1:1G:8:LYS:HD2	1:1G:8:LYS:N	2.06	0.71
1:3I:55:PHE:CA	2:3I:101:LHG:H223	2.20	0.71
1:3K:8:LYS:HD2	1:3K:8:LYS:N	2.06	0.71
1:3M:8:LYS:HD2	1:3M:8:LYS:N	2.06	0.71
1:3P:8:LYS:N	1:3P:8:LYS:HD2	2.06	0.71
1:4E:8:LYS:HD2	1:4E:8:LYS:N	2.06	0.71
1:4I:8:LYS:N	1:4I:8:LYS:HD2	2.06	0.71
1:4O:8:LYS:N	1:4O:8:LYS:HD2	2.06	0.71
1:4P:8:LYS:N	1:4P:8:LYS:HD2	2.06	0.71
1:5M:8:LYS:HD2	1:5M:8:LYS:N	2.06	0.71
1:1B:55:PHE:CA	2:1B:101:LHG:H223	2.20	0.71
1:1D:8:LYS:HD2	1:1D:8:LYS:N	2.06	0.71
1:1O:8:LYS:N	1:1O:8:LYS:HD2	2.06	0.71
1:3A:8:LYS:N	1:3A:8:LYS:HD2	2.06	0.71
1:3E:8:LYS:N	1:3E:8:LYS:HD2	2.06	0.71
1:5A:8:LYS:N	1:5A:8:LYS:HD2	2.06	0.71
1:5D:8:LYS:N	1:5D:8:LYS:HD2	2.06	0.71
1:5L:8:LYS:HD2	1:5L:8:LYS:N	2.06	0.71
1:2D:8:LYS:N	1:2D:8:LYS:HD2	2.06	0.71
1:2I:20:PHE:HE2	2:3J:101:LHG:C37	2.03	0.71
1:2O:8:LYS:N	1:2O:8:LYS:HD2	2.06	0.71
1:3F:8:LYS:N	1:3F:8:LYS:HD2	2.06	0.71
1:4D:55:PHE:HA	2:4D:101:LHG:C22	2.18	0.71
1:4K:8:LYS:HD2	1:4K:8:LYS:N	2.06	0.71
1:5I:8:LYS:HD2	1:5I:8:LYS:N	2.06	0.71
1:5N:8:LYS:N	1:5N:8:LYS:HD2	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2G:8:LYS:N	1:2G:8:LYS:HD2	2.06	0.70
1:2L:8:LYS:N	1:2L:8:LYS:HD2	2.06	0.70
1:3B:8:LYS:HD2	1:3B:8:LYS:N	2.06	0.70
1:3H:8:LYS:N	1:3H:8:LYS:HD2	2.06	0.70
1:3N:55:PHE:CA	2:3N:101:LHG:H223	2.20	0.70
1:4D:8:LYS:HD2	1:4D:8:LYS:N	2.06	0.70
1:5K:8:LYS:N	1:5K:8:LYS:HD2	2.06	0.70
1:1I:8:LYS:HD2	1:1I:8:LYS:N	2.06	0.70
1:1L:55:PHE:CA	2:1L:101:LHG:H223	2.20	0.70
1:2C:8:LYS:HD2	1:2C:8:LYS:N	2.06	0.70
1:2F:55:PHE:CA	2:2F:101:LHG:H223	2.20	0.70
1:2K:55:PHE:CA	2:2K:101:LHG:H223	2.20	0.70
1:4N:8:LYS:N	1:4N:8:LYS:HD2	2.06	0.70
1:5I:55:PHE:CA	2:5I:101:LHG:H223	2.20	0.70
1:1A:8:LYS:HD2	1:1A:8:LYS:N	2.06	0.70
1:2M:8:LYS:HD2	1:2M:8:LYS:N	2.06	0.70
1:3G:55:PHE:HA	2:3G:101:LHG:C22	2.18	0.70
1:4A:8:LYS:HD2	1:4A:8:LYS:N	2.06	0.70
1:4F:55:PHE:CA	2:4F:101:LHG:H223	2.20	0.70
1:5G:8:LYS:HD2	1:5G:8:LYS:N	2.06	0.70
1:1K:55:PHE:HA	2:1K:101:LHG:C22	2.18	0.70
1:1K:8:LYS:HD2	1:1K:8:LYS:N	2.06	0.70
1:2N:55:PHE:HA	2:2N:101:LHG:C22	2.18	0.70
1:2P:8:LYS:HD2	1:2P:8:LYS:N	2.06	0.70
1:3J:8:LYS:HD2	1:3J:8:LYS:N	2.06	0.70
1:4C:8:LYS:N	1:4C:8:LYS:HD2	2.06	0.70
1:4G:8:LYS:N	1:4G:8:LYS:HD2	2.06	0.70
1:5J:55:PHE:CA	2:5J:101:LHG:H223	2.20	0.70
1:5O:8:LYS:N	1:5O:8:LYS:HD2	2.06	0.70
1:1C:55:PHE:CA	2:1C:101:LHG:H223	2.20	0.70
1:1H:55:PHE:CA	2:1H:101:LHG:H223	2.20	0.70
1:1J:8:LYS:N	1:1J:8:LYS:HD2	2.06	0.70
1:2E:8:LYS:N	1:2E:8:LYS:HD2	2.06	0.70
1:2O:55:PHE:CA	2:2O:101:LHG:H223	2.20	0.70
1:3C:55:PHE:CA	2:3C:101:LHG:H223	2.20	0.70
1:4G:55:PHE:CA	2:4G:101:LHG:H223	2.20	0.70
1:5E:55:PHE:CA	2:5E:101:LHG:H223	2.20	0.70
1:1C:8:LYS:HD2	1:1C:8:LYS:N	2.06	0.70
1:1H:8:LYS:N	1:1H:8:LYS:HD2	2.06	0.70
1:2B:8:LYS:N	1:2B:8:LYS:HD2	2.06	0.70
1:2K:8:LYS:HD2	1:2K:8:LYS:N	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2N:8:LYS:HD2	1:2N:8:LYS:N	2.06	0.70
1:3N:8:LYS:N	1:3N:8:LYS:HD2	2.06	0.70
1:1A:55:PHE:CA	2:1A:101:LHG:H223	2.20	0.70
1:1M:55:PHE:CA	2:1M:101:LHG:H223	2.20	0.70
1:2C:20:PHE:HE2	2:3D:101:LHG:C37	2.05	0.70
1:3D:55:PHE:CA	2:3D:101:LHG:H223	2.20	0.70
1:3O:8:LYS:HD2	1:3O:8:LYS:N	2.06	0.70
1:4L:8:LYS:N	1:4L:8:LYS:HD2	2.06	0.70
1:1B:8:LYS:N	1:1B:8:LYS:HD2	2.06	0.70
1:3J:55:PHE:CA	2:3J:101:LHG:H223	2.20	0.70
1:4B:55:PHE:CA	2:4B:101:LHG:H223	2.20	0.70
1:4B:8:LYS:HD2	1:4B:8:LYS:N	2.06	0.70
1:3C:20:PHE:HE2	2:4D:101:LHG:H371	1.57	0.70
1:4F:8:LYS:HD2	1:4F:8:LYS:N	2.06	0.70
1:4M:55:PHE:CA	2:4M:101:LHG:H223	2.20	0.70
1:5E:8:LYS:HD2	1:5E:8:LYS:N	2.06	0.70
1:1M:8:LYS:HD2	1:1M:8:LYS:N	2.06	0.70
1:1N:8:LYS:HD2	1:1N:8:LYS:N	2.06	0.70
1:2F:8:LYS:N	1:2F:8:LYS:HD2	2.06	0.70
1:3C:8:LYS:HD2	1:3C:8:LYS:N	2.06	0.70
1:3C:20:PHE:HE2	2:4D:101:LHG:C37	2.05	0.70
1:4M:8:LYS:HD2	1:4M:8:LYS:N	2.06	0.70
1:5F:8:LYS:N	1:5F:8:LYS:HD2	2.06	0.70
1:5P:8:LYS:HD2	1:5P:8:LYS:N	2.06	0.70
1:2A:55:PHE:CA	2:2A:101:LHG:H223	2.20	0.70
1:2C:55:PHE:CA	2:2C:101:LHG:H223	2.20	0.70
1:2D:55:PHE:CA	2:2D:101:LHG:H223	2.20	0.70
1:3D:55:PHE:HD1	2:3D:101:LHG:H211	1.57	0.70
1:3I:8:LYS:N	1:3I:8:LYS:HD2	2.06	0.70
1:3L:55:PHE:HD1	2:3L:101:LHG:H211	1.57	0.70
1:4C:20:PHE:HE2	2:5D:101:LHG:H371	1.57	0.70
1:1I:20:PHE:HE2	2:2J:101:LHG:C37	2.03	0.69
1:3F:55:PHE:CA	2:3F:101:LHG:H223	2.20	0.69
1:3G:55:PHE:CA	2:3G:101:LHG:H223	2.20	0.69
1:1B:55:PHE:HD1	2:1B:101:LHG:H211	1.57	0.69
2:1E:101:LHG:H371	1:5D:20:PHE:HE2	1.56	0.69
1:1I:55:PHE:HD1	2:1I:101:LHG:H211	1.57	0.69
1:1K:55:PHE:CA	2:1K:101:LHG:H223	2.20	0.69
1:2B:55:PHE:HD1	2:2B:101:LHG:H211	1.58	0.69
1:4C:20:PHE:HE2	2:5D:101:LHG:C37	2.05	0.69
1:4E:55:PHE:HD1	2:4E:101:LHG:H211	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5B:55:PHE:HD1	2:5B:101:LHG:H211	1.57	0.69
1:5G:55:PHE:HD1	2:5G:101:LHG:H211	1.57	0.69
1:1A:55:PHE:HD1	2:1A:101:LHG:H211	1.58	0.69
1:1E:55:PHE:HD1	2:1E:101:LHG:H211	1.58	0.69
1:1F:55:PHE:HD1	2:1F:101:LHG:H211	1.58	0.69
1:2D:55:PHE:HD1	2:2D:101:LHG:H211	1.57	0.69
1:2G:55:PHE:CA	2:2G:101:LHG:H223	2.20	0.69
1:2H:55:PHE:HD1	2:2H:101:LHG:H211	1.58	0.69
1:2I:55:PHE:HD1	2:2I:101:LHG:H211	1.58	0.69
1:2N:55:PHE:CA	2:2N:101:LHG:H223	2.20	0.69
1:3A:55:PHE:HD1	2:3A:101:LHG:H211	1.58	0.69
1:3B:55:PHE:HD1	2:3B:101:LHG:H211	1.58	0.69
1:3C:55:PHE:HD1	2:3C:101:LHG:H211	1.58	0.69
1:4O:55:PHE:HD1	2:4O:101:LHG:H211	1.58	0.69
1:5H:55:PHE:HD1	2:5H:101:LHG:H211	1.57	0.69
1:2A:55:PHE:HD1	2:2A:101:LHG:H211	1.58	0.69
1:2C:55:PHE:HD1	2:2C:101:LHG:H211	1.58	0.69
1:1C:20:PHE:HE2	2:2D:101:LHG:C37	2.05	0.69
1:3G:20:PHE:CE2	2:4H:101:LHG:H371	2.27	0.69
1:3M:55:PHE:HD1	2:3M:101:LHG:H211	1.58	0.69
1:4D:55:PHE:HD1	2:4D:101:LHG:H211	1.57	0.69
1:4F:55:PHE:HD1	2:4F:101:LHG:H211	1.58	0.69
1:4H:55:PHE:CA	2:4H:101:LHG:H223	2.20	0.69
1:5A:55:PHE:HD1	2:5A:101:LHG:H211	1.58	0.69
1:5C:55:PHE:HD1	2:5C:101:LHG:H211	1.58	0.69
1:5H:55:PHE:CA	2:5H:101:LHG:H223	2.20	0.69
1:1H:55:PHE:HD1	2:1H:101:LHG:H211	1.58	0.69
1:1J:55:PHE:HD1	2:1J:101:LHG:H211	1.57	0.69
1:2K:55:PHE:HD1	2:2K:101:LHG:H211	1.57	0.69
1:3O:55:PHE:CA	2:3O:101:LHG:H223	2.20	0.69
1:4J:55:PHE:CA	2:4J:101:LHG:H223	2.20	0.69
1:4M:55:PHE:HD1	2:4M:101:LHG:H211	1.58	0.69
1:5N:55:PHE:HD1	2:5N:101:LHG:H211	1.58	0.69
1:1C:55:PHE:HD1	2:1C:101:LHG:H211	1.58	0.69
1:1N:55:PHE:CA	2:1N:101:LHG:H223	2.20	0.69
1:2J:55:PHE:HD1	2:2J:101:LHG:H211	1.58	0.69
1:3E:55:PHE:HD1	2:3E:101:LHG:H211	1.58	0.69
1:3E:55:PHE:CA	2:3E:101:LHG:H223	2.20	0.69
1:3K:55:PHE:HD1	2:3K:101:LHG:H211	1.58	0.69
1:4I:55:PHE:CA	2:4I:101:LHG:H223	2.20	0.69
1:5K:55:PHE:CA	2:5K:101:LHG:H223	2.20	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5O:55:PHE:HD1	2:5O:101:LHG:H211	1.58	0.69
1:1C:20:PHE:HE2	2:2D:101:LHG:H371	1.57	0.69
1:5F:55:PHE:HD1	2:5F:101:LHG:H211	1.58	0.69
2:1K:101:LHG:C37	1:5J:20:PHE:HE2	2.06	0.69
1:1D:55:PHE:CA	2:1D:101:LHG:H223	2.20	0.69
1:2B:55:PHE:CA	2:2B:101:LHG:H223	2.20	0.69
1:2L:55:PHE:HD1	2:2L:101:LHG:H211	1.57	0.69
1:2L:55:PHE:CA	2:2L:101:LHG:H223	2.20	0.69
1:4G:55:PHE:HD1	2:4G:101:LHG:H211	1.58	0.69
1:4L:55:PHE:HD1	2:4L:101:LHG:H211	1.58	0.69
1:4N:55:PHE:HD1	2:4N:101:LHG:H211	1.58	0.69
2:1H:101:LHG:H371	1:5G:20:PHE:CE2	2.27	0.69
1:5J:8:LYS:HD2	1:5J:8:LYS:N	2.06	0.69
1:1D:55:PHE:HD1	2:1D:101:LHG:H211	1.57	0.69
1:1K:55:PHE:HD1	2:1K:101:LHG:H211	1.57	0.69
1:1O:55:PHE:HD1	2:1O:101:LHG:H211	1.58	0.69
1:2C:20:PHE:HE2	2:3D:101:LHG:H371	1.57	0.69
1:3J:55:PHE:HD1	2:3J:101:LHG:H211	1.57	0.69
1:5L:55:PHE:CA	2:5L:101:LHG:H223	2.20	0.69
1:5M:55:PHE:HD1	2:5M:101:LHG:H211	1.58	0.69
1:1G:55:PHE:HD1	2:1G:101:LHG:H211	1.58	0.69
1:2E:55:PHE:HD1	2:2E:101:LHG:H211	1.58	0.69
1:5A:55:PHE:CA	2:5A:101:LHG:H223	2.20	0.69
1:4B:20:PHE:HE2	2:5C:101:LHG:C37	2.06	0.69
1:5I:55:PHE:HD1	2:5I:101:LHG:H211	1.58	0.69
1:5M:55:PHE:CA	2:5M:101:LHG:H223	2.20	0.69
2:1H:101:LHG:H331	1:5G:24:CYS:SG	2.32	0.69
1:1O:55:PHE:CA	2:1O:101:LHG:H223	2.20	0.69
1:2G:55:PHE:HD1	2:2G:101:LHG:H211	1.57	0.69
1:3F:55:PHE:HD1	2:3F:101:LHG:H211	1.58	0.69
1:3H:20:PHE:CE2	2:4I:101:LHG:H371	2.28	0.69
1:4H:55:PHE:HD1	2:4H:101:LHG:H211	1.57	0.69
1:4J:55:PHE:HD1	2:4J:101:LHG:H211	1.57	0.69
1:5D:55:PHE:HD1	2:5D:101:LHG:H211	1.57	0.69
1:5E:55:PHE:HD1	2:5E:101:LHG:H211	1.58	0.69
1:1I:55:PHE:CA	2:1I:101:LHG:H223	2.20	0.68
1:1J:55:PHE:CA	2:1J:101:LHG:H223	2.20	0.68
1:2M:55:PHE:CA	2:2M:101:LHG:H223	2.20	0.68
1:2N:55:PHE:HD1	2:2N:101:LHG:H211	1.57	0.68
1:3B:20:PHE:HE2	2:4C:101:LHG:C37	2.06	0.68
1:1A:20:PHE:HE2	2:2B:101:LHG:C37	2.06	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2B:20:PHE:HE2	2:3C:101:LHG:H371	1.59	0.68
1:3G:55:PHE:HD1	2:3G:101:LHG:H211	1.58	0.68
1:3N:55:PHE:HD1	2:3N:101:LHG:H211	1.58	0.68
1:4C:55:PHE:HD1	2:4C:101:LHG:H211	1.58	0.68
1:5F:55:PHE:CA	2:5F:101:LHG:H223	2.20	0.68
1:2E:58:VAL:HG23	2:2E:101:LHG:H222	1.75	0.68
1:3H:58:VAL:HG23	2:3H:101:LHG:H222	1.76	0.68
1:3B:20:PHE:HE2	2:4C:101:LHG:H371	1.59	0.68
1:4K:55:PHE:HD1	2:4K:101:LHG:H211	1.57	0.68
2:1G:101:LHG:H331	1:5F:24:CYS:SG	2.33	0.68
1:4K:58:VAL:HG23	2:4K:101:LHG:H222	1.76	0.68
1:5G:55:PHE:CA	2:5G:101:LHG:H223	2.20	0.68
1:1B:58:VAL:HG23	2:1B:101:LHG:H222	1.76	0.68
1:1L:55:PHE:HD1	2:1L:101:LHG:H211	1.57	0.68
1:1N:55:PHE:HD1	2:1N:101:LHG:H211	1.58	0.68
1:2D:58:VAL:HG23	2:2D:101:LHG:H222	1.75	0.68
1:2B:20:PHE:HE2	2:3C:101:LHG:C37	2.06	0.68
1:4C:55:PHE:CA	2:4C:101:LHG:H223	2.20	0.68
1:5J:55:PHE:HD1	2:5J:101:LHG:H211	1.57	0.68
1:1A:58:VAL:HG23	2:1A:101:LHG:H222	1.75	0.68
1:1B:20:PHE:HE2	2:2C:101:LHG:H371	1.59	0.68
1:2M:55:PHE:HD1	2:2M:101:LHG:H211	1.58	0.68
1:2O:55:PHE:HD1	2:2O:101:LHG:H211	1.58	0.68
1:2A:20:PHE:HE2	2:3B:101:LHG:C37	2.06	0.68
1:4I:55:PHE:HD1	2:4I:101:LHG:H211	1.57	0.68
1:4N:55:PHE:CA	2:4N:101:LHG:H223	2.20	0.68
1:5C:3:LEU:HD13	1:5D:13:ALA:O	1.94	0.68
2:1I:101:LHG:H371	1:5H:20:PHE:CE2	2.27	0.68
1:1E:3:LEU:HD13	1:1F:13:ALA:O	1.94	0.68
1:2F:55:PHE:HD1	2:2F:101:LHG:H211	1.58	0.68
1:2F:58:VAL:HG23	2:2F:101:LHG:H222	1.75	0.68
1:2G:3:LEU:HD13	1:2H:13:ALA:O	1.94	0.68
1:3G:58:VAL:HG23	2:3G:101:LHG:H222	1.76	0.68
1:3I:55:PHE:HD1	2:3I:101:LHG:H211	1.57	0.68
1:3I:58:VAL:HG23	2:3I:101:LHG:H222	1.76	0.68
1:3K:55:PHE:CA	2:3K:101:LHG:H223	2.20	0.68
1:4C:3:LEU:HD13	1:4D:13:ALA:O	1.94	0.68
1:4L:58:VAL:HG23	2:4L:101:LHG:H222	1.76	0.68
1:4N:3:LEU:HD13	1:4O:13:ALA:O	1.94	0.68
1:5B:3:LEU:HD13	1:5C:13:ALA:O	1.94	0.68
1:4B:20:PHE:HE2	2:5C:101:LHG:H371	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5N:58:VAL:HG23	2:5N:101:LHG:H222	1.76	0.68
1:1D:3:LEU:HD13	1:1E:13:ALA:O	1.94	0.68
1:2H:3:LEU:HD13	1:2I:13:ALA:O	1.94	0.68
1:2J:3:LEU:HD13	1:2K:13:ALA:O	1.94	0.68
1:4A:55:PHE:HD1	2:4A:101:LHG:H211	1.58	0.68
1:4B:3:LEU:HD13	1:4C:13:ALA:O	1.94	0.68
1:4J:58:VAL:HG23	2:4J:101:LHG:H222	1.76	0.68
1:4J:3:LEU:HD13	1:4K:13:ALA:O	1.94	0.68
1:4K:3:LEU:HD13	1:4L:13:ALA:O	1.94	0.68
1:5L:55:PHE:HD1	2:5L:101:LHG:H211	1.58	0.68
1:5M:3:LEU:HD13	1:5N:13:ALA:O	1.94	0.68
1:1C:58:VAL:HG23	2:1C:101:LHG:H222	1.75	0.68
1:1H:3:LEU:HD13	1:1I:13:ALA:O	1.94	0.68
1:2K:3:LEU:HD13	1:2L:13:ALA:O	1.94	0.68
1:2L:3:LEU:HD13	1:2M:13:ALA:O	1.94	0.68
1:3H:55:PHE:HD1	2:3H:101:LHG:H211	1.58	0.68
1:3K:3:LEU:HD13	1:3L:13:ALA:O	1.94	0.68
1:3M:3:LEU:HD13	1:3N:13:ALA:O	1.94	0.68
1:4A:20:PHE:HE2	2:5B:101:LHG:C37	2.06	0.68
1:5E:3:LEU:HD13	1:5F:13:ALA:O	1.94	0.68
1:5F:3:LEU:HD13	1:5G:13:ALA:O	1.94	0.68
1:5O:3:LEU:HD13	1:5P:13:ALA:O	1.94	0.68
1:1A:20:PHE:HE2	2:2B:101:LHG:H371	1.59	0.68
1:1B:20:PHE:HE2	2:2C:101:LHG:C37	2.06	0.68
1:1F:3:LEU:HD13	1:1G:13:ALA:O	1.94	0.68
1:1I:3:LEU:HD13	1:1J:13:ALA:O	1.94	0.68
1:2D:3:LEU:HD13	1:2E:13:ALA:O	1.94	0.68
1:2H:55:PHE:CA	2:2H:101:LHG:H223	2.20	0.68
1:3G:3:LEU:HD13	1:3H:13:ALA:O	1.94	0.68
1:3N:3:LEU:HD13	1:3O:13:ALA:O	1.94	0.68
1:3O:55:PHE:HD1	2:3O:101:LHG:H211	1.58	0.68
1:3O:3:LEU:HD13	1:3P:13:ALA:O	1.94	0.68
1:3A:20:PHE:HE2	2:4B:101:LHG:C37	2.06	0.68
1:5A:3:LEU:HD13	1:5B:13:ALA:O	1.94	0.68
1:5O:58:VAL:HG23	2:5O:101:LHG:H222	1.76	0.68
1:1G:3:LEU:HD13	1:1H:13:ALA:O	1.94	0.67
1:2A:20:PHE:HE2	2:3B:101:LHG:H371	1.59	0.67
1:3H:3:LEU:HD13	1:3I:13:ALA:O	1.94	0.67
1:3J:3:LEU:HD13	1:3K:13:ALA:O	1.94	0.67
1:4D:55:PHE:CA	2:4D:101:LHG:H223	2.20	0.67
1:4M:3:LEU:HD13	1:4N:13:ALA:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5M:58:VAL:HG23	2:5M:101:LHG:H222	1.76	0.67
1:1A:3:LEU:HD13	1:1B:13:ALA:O	1.94	0.67
1:1M:55:PHE:HD1	2:1M:101:LHG:H211	1.58	0.67
1:3C:3:LEU:HD13	1:3D:13:ALA:O	1.94	0.67
1:4B:55:PHE:HD1	2:4B:101:LHG:H211	1.57	0.67
1:5K:55:PHE:HD1	2:5K:101:LHG:H211	1.57	0.67
1:5N:3:LEU:HD13	1:5O:13:ALA:O	1.94	0.67
1:1C:3:LEU:HD13	1:1D:13:ALA:O	1.94	0.67
1:1O:3:LEU:HD13	1:1P:13:ALA:O	1.94	0.67
1:3B:3:LEU:HD13	1:3C:13:ALA:O	1.94	0.67
1:4O:3:LEU:HD13	1:4P:13:ALA:O	1.94	0.67
1:2E:3:LEU:HD13	1:2F:13:ALA:O	1.94	0.67
1:2I:3:LEU:HD13	1:2J:13:ALA:O	1.94	0.67
1:4A:58:VAL:HG23	2:4A:101:LHG:H222	1.76	0.67
1:4L:3:LEU:HD13	1:4M:13:ALA:O	1.94	0.67
1:5B:55:PHE:CA	2:5B:101:LHG:H223	2.20	0.67
1:5C:58:VAL:HG23	2:5C:101:LHG:H222	1.75	0.67
1:1E:55:PHE:CA	2:1E:101:LHG:H223	2.20	0.67
2:1I:101:LHG:H331	1:5H:24:CYS:SG	2.34	0.67
1:1M:58:VAL:HG23	2:1M:101:LHG:H222	1.76	0.67
1:1L:3:LEU:HD13	1:1M:13:ALA:O	1.94	0.67
1:2C:58:VAL:HG23	2:2C:101:LHG:H222	1.76	0.67
1:2O:3:LEU:HD13	1:2P:13:ALA:O	1.94	0.67
1:3A:3:LEU:HD13	1:3B:13:ALA:O	1.94	0.67
1:3J:58:VAL:HG23	2:3J:101:LHG:H222	1.76	0.67
1:3L:3:LEU:HD13	1:3M:13:ALA:O	1.94	0.67
1:4F:3:LEU:HD13	1:4G:13:ALA:O	1.94	0.67
1:4M:58:VAL:HG23	2:4M:101:LHG:H222	1.76	0.67
1:4A:20:PHE:HE2	2:5B:101:LHG:H371	1.59	0.67
1:5L:3:LEU:HD13	1:5M:13:ALA:O	1.94	0.67
1:1B:3:LEU:HD13	1:1C:13:ALA:O	1.94	0.67
1:2A:3:LEU:HD13	1:2B:13:ALA:O	1.94	0.67
1:2G:58:VAL:HG23	2:2G:101:LHG:H222	1.75	0.67
1:2O:58:VAL:HG23	2:2O:101:LHG:H222	1.76	0.67
1:3F:58:VAL:HG23	2:3F:101:LHG:H222	1.76	0.67
1:3O:58:VAL:HG23	2:3O:101:LHG:H222	1.76	0.67
1:4G:20:PHE:CE2	2:5H:101:LHG:H371	2.27	0.67
2:1D:101:LHG:H371	1:5C:20:PHE:HE2	1.59	0.67
1:5D:58:VAL:HG23	2:5D:101:LHG:H222	1.75	0.67
1:5I:3:LEU:HD13	1:5J:13:ALA:O	1.94	0.67
1:1F:58:VAL:HG23	2:1F:101:LHG:H222	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1M:3:LEU:HD13	1:1N:13:ALA:O	1.94	0.67
1:2G:20:PHE:CE2	2:3H:101:LHG:H371	2.27	0.67
1:3D:3:LEU:HD13	1:3E:13:ALA:O	1.94	0.67
1:3N:58:VAL:HG23	2:3N:101:LHG:H222	1.76	0.67
1:4E:3:LEU:HD13	1:4F:13:ALA:O	1.94	0.67
1:4I:58:VAL:HG23	2:4I:101:LHG:H222	1.75	0.67
1:4I:3:LEU:HD13	1:4J:13:ALA:O	1.94	0.67
1:5D:3:LEU:HD13	1:5E:13:ALA:O	1.94	0.67
1:5J:3:LEU:HD13	1:5K:13:ALA:O	1.94	0.67
1:1D:58:VAL:HG23	2:1D:101:LHG:H222	1.75	0.67
1:2C:3:LEU:HD13	1:2D:13:ALA:O	1.94	0.67
1:2K:58:VAL:HG23	2:2K:101:LHG:H222	1.76	0.67
1:2L:58:VAL:HG23	2:2L:101:LHG:H222	1.76	0.67
1:2M:3:LEU:HD13	1:2N:13:ALA:O	1.94	0.67
1:3L:55:PHE:HD1	2:3L:101:LHG:C21	2.08	0.67
1:4D:3:LEU:HD13	1:4E:13:ALA:O	1.94	0.67
1:4G:3:LEU:HD13	1:4H:13:ALA:O	1.94	0.67
1:4M:55:PHE:HD1	2:4M:101:LHG:C21	2.08	0.67
1:5B:58:VAL:HG23	2:5B:101:LHG:H222	1.75	0.67
1:5J:58:VAL:HG23	2:5J:101:LHG:H222	1.76	0.67
1:1I:55:PHE:HD1	2:1I:101:LHG:C21	2.08	0.67
1:1J:55:PHE:HD1	2:1J:101:LHG:C21	2.08	0.67
1:1L:58:VAL:HG23	2:1L:101:LHG:H222	1.76	0.67
1:1N:58:VAL:HG23	2:1N:101:LHG:H222	1.76	0.67
1:2K:55:PHE:HD1	2:2K:101:LHG:C21	2.08	0.67
1:2L:55:PHE:HD1	2:2L:101:LHG:C21	2.08	0.67
1:3D:55:PHE:HD1	2:3D:101:LHG:C21	2.08	0.67
1:3F:3:LEU:HD13	1:3G:13:ALA:O	1.94	0.67
1:3M:55:PHE:HD1	2:3M:101:LHG:C21	2.08	0.67
1:4N:55:PHE:HD1	2:4N:101:LHG:C21	2.08	0.67
1:4O:55:PHE:HD1	2:4O:101:LHG:C21	2.08	0.67
1:5G:3:LEU:HD13	1:5H:13:ALA:O	1.94	0.67
1:5H:55:PHE:HD1	2:5H:101:LHG:C21	2.08	0.67
1:1E:55:PHE:HD1	2:1E:101:LHG:C21	2.08	0.67
1:1I:58:VAL:HG23	2:1I:101:LHG:H222	1.76	0.67
1:1J:3:LEU:HD13	1:1K:13:ALA:O	1.94	0.67
1:2M:58:VAL:HG23	2:2M:101:LHG:H222	1.76	0.67
1:3M:58:VAL:HG23	2:3M:101:LHG:H222	1.76	0.67
1:3A:20:PHE:HE2	2:4B:101:LHG:H371	1.59	0.67
1:4A:3:LEU:HD13	1:4B:13:ALA:O	1.94	0.67
1:4F:55:PHE:HD1	2:4F:101:LHG:C21	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5A:58:VAL:HG23	2:5A:101:LHG:H222	1.75	0.67
1:5G:55:PHE:HD1	2:5G:101:LHG:C21	2.08	0.67
1:1F:55:PHE:HD1	2:1F:101:LHG:C21	2.08	0.66
1:1J:58:VAL:HG23	2:1J:101:LHG:H222	1.76	0.66
1:1K:55:PHE:HD1	2:1K:101:LHG:C21	2.08	0.66
1:2A:55:PHE:HD1	2:2A:101:LHG:C21	2.08	0.66
1:2J:55:PHE:HD1	2:2J:101:LHG:C21	2.08	0.66
1:3N:55:PHE:HD1	2:3N:101:LHG:C21	2.08	0.66
1:4E:55:PHE:HD1	2:4E:101:LHG:C21	2.08	0.66
1:4L:55:PHE:HD1	2:4L:101:LHG:C21	2.08	0.66
1:5A:55:PHE:HD1	2:5A:101:LHG:C21	2.08	0.66
1:5B:55:PHE:HD1	2:5B:101:LHG:C21	2.08	0.66
1:1D:55:PHE:HD1	2:1D:101:LHG:C21	2.08	0.66
1:1E:58:VAL:HG23	2:1E:101:LHG:H222	1.75	0.66
1:1H:55:PHE:HD1	2:1H:101:LHG:C21	2.08	0.66
1:2B:55:PHE:HD1	2:2B:101:LHG:C21	2.08	0.66
1:2F:3:LEU:HD13	1:2G:13:ALA:O	1.94	0.66
1:3C:55:PHE:HD1	2:3C:101:LHG:C21	2.09	0.66
1:3E:3:LEU:HD13	1:3F:13:ALA:O	1.94	0.66
1:5K:58:VAL:HG23	2:5K:101:LHG:H222	1.76	0.66
1:5L:58:VAL:HG23	2:5L:101:LHG:H222	1.76	0.66
1:5O:55:PHE:HD1	2:5O:101:LHG:C21	2.08	0.66
1:1B:55:PHE:HD1	2:1B:101:LHG:C21	2.08	0.66
1:1C:55:PHE:HD1	2:1C:101:LHG:C21	2.08	0.66
1:2C:55:PHE:HD1	2:2C:101:LHG:C21	2.08	0.66
1:2D:55:PHE:HD1	2:2D:101:LHG:C21	2.08	0.66
1:2I:58:VAL:HG23	2:2I:101:LHG:H222	1.76	0.66
1:2J:58:VAL:HG23	2:2J:101:LHG:H222	1.76	0.66
1:2M:55:PHE:HD1	2:2M:101:LHG:C21	2.08	0.66
1:3E:55:PHE:HD1	2:3E:101:LHG:C21	2.08	0.66
1:4A:55:PHE:HD1	2:4A:101:LHG:C21	2.08	0.66
1:4D:55:PHE:HD1	2:4D:101:LHG:C21	2.08	0.66
1:4G:55:PHE:HD1	2:4G:101:LHG:C21	2.08	0.66
1:4H:3:LEU:HD13	1:4I:13:ALA:O	1.94	0.66
1:5I:55:PHE:HD1	2:5I:101:LHG:C21	2.08	0.66
1:1A:55:PHE:HD1	2:1A:101:LHG:C21	2.08	0.66
1:1G:55:PHE:HD1	2:1G:101:LHG:C21	2.08	0.66
1:1H:58:VAL:HG23	2:1H:101:LHG:H222	1.76	0.66
1:1K:3:LEU:HD13	1:1L:13:ALA:O	1.94	0.66
1:2N:3:LEU:HD13	1:2O:13:ALA:O	1.94	0.66
1:3I:3:LEU:HD13	1:3J:13:ALA:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3K:55:PHE:HD1	2:3K:101:LHG:C21	2.08	0.66
1:3O:55:PHE:HD1	2:3O:101:LHG:C21	2.08	0.66
1:5C:55:PHE:HD1	2:5C:101:LHG:C21	2.08	0.66
1:5F:55:PHE:HD1	2:5F:101:LHG:C21	2.09	0.66
1:5H:3:LEU:HD13	1:5I:13:ALA:O	1.94	0.66
1:1K:58:VAL:HG23	2:1K:101:LHG:H222	1.76	0.66
1:2N:58:VAL:HG23	2:2N:101:LHG:H222	1.76	0.66
1:3A:55:PHE:HD1	2:3A:101:LHG:C21	2.08	0.66
1:3B:55:PHE:HD1	2:3B:101:LHG:C21	2.08	0.66
1:4O:58:VAL:HG23	2:4O:101:LHG:H222	1.76	0.66
1:5G:58:VAL:HG23	2:5G:101:LHG:H222	1.76	0.66
1:5K:3:LEU:HD13	1:5L:13:ALA:O	1.94	0.66
1:1O:58:VAL:HG23	2:1O:101:LHG:H222	1.76	0.66
1:2E:55:PHE:HD1	2:2E:101:LHG:C21	2.09	0.66
1:3F:55:PHE:HD1	2:3F:101:LHG:C21	2.08	0.66
1:4H:55:PHE:HD1	2:4H:101:LHG:C21	2.08	0.66
1:5D:55:PHE:HD1	2:5D:101:LHG:C21	2.08	0.66
1:5F:58:VAL:HG23	2:5F:101:LHG:H222	1.75	0.66
1:5N:55:PHE:HD1	2:5N:101:LHG:C21	2.08	0.66
1:1L:55:PHE:HD1	2:1L:101:LHG:C21	2.08	0.66
1:1N:3:LEU:HD13	1:1O:13:ALA:O	1.94	0.66
1:2I:55:PHE:HD1	2:2I:101:LHG:C21	2.08	0.66
1:3L:58:VAL:HG23	2:3L:101:LHG:H222	1.76	0.66
1:4K:55:PHE:HD1	2:4K:101:LHG:C21	2.08	0.66
1:5E:55:PHE:HD1	2:5E:101:LHG:C21	2.08	0.66
1:5H:58:VAL:HG23	2:5H:101:LHG:H222	1.76	0.66
1:5J:55:PHE:HD1	2:5J:101:LHG:C21	2.08	0.66
1:1H:20:PHE:CE2	2:2I:101:LHG:H371	2.28	0.66
1:2B:3:LEU:HD13	1:2C:13:ALA:O	1.94	0.66
1:2F:55:PHE:HD1	2:2F:101:LHG:C21	2.09	0.66
1:2H:58:VAL:HG23	2:2H:101:LHG:H222	1.76	0.66
1:3G:55:PHE:HD1	2:3G:101:LHG:C21	2.08	0.66
1:3J:55:PHE:HD1	2:3J:101:LHG:C21	2.08	0.66
1:4H:20:PHE:CE2	2:5I:101:LHG:H371	2.28	0.66
1:2G:55:PHE:HD1	2:2G:101:LHG:C21	2.08	0.66
1:2N:55:PHE:HD1	2:2N:101:LHG:C21	2.08	0.66
1:4B:55:PHE:HD1	2:4B:101:LHG:C21	2.08	0.66
1:3F:24:CYS:SG	2:4G:101:LHG:H331	2.36	0.66
1:4G:24:CYS:SG	2:5H:101:LHG:H331	2.36	0.66
1:1G:58:VAL:HG23	2:1G:101:LHG:H222	1.76	0.66
1:1G:24:CYS:SG	2:2H:101:LHG:H331	2.36	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5E:58:VAL:HG23	2:5E:101:LHG:H222	1.75	0.66
1:1O:55:PHE:HD1	2:1O:101:LHG:C21	2.08	0.65
1:2A:58:VAL:HG23	2:2A:101:LHG:H222	1.75	0.65
1:2B:58:VAL:HG23	2:2B:101:LHG:H222	1.76	0.65
1:3A:58:VAL:HG23	2:3A:101:LHG:H222	1.75	0.65
1:3B:58:VAL:HG23	2:3B:101:LHG:H222	1.75	0.65
1:3E:58:VAL:HG23	2:3E:101:LHG:H222	1.75	0.65
1:3H:55:PHE:HD1	2:3H:101:LHG:C21	2.08	0.65
1:4E:58:VAL:HG23	2:4E:101:LHG:H222	1.75	0.65
1:4I:55:PHE:HD1	2:4I:101:LHG:C21	2.08	0.65
2:1F:101:LHG:H331	1:5E:24:CYS:SG	2.36	0.65
1:1G:20:PHE:CE2	2:2H:101:LHG:H371	2.27	0.65
1:2H:20:PHE:CE2	2:3I:101:LHG:H371	2.28	0.65
1:3I:55:PHE:HD1	2:3I:101:LHG:C21	2.08	0.65
1:4C:55:PHE:HD1	2:4C:101:LHG:C21	2.08	0.65
1:4D:58:VAL:HG23	2:4D:101:LHG:H222	1.75	0.65
1:3G:24:CYS:SG	2:4H:101:LHG:H331	2.36	0.65
1:4J:55:PHE:HD1	2:4J:101:LHG:C21	2.08	0.65
1:5K:55:PHE:HD1	2:5K:101:LHG:C21	2.08	0.65
1:2H:55:PHE:HD1	2:2H:101:LHG:C21	2.08	0.65
1:4H:58:VAL:HG23	2:4H:101:LHG:H222	1.75	0.65
1:4N:58:VAL:HG23	2:4N:101:LHG:H222	1.76	0.65
1:5I:58:VAL:HG23	2:5I:101:LHG:H222	1.76	0.65
1:5M:55:PHE:HD1	2:5M:101:LHG:C21	2.08	0.65
1:2F:20:PHE:CE2	2:3G:101:LHG:H371	2.30	0.65
1:4F:24:CYS:SG	2:5G:101:LHG:H331	2.36	0.65
2:1L:101:LHG:H371	1:5K:20:PHE:HE2	1.62	0.65
1:5M:9:ASP:OD2	1:5N:23:MET:SD	2.55	0.65
1:1D:9:ASP:OD2	1:1E:23:MET:SD	2.55	0.65
1:1O:9:ASP:OD2	1:1P:23:MET:SD	2.55	0.65
1:2D:9:ASP:OD2	1:2E:23:MET:SD	2.55	0.65
1:2O:55:PHE:HD1	2:2O:101:LHG:C21	2.08	0.65
1:3C:58:VAL:HG23	2:3C:101:LHG:H222	1.75	0.65
1:2F:24:CYS:SG	2:3G:101:LHG:H331	2.36	0.65
1:3G:9:ASP:OD2	1:3H:23:MET:SD	2.55	0.65
1:3K:58:VAL:HG23	2:3K:101:LHG:H222	1.76	0.65
1:5A:9:ASP:OD2	1:5B:23:MET:SD	2.55	0.65
1:5L:55:PHE:HD1	2:5L:101:LHG:C21	2.08	0.65
1:4K:20:PHE:HE2	2:5L:101:LHG:H371	1.62	0.65
1:5O:9:ASP:OD2	1:5P:23:MET:SD	2.55	0.65
1:1A:9:ASP:OD2	1:1B:23:MET:SD	2.55	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1F:9:ASP:OD2	1:1G:23:MET:SD	2.55	0.65
1:1M:55:PHE:HD1	2:1M:101:LHG:C21	2.08	0.65
1:1N:55:PHE:HD1	2:1N:101:LHG:C21	2.08	0.65
1:2G:9:ASP:OD2	1:2H:23:MET:SD	2.55	0.65
1:2L:9:ASP:OD2	1:2M:23:MET:SD	2.55	0.65
1:2M:9:ASP:OD2	1:2N:23:MET:SD	2.55	0.65
1:4A:9:ASP:OD2	1:4B:23:MET:SD	2.55	0.65
1:4C:58:VAL:HG23	2:4C:101:LHG:H222	1.75	0.65
1:4E:9:ASP:OD2	1:4F:23:MET:SD	2.55	0.65
1:4J:9:ASP:OD2	1:4K:23:MET:SD	2.55	0.65
1:4L:9:ASP:OD2	1:4M:23:MET:SD	2.55	0.65
1:4M:9:ASP:OD2	1:4N:23:MET:SD	2.55	0.65
1:5C:9:ASP:OD2	1:5D:23:MET:SD	2.55	0.65
1:1F:24:CYS:SG	2:2G:101:LHG:H331	2.36	0.65
1:1M:9:ASP:OD2	1:1N:23:MET:SD	2.55	0.65
1:2F:9:ASP:OD2	1:2G:23:MET:SD	2.55	0.65
1:3I:9:ASP:OD2	1:3J:23:MET:SD	2.55	0.65
1:3J:9:ASP:OD2	1:3K:23:MET:SD	2.55	0.65
1:3L:9:ASP:OD2	1:3M:23:MET:SD	2.55	0.65
1:4D:9:ASP:OD2	1:4E:23:MET:SD	2.55	0.65
1:4F:20:PHE:CE2	2:5G:101:LHG:H371	2.30	0.65
1:4F:9:ASP:OD2	1:4G:23:MET:SD	2.55	0.65
1:4K:9:ASP:OD2	1:4L:23:MET:SD	2.55	0.65
1:4O:9:ASP:OD2	1:4P:23:MET:SD	2.55	0.65
2:1B:101:LHG:H371	1:5A:20:PHE:HE2	1.61	0.65
1:5L:9:ASP:OD2	1:5M:23:MET:SD	2.55	0.65
1:1C:9:ASP:OD2	1:1D:23:MET:SD	2.55	0.65
1:2I:9:ASP:OD2	1:2J:23:MET:SD	2.55	0.65
1:4F:58:VAL:HG23	2:4F:101:LHG:H222	1.76	0.65
1:2N:9:ASP:OD2	1:2O:23:MET:SD	2.55	0.65
1:2G:24:CYS:SG	2:3H:101:LHG:H331	2.36	0.65
1:5D:9:ASP:OD2	1:5E:23:MET:SD	2.55	0.65
1:2K:9:ASP:OD2	1:2L:23:MET:SD	2.55	0.65
1:2K:20:PHE:HE2	2:3L:101:LHG:H371	1.62	0.65
1:3O:9:ASP:OD2	1:3P:23:MET:SD	2.55	0.65
1:4I:9:ASP:OD2	1:4J:23:MET:SD	2.55	0.65
1:5J:9:ASP:OD2	1:5K:23:MET:SD	2.55	0.65
1:1B:9:ASP:OD2	1:1C:23:MET:SD	2.55	0.64
1:1K:20:PHE:HE2	2:2L:101:LHG:H371	1.62	0.64
1:3F:9:ASP:OD2	1:3G:23:MET:SD	2.55	0.64
1:4C:9:ASP:OD2	1:4D:23:MET:SD	2.55	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1E:9:ASP:OD2	1:1F:23:MET:SD	2.55	0.64
1:1G:9:ASP:OD2	1:1H:23:MET:SD	2.55	0.64
1:3A:9:ASP:OD2	1:3B:23:MET:SD	2.55	0.64
1:3B:9:ASP:OD2	1:3C:23:MET:SD	2.55	0.64
1:4G:9:ASP:OD2	1:4H:23:MET:SD	2.55	0.64
1:5B:9:ASP:OD2	1:5C:23:MET:SD	2.55	0.64
1:5I:9:ASP:OD2	1:5J:23:MET:SD	2.55	0.64
1:5N:9:ASP:OD2	1:5O:23:MET:SD	2.55	0.64
1:2B:9:ASP:OD2	1:2C:23:MET:SD	2.55	0.64
1:3D:58:VAL:HG23	2:3D:101:LHG:H222	1.75	0.64
1:3E:9:ASP:OD2	1:3F:23:MET:SD	2.55	0.64
1:3N:9:ASP:OD2	1:3O:23:MET:SD	2.55	0.64
1:4B:58:VAL:HG23	2:4B:101:LHG:H222	1.75	0.64
1:4G:58:VAL:HG23	2:4G:101:LHG:H222	1.76	0.64
1:4N:9:ASP:OD2	1:4O:23:MET:SD	2.55	0.64
1:5G:9:ASP:OD2	1:5H:23:MET:SD	2.55	0.64
1:5H:9:ASP:OD2	1:5I:23:MET:SD	2.55	0.64
1:5K:9:ASP:OD2	1:5L:23:MET:SD	2.55	0.64
1:1I:9:ASP:OD2	1:1J:23:MET:SD	2.55	0.64
1:2A:9:ASP:OD2	1:2B:23:MET:SD	2.55	0.64
1:2C:9:ASP:OD2	1:2D:23:MET:SD	2.55	0.64
1:2E:9:ASP:OD2	1:2F:23:MET:SD	2.55	0.64
1:2O:9:ASP:OD2	1:2P:23:MET:SD	2.55	0.64
1:3C:9:ASP:OD2	1:3D:23:MET:SD	2.55	0.64
1:2H:24:CYS:SG	2:3I:101:LHG:H331	2.38	0.64
1:3K:9:ASP:OD2	1:3L:23:MET:SD	2.55	0.64
1:4H:9:ASP:OD2	1:4I:23:MET:SD	2.55	0.64
1:5F:9:ASP:OD2	1:5G:23:MET:SD	2.55	0.64
1:1H:9:ASP:OD2	1:1I:23:MET:SD	2.55	0.64
1:1J:9:ASP:OD2	1:1K:23:MET:SD	2.55	0.64
1:1K:9:ASP:OD2	1:1L:23:MET:SD	2.55	0.64
1:1N:9:ASP:OD2	1:1O:23:MET:SD	2.55	0.64
1:3D:9:ASP:OD2	1:3E:23:MET:SD	2.55	0.64
1:2H:9:ASP:OD2	1:2I:23:MET:SD	2.55	0.64
1:2J:9:ASP:OD2	1:2K:23:MET:SD	2.55	0.64
1:3H:9:ASP:OD2	1:3I:23:MET:SD	2.55	0.64
2:1C:101:LHG:H371	1:5B:20:PHE:HE2	1.61	0.64
1:4B:9:ASP:OD2	1:4C:23:MET:SD	2.55	0.64
1:5E:9:ASP:OD2	1:5F:23:MET:SD	2.55	0.64
1:3M:9:ASP:OD2	1:3N:23:MET:SD	2.55	0.64
2:1G:101:LHG:H371	1:5F:20:PHE:CE2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1L:9:ASP:OD2	1:1M:23:MET:SD	2.55	0.64
1:3H:24:CYS:SG	2:4I:101:LHG:H331	2.38	0.64
1:3K:20:PHE:HE2	2:4L:101:LHG:H371	1.62	0.64
2:1J:101:LHG:H371	1:5I:20:PHE:CE2	2.31	0.63
1:3F:20:PHE:CE2	2:4G:101:LHG:H371	2.30	0.63
1:1H:24:CYS:SG	2:2I:101:LHG:H331	2.38	0.63
1:4H:24:CYS:SG	2:5I:101:LHG:H331	2.38	0.63
1:3J:20:PHE:HE2	2:4K:101:LHG:C37	2.12	0.63
1:1E:24:CYS:SG	2:2F:101:LHG:H331	2.39	0.63
1:2E:24:CYS:SG	2:3F:101:LHG:H331	2.39	0.63
1:3E:24:CYS:SG	2:4F:101:LHG:H331	2.39	0.63
1:2J:20:PHE:HE2	2:3K:101:LHG:C37	2.12	0.63
2:4L:101:LHG:C21	2:4L:101:LHG:H372	2.25	0.63
2:5O:101:LHG:C21	2:5O:101:LHG:H372	2.25	0.63
1:1J:20:PHE:HE2	2:2K:101:LHG:C37	2.12	0.62
2:3I:101:LHG:C21	2:3I:101:LHG:H372	2.25	0.62
1:1I:20:PHE:CE2	2:2J:101:LHG:H371	2.32	0.62
1:2E:20:PHE:CE2	2:3F:101:LHG:H371	2.34	0.62
1:1F:20:PHE:CE2	2:2G:101:LHG:H371	2.30	0.62
1:4E:24:CYS:SG	2:5F:101:LHG:H331	2.39	0.62
2:1G:101:LHG:H372	1:5F:20:PHE:HE2	1.62	0.62
2:2F:101:LHG:H372	2:2F:101:LHG:C21	2.25	0.62
2:1J:101:LHG:H331	1:5I:24:CYS:SG	2.39	0.62
2:1C:101:LHG:C21	2:1C:101:LHG:H372	2.25	0.62
2:1E:101:LHG:H331	1:5D:24:CYS:SG	2.39	0.62
2:2J:101:LHG:H372	2:2J:101:LHG:C21	2.25	0.62
2:3E:101:LHG:C21	2:3E:101:LHG:H372	2.25	0.62
2:3M:101:LHG:C21	2:3M:101:LHG:H372	2.25	0.62
1:4J:20:PHE:HE2	2:5K:101:LHG:C37	2.12	0.62
2:2B:101:LHG:H372	2:2B:101:LHG:C21	2.25	0.62
2:1G:101:LHG:H372	2:1G:101:LHG:C21	2.25	0.61
2:5D:101:LHG:C21	2:5D:101:LHG:H372	2.25	0.61
2:1H:101:LHG:H372	1:5G:20:PHE:HE2	1.63	0.61
2:4A:101:LHG:C21	2:4A:101:LHG:H372	2.25	0.61
2:4H:101:LHG:C21	2:4H:101:LHG:H372	2.25	0.61
2:5K:101:LHG:C21	2:5K:101:LHG:H372	2.25	0.61
2:2M:101:LHG:C21	2:2M:101:LHG:H372	2.25	0.61
1:4I:20:PHE:CE2	2:5J:101:LHG:H371	2.32	0.61
2:1N:101:LHG:C21	2:1N:101:LHG:H372	2.25	0.61
1:4E:20:PHE:CE2	2:5F:101:LHG:H371	2.34	0.61
2:1J:101:LHG:C21	2:1J:101:LHG:H372	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1H:101:LHG:C37	1:5G:20:PHE:CE2	2.81	0.60
2:1F:101:LHG:H372	1:5E:20:PHE:HE2	1.63	0.60
2:5G:101:LHG:C21	2:5G:101:LHG:H372	2.25	0.60
2:5H:101:LHG:C21	2:5H:101:LHG:H372	2.25	0.60
1:2I:20:PHE:CE2	2:3J:101:LHG:H371	2.32	0.60
2:3B:101:LHG:C21	2:3B:101:LHG:H372	2.25	0.60
2:1K:101:LHG:C21	2:1K:101:LHG:H372	2.25	0.60
2:4E:101:LHG:H372	2:4E:101:LHG:C21	2.25	0.60
2:2N:101:LHG:C21	2:2N:101:LHG:H372	2.25	0.60
1:3E:20:PHE:CE2	2:4F:101:LHG:H371	2.34	0.60
2:1D:101:LHG:H331	1:5C:24:CYS:SG	2.41	0.60
2:1F:101:LHG:H371	1:5E:20:PHE:CE2	2.34	0.60
1:1O:55:PHE:CG	2:1O:101:LHG:H223	2.37	0.60
2:1O:101:LHG:H372	2:1O:101:LHG:C21	2.25	0.60
2:4I:101:LHG:C21	2:4I:101:LHG:H372	2.25	0.60
1:1N:55:PHE:CG	2:1N:101:LHG:H223	2.37	0.60
1:2B:55:PHE:CG	2:2B:101:LHG:H223	2.37	0.60
1:1D:24:CYS:SG	2:2E:101:LHG:H331	2.42	0.60
2:4D:101:LHG:H372	2:4D:101:LHG:C21	2.25	0.60
2:4M:101:LHG:C21	2:4M:101:LHG:H372	2.25	0.60
2:1B:101:LHG:H331	1:5A:24:CYS:SG	2.42	0.60
2:5L:101:LHG:H372	2:5L:101:LHG:C21	2.25	0.60
1:1C:55:PHE:CG	2:1C:101:LHG:H223	2.37	0.59
1:2G:55:PHE:CG	2:2G:101:LHG:H223	2.37	0.59
1:2D:24:CYS:SG	2:3E:101:LHG:H331	2.42	0.59
1:3E:55:PHE:CG	2:3E:101:LHG:H223	2.38	0.59
2:3J:101:LHG:H372	2:3J:101:LHG:C21	2.25	0.59
1:4H:55:PHE:CG	2:4H:101:LHG:H223	2.37	0.59
1:5A:55:PHE:CG	2:5A:101:LHG:H223	2.37	0.59
1:5L:55:PHE:CG	2:5L:101:LHG:H223	2.37	0.59
1:1D:55:PHE:CG	2:1D:101:LHG:H223	2.38	0.59
1:2F:55:PHE:CG	2:2F:101:LHG:H223	2.37	0.59
2:2G:101:LHG:H372	2:2G:101:LHG:C21	2.25	0.59
1:3F:55:PHE:CG	2:3F:101:LHG:H223	2.37	0.59
1:4I:55:PHE:CG	2:4I:101:LHG:H223	2.38	0.59
2:1B:101:LHG:H372	1:5A:20:PHE:HE2	1.67	0.59
2:1C:101:LHG:H331	1:5B:24:CYS:SG	2.42	0.59
1:5K:55:PHE:CG	2:5K:101:LHG:H223	2.37	0.59
1:2A:55:PHE:CG	2:2A:101:LHG:H223	2.37	0.59
1:2C:55:PHE:CG	2:2C:101:LHG:H223	2.37	0.59
1:2K:55:PHE:CD1	2:2K:101:LHG:H211	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2M:55:PHE:CG	2:2M:101:LHG:H223	2.37	0.59
1:3J:55:PHE:CG	2:3J:101:LHG:H223	2.38	0.59
1:3L:55:PHE:CD1	2:3L:101:LHG:H211	2.38	0.59
1:3D:24:CYS:SG	2:4E:101:LHG:H331	2.42	0.59
1:4M:55:PHE:CG	2:4M:101:LHG:H223	2.37	0.59
2:2I:101:LHG:H372	2:2I:101:LHG:C21	2.25	0.59
1:2N:55:PHE:CG	2:2N:101:LHG:H223	2.37	0.59
2:3A:101:LHG:H372	2:3A:101:LHG:C21	2.25	0.59
1:3I:55:PHE:CG	2:3I:101:LHG:H223	2.38	0.59
1:3M:55:PHE:CD1	2:3M:101:LHG:H211	2.38	0.59
1:4D:24:CYS:SG	2:5E:101:LHG:H331	2.42	0.59
1:4L:55:PHE:CG	2:4L:101:LHG:H223	2.37	0.59
1:1E:20:PHE:CE2	2:2F:101:LHG:H371	2.34	0.59
1:1I:55:PHE:CD1	2:1I:101:LHG:H211	2.38	0.59
1:2J:55:PHE:CD1	2:2J:101:LHG:H211	2.38	0.59
2:3F:101:LHG:C21	2:3F:101:LHG:H372	2.25	0.59
1:4G:55:PHE:CG	2:4G:101:LHG:H223	2.37	0.59
1:3I:20:PHE:CE2	2:4J:101:LHG:H371	2.32	0.59
1:4M:55:PHE:CD1	2:4M:101:LHG:H211	2.38	0.59
1:4O:55:PHE:CD1	2:4O:101:LHG:H211	2.38	0.59
1:5O:55:PHE:CG	2:5O:101:LHG:H223	2.37	0.59
1:1B:55:PHE:CG	2:1B:101:LHG:H223	2.37	0.59
1:1H:55:PHE:CD1	2:1H:101:LHG:H211	2.38	0.59
1:1J:55:PHE:CG	2:1J:101:LHG:H223	2.37	0.59
1:1M:55:PHE:CG	2:1M:101:LHG:H223	2.37	0.59
1:2H:55:PHE:CG	2:2H:101:LHG:H223	2.37	0.59
1:3D:55:PHE:CG	2:3D:101:LHG:H223	2.38	0.59
1:3K:55:PHE:CD1	2:3K:101:LHG:H211	2.38	0.59
1:3O:55:PHE:CG	2:3O:101:LHG:H223	2.37	0.59
1:4N:55:PHE:CG	2:4N:101:LHG:H223	2.37	0.59
1:4N:55:PHE:CD1	2:4N:101:LHG:H211	2.38	0.59
1:5B:55:PHE:CG	2:5B:101:LHG:H223	2.37	0.59
1:5M:55:PHE:CG	2:5M:101:LHG:H223	2.37	0.59
1:1E:55:PHE:CG	2:1E:101:LHG:H223	2.37	0.59
1:1K:55:PHE:CG	2:1K:101:LHG:H223	2.37	0.59
1:2E:55:PHE:CG	2:2E:101:LHG:H223	2.37	0.59
1:2L:55:PHE:CG	2:2L:101:LHG:H223	2.37	0.59
1:3K:55:PHE:CG	2:3K:101:LHG:H223	2.38	0.59
1:5G:55:PHE:CG	2:5G:101:LHG:H223	2.37	0.59
1:5J:55:PHE:CG	2:5J:101:LHG:H223	2.37	0.59
2:1D:101:LHG:H372	2:1D:101:LHG:C21	2.25	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1I:55:PHE:CG	2:1I:101:LHG:H223	2.37	0.59
2:2C:101:LHG:H372	2:2C:101:LHG:C21	2.25	0.59
1:2I:55:PHE:CD1	2:2I:101:LHG:H211	2.38	0.59
1:3J:55:PHE:CD1	2:3J:101:LHG:H211	2.38	0.59
1:4C:55:PHE:CG	2:4C:101:LHG:H223	2.37	0.59
1:4J:55:PHE:CG	2:4J:101:LHG:H223	2.38	0.59
2:5A:101:LHG:C21	2:5A:101:LHG:H372	2.25	0.59
2:1F:101:LHG:H372	2:1F:101:LHG:C21	2.25	0.59
1:3G:55:PHE:CG	2:3G:101:LHG:H223	2.37	0.59
1:4A:55:PHE:CG	2:4A:101:LHG:H223	2.37	0.59
1:4B:55:PHE:CG	2:4B:101:LHG:H223	2.37	0.59
2:5C:101:LHG:H372	2:5C:101:LHG:C21	2.25	0.59
1:5F:55:PHE:CG	2:5F:101:LHG:H223	2.37	0.59
1:1G:55:PHE:CD1	2:1G:101:LHG:H211	2.38	0.59
1:2O:55:PHE:CG	2:2O:101:LHG:H223	2.37	0.59
1:3H:55:PHE:CG	2:3H:101:LHG:H223	2.37	0.59
1:3I:24:CYS:SG	2:4J:101:LHG:H331	2.43	0.59
1:5E:55:PHE:CG	2:5E:101:LHG:H223	2.37	0.59
1:5F:55:PHE:CD1	2:5F:101:LHG:H211	2.38	0.59
1:5H:55:PHE:CG	2:5H:101:LHG:H223	2.38	0.59
1:1H:55:PHE:CG	2:1H:101:LHG:H223	2.37	0.58
1:2H:55:PHE:CD1	2:2H:101:LHG:H211	2.38	0.58
1:3A:55:PHE:CG	2:3A:101:LHG:H223	2.37	0.58
1:4D:55:PHE:CG	2:4D:101:LHG:H223	2.37	0.58
1:4I:24:CYS:SG	2:5J:101:LHG:H331	2.43	0.58
2:1L:101:LHG:C37	1:5K:20:PHE:HE2	2.15	0.58
2:1C:101:LHG:H372	1:5B:20:PHE:HE2	1.68	0.58
2:1I:101:LHG:C37	1:5H:20:PHE:CE2	2.82	0.58
1:2D:55:PHE:CG	2:2D:101:LHG:H223	2.38	0.58
1:3C:55:PHE:CG	2:3C:101:LHG:H223	2.37	0.58
1:4A:55:PHE:CD1	2:4A:101:LHG:H211	2.38	0.58
1:4D:55:PHE:CD1	2:4D:101:LHG:H211	2.38	0.58
1:5E:55:PHE:CD1	2:5E:101:LHG:H211	2.38	0.58
1:2I:24:CYS:SG	2:3J:101:LHG:H331	2.43	0.58
1:2K:55:PHE:CG	2:2K:101:LHG:H223	2.38	0.58
2:2K:101:LHG:C21	2:2K:101:LHG:H372	2.25	0.58
1:4E:55:PHE:CG	2:4E:101:LHG:H223	2.37	0.58
1:4K:55:PHE:CG	2:4K:101:LHG:H223	2.38	0.58
1:4O:55:PHE:CG	2:4O:101:LHG:H223	2.37	0.58
2:5E:101:LHG:H372	2:5E:101:LHG:C21	2.25	0.58
1:5N:55:PHE:CG	2:5N:101:LHG:H223	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1F:55:PHE:CD1	2:1F:101:LHG:H211	2.38	0.58
2:1H:101:LHG:H372	2:1H:101:LHG:C21	2.25	0.58
1:3N:55:PHE:CG	2:3N:101:LHG:H223	2.37	0.58
2:3N:101:LHG:H372	2:3N:101:LHG:C21	2.25	0.58
1:4H:55:PHE:CD1	2:4H:101:LHG:H211	2.38	0.58
1:5D:55:PHE:CG	2:5D:101:LHG:H223	2.37	0.58
1:1G:55:PHE:CG	2:1G:101:LHG:H223	2.37	0.58
1:2D:55:PHE:CD1	2:2D:101:LHG:H211	2.38	0.58
1:2I:55:PHE:CG	2:2I:101:LHG:H223	2.37	0.58
1:3L:55:PHE:CG	2:3L:101:LHG:H223	2.38	0.58
1:4C:55:PHE:CD1	2:4C:101:LHG:H211	2.38	0.58
1:4F:55:PHE:CG	2:4F:101:LHG:H223	2.37	0.58
1:5D:55:PHE:CD1	2:5D:101:LHG:H211	2.38	0.58
2:1D:101:LHG:H372	1:5C:20:PHE:HE2	1.67	0.58
1:3B:55:PHE:CG	2:3B:101:LHG:H223	2.37	0.58
1:4B:55:PHE:CD1	2:4B:101:LHG:H211	2.38	0.58
2:1E:101:LHG:H372	1:5D:20:PHE:HE2	1.65	0.58
1:5J:55:PHE:CD1	2:5J:101:LHG:H211	2.38	0.58
1:1A:55:PHE:CG	2:1A:101:LHG:H223	2.37	0.58
1:2G:55:PHE:CD1	2:2G:101:LHG:H211	2.38	0.58
2:4B:101:LHG:C21	2:4B:101:LHG:H372	2.25	0.58
1:5K:55:PHE:CD1	2:5K:101:LHG:H211	2.38	0.58
1:1B:55:PHE:CD1	2:1B:101:LHG:H211	2.38	0.58
1:1L:55:PHE:CG	2:1L:101:LHG:H223	2.38	0.58
1:1L:55:PHE:CD1	2:1L:101:LHG:H211	2.38	0.58
1:3B:55:PHE:CD1	2:3B:101:LHG:H211	2.38	0.58
1:3F:55:PHE:CD1	2:3F:101:LHG:H211	2.38	0.58
1:4I:55:PHE:CD1	2:4I:101:LHG:H211	2.38	0.58
1:5C:55:PHE:CG	2:5C:101:LHG:H223	2.37	0.58
2:1E:101:LHG:H371	1:5D:20:PHE:CE2	2.38	0.58
1:5I:55:PHE:CG	2:5I:101:LHG:H223	2.38	0.58
1:1M:55:PHE:CD1	2:1M:101:LHG:H211	2.38	0.58
1:2J:55:PHE:CG	2:2J:101:LHG:H223	2.37	0.58
1:1A:55:PHE:CD1	2:1A:101:LHG:H211	2.38	0.58
1:1E:55:PHE:CD1	2:1E:101:LHG:H211	2.38	0.58
1:3A:55:PHE:CD1	2:3A:101:LHG:H211	2.38	0.58
1:3G:55:PHE:CD1	2:3G:101:LHG:H211	2.38	0.58
1:1I:24:CYS:SG	2:2J:101:LHG:H331	2.43	0.57
1:2C:55:PHE:CD1	2:2C:101:LHG:H211	2.38	0.57
1:2N:55:PHE:CD1	2:2N:101:LHG:H211	2.38	0.57
1:2O:55:PHE:CD1	2:2O:101:LHG:H211	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3E:55:PHE:CD1	2:3E:101:LHG:H211	2.38	0.57
1:4C:24:CYS:SG	2:5D:101:LHG:H331	2.44	0.57
1:3M:55:PHE:CG	2:3M:101:LHG:H223	2.37	0.57
1:4G:55:PHE:CD1	2:4G:101:LHG:H211	2.38	0.57
1:1F:55:PHE:CG	2:1F:101:LHG:H223	2.37	0.57
2:1I:101:LHG:H372	1:5H:20:PHE:HE2	1.67	0.57
1:5C:55:PHE:CD1	2:5C:101:LHG:H211	2.38	0.57
1:5I:55:PHE:CD1	2:5I:101:LHG:H211	2.38	0.57
1:5L:55:PHE:HD1	2:5L:101:LHG:C22	2.17	0.57
1:1C:55:PHE:HD1	2:1C:101:LHG:C22	2.18	0.57
1:3C:24:CYS:SG	2:4D:101:LHG:H331	2.44	0.57
1:4K:55:PHE:HD1	2:4K:101:LHG:C22	2.18	0.57
1:2E:55:PHE:CD1	2:2E:101:LHG:H211	2.38	0.57
1:1D:20:PHE:CE2	2:2E:101:LHG:H371	2.38	0.57
1:1D:55:PHE:CD1	2:1D:101:LHG:H211	2.38	0.57
1:2C:24:CYS:SG	2:3D:101:LHG:H331	2.44	0.57
1:1K:55:PHE:CD1	2:1K:101:LHG:H211	2.38	0.57
1:5M:55:PHE:CD1	2:5M:101:LHG:H211	2.38	0.57
1:1C:55:PHE:CD1	2:1C:101:LHG:H211	2.38	0.57
1:1G:47:LEU:HD11	1:5F:31:ILE:HD11	1.87	0.57
1:1G:55:PHE:CD1	2:1G:101:LHG:C21	2.88	0.57
1:1N:55:PHE:CD1	2:1N:101:LHG:H211	2.38	0.57
1:1O:55:PHE:CD1	2:1O:101:LHG:H211	2.38	0.57
1:2A:55:PHE:CD1	2:2A:101:LHG:H211	2.38	0.57
1:3N:55:PHE:CD1	2:3N:101:LHG:C21	2.88	0.57
1:4C:55:PHE:CD1	2:4C:101:LHG:C21	2.88	0.57
1:1C:24:CYS:SG	2:2D:101:LHG:H331	2.44	0.57
1:2J:55:PHE:CD1	2:2J:101:LHG:C21	2.88	0.57
1:3D:20:PHE:CE2	2:4E:101:LHG:H371	2.38	0.57
1:4K:55:PHE:CD1	2:4K:101:LHG:H211	2.38	0.57
1:4L:55:PHE:HD1	2:4L:101:LHG:C22	2.17	0.57
1:4N:55:PHE:CD1	2:4N:101:LHG:C21	2.88	0.57
1:5C:55:PHE:CD1	2:5C:101:LHG:C21	2.88	0.57
1:4B:24:CYS:SG	2:5C:101:LHG:H331	2.45	0.57
1:5G:55:PHE:CD1	2:5G:101:LHG:C21	2.88	0.57
2:5I:101:LHG:C21	2:5I:101:LHG:H372	2.25	0.57
1:5N:55:PHE:CD1	2:5N:101:LHG:H211	2.38	0.57
1:4D:20:PHE:CE2	2:5E:101:LHG:H371	2.38	0.57
1:4J:55:PHE:CD1	2:4J:101:LHG:H211	2.38	0.57
1:5B:55:PHE:CD1	2:5B:101:LHG:H211	2.38	0.57
1:5L:55:PHE:CD1	2:5L:101:LHG:H211	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1B:10:ASP:O	1:1B:13:ALA:N	2.38	0.56
1:1D:55:PHE:HD1	2:1D:101:LHG:C22	2.17	0.56
1:1F:55:PHE:CD1	2:1F:101:LHG:C21	2.88	0.56
1:2B:55:PHE:CD1	2:2B:101:LHG:H211	2.38	0.56
1:2C:10:ASP:O	1:2C:13:ALA:N	2.38	0.56
2:2O:101:LHG:H372	2:2O:101:LHG:C21	2.25	0.56
1:3C:55:PHE:CD1	2:3C:101:LHG:H211	2.38	0.56
1:4B:55:PHE:CD1	2:4B:101:LHG:C21	2.88	0.56
1:5F:55:PHE:CD1	2:5F:101:LHG:C21	2.88	0.56
2:5M:101:LHG:H372	2:5M:101:LHG:C21	2.25	0.56
2:1L:101:LHG:H372	2:1L:101:LHG:C21	2.25	0.56
1:1N:55:PHE:HD1	2:1N:101:LHG:C22	2.17	0.56
1:1A:24:CYS:SG	2:2B:101:LHG:H331	2.45	0.56
1:3D:55:PHE:CD1	2:3D:101:LHG:H211	2.38	0.56
1:3I:55:PHE:CD1	2:3I:101:LHG:H211	2.38	0.56
2:4F:101:LHG:H372	2:4F:101:LHG:C21	2.25	0.56
1:2A:24:CYS:SG	2:3B:101:LHG:H331	2.45	0.56
1:3M:55:PHE:CD1	2:3M:101:LHG:C21	2.88	0.56
1:4E:55:PHE:CD1	2:4E:101:LHG:H211	2.38	0.56
2:4J:101:LHG:H372	2:4J:101:LHG:C21	2.25	0.56
1:4L:55:PHE:CD1	2:4L:101:LHG:H211	2.38	0.56
1:5A:55:PHE:CD1	2:5A:101:LHG:H211	2.38	0.56
1:1M:10:ASP:O	1:1M:13:ALA:N	2.39	0.56
1:3A:10:ASP:O	1:3A:13:ALA:N	2.38	0.56
1:3B:55:PHE:CD1	2:3B:101:LHG:C21	2.88	0.56
2:3C:101:LHG:H372	2:3C:101:LHG:C21	2.25	0.56
1:3G:10:ASP:O	1:3G:13:ALA:N	2.39	0.56
1:2L:20:PHE:HE2	2:3M:101:LHG:H371	1.71	0.56
1:3B:24:CYS:SG	2:4C:101:LHG:H331	2.45	0.56
1:4H:10:ASP:O	1:4H:13:ALA:N	2.39	0.56
1:1O:10:ASP:O	1:1O:13:ALA:N	2.39	0.56
1:2A:10:ASP:O	1:2A:13:ALA:N	2.38	0.56
1:2E:10:ASP:O	1:2E:13:ALA:N	2.39	0.56
1:2M:55:PHE:CD1	2:2M:101:LHG:H211	2.38	0.56
1:4J:10:ASP:O	1:4J:13:ALA:N	2.39	0.56
1:5E:10:ASP:O	1:5E:13:ALA:N	2.38	0.56
1:5G:55:PHE:CD1	2:5G:101:LHG:H211	2.38	0.56
2:1K:101:LHG:H371	1:5J:20:PHE:CE2	2.38	0.56
1:4L:20:PHE:HE2	2:5M:101:LHG:H371	1.71	0.56
1:1D:10:ASP:O	1:1D:13:ALA:N	2.38	0.56
1:1F:47:LEU:HD11	1:5E:31:ILE:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1I:55:PHE:CD1	2:1I:101:LHG:C21	2.88	0.56
1:1L:20:PHE:HE2	2:2M:101:LHG:H371	1.71	0.56
1:2I:55:PHE:CD1	2:2I:101:LHG:C21	2.88	0.56
1:3E:10:ASP:O	1:3E:13:ALA:N	2.39	0.56
1:3H:55:PHE:CD1	2:3H:101:LHG:H211	2.38	0.56
1:4A:10:ASP:O	1:4A:13:ALA:N	2.38	0.56
1:4F:10:ASP:O	1:4F:13:ALA:N	2.38	0.56
1:2P:10:ASP:O	1:2P:13:ALA:N	2.39	0.56
1:3I:10:ASP:O	1:3I:13:ALA:N	2.39	0.56
1:5L:10:ASP:O	1:5L:13:ALA:N	2.39	0.56
1:1B:24:CYS:SG	2:2C:101:LHG:H331	2.45	0.56
1:2D:10:ASP:O	1:2D:13:ALA:N	2.38	0.56
1:2J:10:ASP:O	1:2J:13:ALA:N	2.39	0.56
2:3G:101:LHG:C21	2:3G:101:LHG:H372	2.25	0.56
1:3G:55:PHE:CD1	2:3G:101:LHG:C21	2.88	0.56
2:3K:101:LHG:C21	2:3K:101:LHG:H372	2.25	0.56
1:5A:10:ASP:O	1:5A:13:ALA:N	2.38	0.56
1:5D:10:ASP:O	1:5D:13:ALA:N	2.38	0.56
1:5E:55:PHE:CD1	2:5E:101:LHG:C21	2.88	0.56
1:5F:10:ASP:O	1:5F:13:ALA:N	2.39	0.56
1:1H:47:LEU:HD11	1:5G:31:ILE:HD11	1.88	0.56
1:5H:55:PHE:CD1	2:5H:101:LHG:H211	2.38	0.56
1:1J:55:PHE:CD1	2:1J:101:LHG:H211	2.38	0.56
1:1K:10:ASP:O	1:1K:13:ALA:N	2.39	0.56
1:2I:10:ASP:O	1:2I:13:ALA:N	2.39	0.56
1:2B:24:CYS:SG	2:3C:101:LHG:H331	2.45	0.56
1:3F:10:ASP:O	1:3F:13:ALA:N	2.39	0.56
1:3N:10:ASP:O	1:3N:13:ALA:N	2.39	0.56
1:4B:10:ASP:O	1:4B:13:ALA:N	2.38	0.56
1:4F:55:PHE:CD1	2:4F:101:LHG:H211	2.38	0.56
1:4H:55:PHE:CD1	2:4H:101:LHG:C21	2.88	0.56
2:4N:101:LHG:C21	2:4N:101:LHG:H372	2.25	0.56
1:4N:10:ASP:O	1:4N:13:ALA:N	2.39	0.56
1:4O:10:ASP:O	1:4O:13:ALA:N	2.39	0.56
1:4A:24:CYS:SG	2:5B:101:LHG:H331	2.45	0.56
2:1D:101:LHG:H371	1:5C:20:PHE:CE2	2.41	0.56
1:5I:10:ASP:O	1:5I:13:ALA:N	2.39	0.56
1:5J:10:ASP:O	1:5J:13:ALA:N	2.39	0.56
1:5K:10:ASP:O	1:5K:13:ALA:N	2.39	0.56
1:5N:10:ASP:O	1:5N:13:ALA:N	2.39	0.56
1:1I:10:ASP:O	1:1I:13:ALA:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2H:101:LHG:C21	2:2H:101:LHG:H372	2.25	0.56
1:2N:10:ASP:O	1:2N:13:ALA:N	2.39	0.56
1:3D:10:ASP:O	1:3D:13:ALA:N	2.38	0.56
1:3O:55:PHE:CD1	2:3O:101:LHG:H211	2.38	0.56
1:4D:10:ASP:O	1:4D:13:ALA:N	2.38	0.56
1:1E:10:ASP:O	1:1E:13:ALA:N	2.38	0.56
1:1F:10:ASP:O	1:1F:13:ALA:N	2.39	0.56
1:2F:10:ASP:O	1:2F:13:ALA:N	2.39	0.56
1:3B:10:ASP:O	1:3B:13:ALA:N	2.38	0.56
1:3C:10:ASP:O	1:3C:13:ALA:N	2.38	0.56
1:3M:10:ASP:O	1:3M:13:ALA:N	2.39	0.56
1:4K:55:PHE:CD1	2:4K:101:LHG:C21	2.88	0.56
1:1A:10:ASP:O	1:1A:13:ALA:N	2.38	0.55
1:1C:20:PHE:CE2	2:2D:101:LHG:H371	2.41	0.55
2:2D:101:LHG:C21	2:2D:101:LHG:H372	2.25	0.55
1:2G:10:ASP:O	1:2G:13:ALA:N	2.39	0.55
1:1J:20:PHE:CE2	2:2K:101:LHG:H371	2.39	0.55
1:2L:55:PHE:CD1	2:2L:101:LHG:H211	2.38	0.55
1:3P:10:ASP:O	1:3P:13:ALA:N	2.39	0.55
1:4E:10:ASP:O	1:4E:13:ALA:N	2.39	0.55
1:4G:55:PHE:CD1	2:4G:101:LHG:C21	2.88	0.55
1:4L:10:ASP:O	1:4L:13:ALA:N	2.39	0.55
1:5K:55:PHE:CD1	2:5K:101:LHG:C21	2.88	0.55
1:5N:55:PHE:CD1	2:5N:101:LHG:C21	2.88	0.55
1:1C:55:PHE:CD1	2:1C:101:LHG:C21	2.88	0.55
1:1J:10:ASP:O	1:1J:13:ALA:N	2.39	0.55
1:2F:55:PHE:CD1	2:2F:101:LHG:H211	2.38	0.55
1:2K:10:ASP:O	1:2K:13:ALA:N	2.39	0.55
1:2O:55:PHE:CD1	2:2O:101:LHG:C21	2.88	0.55
1:3A:55:PHE:CD1	2:3A:101:LHG:C21	2.88	0.55
1:3O:10:ASP:O	1:3O:13:ALA:N	2.39	0.55
1:3A:24:CYS:SG	2:4B:101:LHG:H331	2.45	0.55
1:4J:55:PHE:CD1	2:4J:101:LHG:C21	2.88	0.55
1:3L:20:PHE:HE2	2:4M:101:LHG:H371	1.71	0.55
2:5B:101:LHG:H372	2:5B:101:LHG:C21	2.25	0.55
1:5O:55:PHE:CD1	2:5O:101:LHG:H211	2.38	0.55
2:1E:101:LHG:C21	2:1E:101:LHG:H372	2.25	0.55
1:1H:10:ASP:O	1:1H:13:ALA:N	2.39	0.55
1:2O:10:ASP:O	1:2O:13:ALA:N	2.39	0.55
1:4K:10:ASP:O	1:4K:13:ALA:N	2.39	0.55
1:4M:10:ASP:O	1:4M:13:ALA:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5B:10:ASP:O	1:5B:13:ALA:N	2.38	0.55
1:5C:10:ASP:O	1:5C:13:ALA:N	2.38	0.55
2:1A:101:LHG:H372	2:1A:101:LHG:C21	2.25	0.55
1:2H:10:ASP:O	1:2H:13:ALA:N	2.39	0.55
1:3E:55:PHE:CD1	2:3E:101:LHG:C21	2.88	0.55
1:3J:10:ASP:O	1:3J:13:ALA:N	2.39	0.55
1:3O:55:PHE:HD1	2:3O:101:LHG:C22	2.17	0.55
1:4C:10:ASP:O	1:4C:13:ALA:N	2.38	0.55
1:4I:10:ASP:O	1:4I:13:ALA:N	2.39	0.55
2:1M:101:LHG:H371	1:5L:20:PHE:HE2	1.71	0.55
1:5M:10:ASP:O	1:5M:13:ALA:N	2.39	0.55
1:1M:55:PHE:CD1	2:1M:101:LHG:C21	2.88	0.55
1:2B:10:ASP:O	1:2B:13:ALA:N	2.38	0.55
1:2F:55:PHE:CD1	2:2F:101:LHG:C21	2.88	0.55
1:3K:10:ASP:O	1:3K:13:ALA:N	2.39	0.55
1:3N:55:PHE:CD1	2:3N:101:LHG:H211	2.38	0.55
1:4P:10:ASP:O	1:4P:13:ALA:N	2.39	0.55
1:5G:10:ASP:O	1:5G:13:ALA:N	2.39	0.55
1:5H:10:ASP:O	1:5H:13:ALA:N	2.39	0.55
1:1G:10:ASP:O	1:1G:13:ALA:N	2.39	0.55
1:2D:20:PHE:CE2	2:3E:101:LHG:H371	2.38	0.55
1:2J:12:LYS:HB2	1:2K:23:MET:CE	2.37	0.55
1:3H:55:PHE:CD1	2:3H:101:LHG:C21	2.88	0.55
1:3J:55:PHE:CD1	2:3J:101:LHG:C21	2.88	0.55
1:4O:12:LYS:HB2	1:4P:23:MET:CE	2.37	0.55
1:5M:12:LYS:HB2	1:5N:23:MET:CE	2.37	0.55
1:1B:55:PHE:CD1	2:1B:101:LHG:C21	2.88	0.55
1:1G:12:LYS:HB2	1:1H:23:MET:CE	2.37	0.55
1:1F:12:LYS:HB2	1:1G:23:MET:CE	2.37	0.55
1:2K:12:LYS:HB2	1:2L:23:MET:CE	2.37	0.55
1:3H:12:LYS:HB2	1:3I:23:MET:CE	2.37	0.55
1:3I:12:LYS:HB2	1:3J:23:MET:CE	2.37	0.55
1:4C:12:LYS:HB2	1:4D:23:MET:CE	2.37	0.55
1:4J:12:LYS:HB2	1:4K:23:MET:CE	2.37	0.55
1:4K:12:LYS:HB2	1:4L:23:MET:CE	2.37	0.55
1:4L:12:LYS:HB2	1:4M:23:MET:CE	2.37	0.55
1:4M:12:LYS:HB2	1:4N:23:MET:CE	2.37	0.55
1:5A:12:LYS:HB2	1:5B:23:MET:CE	2.37	0.55
1:5G:55:PHE:HD1	2:5G:101:LHG:C22	2.18	0.55
1:5O:12:LYS:HB2	1:5P:23:MET:CE	2.37	0.55
1:1A:55:PHE:CD1	2:1A:101:LHG:C21	2.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1E:12:LYS:HB2	1:1F:23:MET:CE	2.37	0.55
1:1N:10:ASP:O	1:1N:13:ALA:N	2.39	0.55
1:1N:55:PHE:CD1	2:1N:101:LHG:C21	2.88	0.55
1:1O:12:LYS:HB2	1:1P:23:MET:CE	2.37	0.55
1:1O:55:PHE:CD1	2:1O:101:LHG:C21	2.88	0.55
1:1P:10:ASP:O	1:1P:13:ALA:N	2.39	0.55
1:3H:10:ASP:O	1:3H:13:ALA:N	2.39	0.55
1:3J:12:LYS:HB2	1:3K:23:MET:CE	2.37	0.55
1:3M:12:LYS:HB2	1:3N:23:MET:CE	2.37	0.55
1:4B:12:LYS:HB2	1:4C:23:MET:CE	2.37	0.55
1:4I:55:PHE:CD1	2:4I:101:LHG:C21	2.88	0.55
1:4N:12:LYS:HB2	1:4O:23:MET:CE	2.37	0.55
1:5B:12:LYS:HB2	1:5C:23:MET:CE	2.37	0.55
1:5O:10:ASP:O	1:5O:13:ALA:N	2.39	0.55
1:5N:12:LYS:HB2	1:5O:23:MET:CE	2.37	0.55
1:1C:10:ASP:O	1:1C:13:ALA:N	2.38	0.55
1:1L:55:PHE:CD1	2:1L:101:LHG:C21	2.88	0.55
1:1L:10:ASP:O	1:1L:13:ALA:N	2.39	0.55
1:2M:10:ASP:O	1:2M:13:ALA:N	2.39	0.55
1:3F:55:PHE:CD1	2:3F:101:LHG:C21	2.88	0.55
1:3I:55:PHE:CD1	2:3I:101:LHG:C21	2.88	0.55
1:3K:12:LYS:HB2	1:3L:23:MET:CE	2.37	0.55
1:3L:12:LYS:HB2	1:3M:23:MET:CE	2.37	0.55
1:3N:12:LYS:HB2	1:3O:23:MET:CE	2.37	0.55
1:3O:12:LYS:HB2	1:3P:23:MET:CE	2.37	0.55
1:4G:10:ASP:O	1:4G:13:ALA:N	2.39	0.55
1:5L:12:LYS:HB2	1:5M:23:MET:CE	2.37	0.55
1:5M:55:PHE:CD1	2:5M:101:LHG:C21	2.88	0.55
1:1D:12:LYS:HB2	1:1E:23:MET:CE	2.37	0.55
1:1N:12:LYS:HB2	1:1O:23:MET:CE	2.37	0.55
1:2I:12:LYS:HB2	1:2J:23:MET:CE	2.37	0.55
1:2L:12:LYS:HB2	1:2M:23:MET:CE	2.37	0.55
1:3A:12:LYS:HB2	1:3B:23:MET:CE	2.37	0.55
1:3L:10:ASP:O	1:3L:13:ALA:N	2.39	0.55
1:3N:55:PHE:HD1	2:3N:101:LHG:C22	2.17	0.55
1:4I:12:LYS:HB2	1:4J:23:MET:CE	2.37	0.55
1:1E:47:LEU:HD11	1:5D:31:ILE:HD11	1.89	0.55
1:5G:12:LYS:HB2	1:5H:23:MET:CE	2.37	0.55
1:5I:55:PHE:CD1	2:5I:101:LHG:C21	2.88	0.55
1:5K:12:LYS:HB2	1:5L:23:MET:CE	2.37	0.55
2:1C:101:LHG:H371	1:5B:20:PHE:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1M:12:LYS:HB2	1:1N:23:MET:CE	2.37	0.54
1:2E:12:LYS:HB2	1:2F:23:MET:CE	2.37	0.54
1:2L:10:ASP:O	1:2L:13:ALA:N	2.39	0.54
1:2O:12:LYS:HB2	1:2P:23:MET:CE	2.37	0.54
1:4D:12:LYS:HB2	1:4E:23:MET:CE	2.37	0.54
1:5H:55:PHE:CD1	2:5H:101:LHG:C21	2.88	0.54
1:5P:10:ASP:O	1:5P:13:ALA:N	2.39	0.54
1:1H:12:LYS:HB2	1:1I:23:MET:CE	2.37	0.54
1:2F:12:LYS:HB2	1:2G:23:MET:CE	2.37	0.54
1:2G:12:LYS:HB2	1:2H:23:MET:CE	2.37	0.54
1:2N:12:LYS:HB2	1:2O:23:MET:CE	2.37	0.54
1:2M:12:LYS:HB2	1:2N:23:MET:CE	2.37	0.54
1:4O:55:PHE:HD1	2:4O:101:LHG:C22	2.17	0.54
1:5B:55:PHE:CD1	2:5B:101:LHG:C21	2.88	0.54
1:5F:55:PHE:HD1	2:5F:101:LHG:C22	2.18	0.54
1:5F:12:LYS:HB2	1:5G:23:MET:CE	2.37	0.54
1:5J:55:PHE:CD1	2:5J:101:LHG:C21	2.88	0.54
1:1K:12:LYS:HB2	1:1L:23:MET:CE	2.37	0.54
1:1L:12:LYS:HB2	1:1M:23:MET:CE	2.37	0.54
1:1P:12:LYS:NZ	1:1P:64:LYS:HE2	2.23	0.54
1:2D:12:LYS:HB2	1:2E:23:MET:CE	2.37	0.54
1:2H:12:LYS:HB2	1:2I:23:MET:CE	2.37	0.54
1:3B:12:LYS:HB2	1:3C:23:MET:CE	2.37	0.54
1:3G:12:LYS:HB2	1:3H:23:MET:CE	2.37	0.54
1:4A:12:LYS:HB2	1:4B:23:MET:CE	2.37	0.54
1:4K:20:PHE:HE2	2:5L:101:LHG:C37	2.21	0.54
1:5C:12:LYS:HB2	1:5D:23:MET:CE	2.37	0.54
2:1I:101:LHG:H372	2:1I:101:LHG:C21	2.25	0.54
1:2A:55:PHE:CD1	2:2A:101:LHG:C21	2.88	0.54
1:2E:55:PHE:CD1	2:2E:101:LHG:C21	2.88	0.54
2:3O:101:LHG:H372	2:3O:101:LHG:C21	2.25	0.54
1:3P:12:LYS:NZ	1:3P:64:LYS:HE2	2.23	0.54
1:4H:12:LYS:HB2	1:4I:23:MET:CE	2.37	0.54
1:1B:47:LEU:HD11	1:5A:31:ILE:HD11	1.89	0.54
2:5F:101:LHG:C21	2:5F:101:LHG:H372	2.25	0.54
1:5L:55:PHE:CD1	2:5L:101:LHG:C21	2.88	0.54
1:1D:12:LYS:NZ	1:1D:64:LYS:HE2	2.23	0.54
1:1I:12:LYS:HB2	1:1J:23:MET:CE	2.37	0.54
1:1J:12:LYS:HB2	1:1K:23:MET:CE	2.37	0.54
1:2B:55:PHE:CD1	2:2B:101:LHG:C21	2.88	0.54
1:2C:55:PHE:CD1	2:2C:101:LHG:C21	2.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2L:101:LHG:C21	2:2L:101:LHG:H372	2.25	0.54
1:2G:20:PHE:CE2	2:3H:101:LHG:C37	2.85	0.54
1:2J:20:PHE:CE2	2:3K:101:LHG:H371	2.39	0.54
2:4C:101:LHG:C21	2:4C:101:LHG:H372	2.25	0.54
1:5J:12:LYS:HB2	1:5K:23:MET:CE	2.37	0.54
1:5N:12:LYS:NZ	1:5N:64:LYS:HE2	2.23	0.54
1:1C:12:LYS:NZ	1:1C:64:LYS:HE2	2.23	0.54
1:2A:12:LYS:HB2	1:2B:23:MET:CE	2.37	0.54
1:2A:12:LYS:NZ	1:2A:64:LYS:HE2	2.23	0.54
1:2D:55:PHE:CD1	2:2D:101:LHG:C21	2.88	0.54
1:2N:12:LYS:NZ	1:2N:64:LYS:HE2	2.23	0.54
1:3B:12:LYS:NZ	1:3B:64:LYS:HE2	2.23	0.54
1:3D:12:LYS:NZ	1:3D:64:LYS:HE2	2.23	0.54
1:3J:12:LYS:NZ	1:3J:64:LYS:HE2	2.23	0.54
1:3O:12:LYS:NZ	1:3O:64:LYS:HE2	2.23	0.54
1:4L:12:LYS:NZ	1:4L:64:LYS:HE2	2.23	0.54
1:5A:12:LYS:NZ	1:5A:64:LYS:HE2	2.23	0.54
1:5I:12:LYS:NZ	1:5I:64:LYS:HE2	2.23	0.54
1:1A:12:LYS:HB2	1:1B:23:MET:CE	2.37	0.54
1:1B:12:LYS:NZ	1:1B:64:LYS:HE2	2.23	0.54
1:1C:12:LYS:HB2	1:1D:23:MET:CE	2.37	0.54
1:1E:12:LYS:NZ	1:1E:64:LYS:HE2	2.23	0.54
1:1H:12:LYS:NZ	1:1H:64:LYS:HE2	2.23	0.54
1:1K:12:LYS:NZ	1:1K:64:LYS:HE2	2.23	0.54
1:1N:12:LYS:NZ	1:1N:64:LYS:HE2	2.23	0.54
1:1O:12:LYS:NZ	1:1O:64:LYS:HE2	2.23	0.54
1:2G:12:LYS:NZ	1:2G:64:LYS:HE2	2.23	0.54
1:3C:20:PHE:CE2	2:4D:101:LHG:H371	2.41	0.54
1:3I:12:LYS:NZ	1:3I:64:LYS:HE2	2.23	0.54
1:4A:12:LYS:NZ	1:4A:64:LYS:HE2	2.23	0.54
1:4D:12:LYS:NZ	1:4D:64:LYS:HE2	2.23	0.54
1:4O:12:LYS:NZ	1:4O:64:LYS:HE2	2.23	0.54
1:5F:12:LYS:NZ	1:5F:64:LYS:HE2	2.23	0.54
1:5I:12:LYS:HB2	1:5J:23:MET:CE	2.37	0.54
1:5K:12:LYS:NZ	1:5K:64:LYS:HE2	2.23	0.54
1:1G:55:PHE:HD1	2:1G:101:LHG:C22	2.18	0.54
1:1L:12:LYS:NZ	1:1L:64:LYS:HE2	2.23	0.54
1:2B:12:LYS:NZ	1:2B:64:LYS:HE2	2.23	0.54
1:2D:12:LYS:NZ	1:2D:64:LYS:HE2	2.23	0.54
1:2F:12:LYS:NZ	1:2F:64:LYS:HE2	2.23	0.54
1:2H:12:LYS:NZ	1:2H:64:LYS:HE2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2J:12:LYS:NZ	1:2J:64:LYS:HE2	2.23	0.54
1:2M:12:LYS:NZ	1:2M:64:LYS:HE2	2.23	0.54
1:3E:12:LYS:NZ	1:3E:64:LYS:HE2	2.23	0.54
1:3F:12:LYS:NZ	1:3F:64:LYS:HE2	2.23	0.54
1:4G:12:LYS:NZ	1:4G:64:LYS:HE2	2.23	0.54
1:4H:12:LYS:NZ	1:4H:64:LYS:HE2	2.23	0.54
1:4K:12:LYS:NZ	1:4K:64:LYS:HE2	2.23	0.54
1:4L:55:PHE:CD1	2:4L:101:LHG:C21	2.88	0.54
1:5C:12:LYS:NZ	1:5C:64:LYS:HE2	2.23	0.54
1:5D:12:LYS:HB2	1:5E:23:MET:CE	2.37	0.54
1:5E:12:LYS:HB2	1:5F:23:MET:CE	2.37	0.54
1:5H:12:LYS:HB2	1:5I:23:MET:CE	2.37	0.54
1:5J:12:LYS:NZ	1:5J:64:LYS:HE2	2.23	0.54
1:1A:12:LYS:NZ	1:1A:64:LYS:HE2	2.23	0.54
1:1I:12:LYS:NZ	1:1I:64:LYS:HE2	2.23	0.54
1:2C:12:LYS:NZ	1:2C:64:LYS:HE2	2.23	0.54
1:2K:12:LYS:NZ	1:2K:64:LYS:HE2	2.23	0.54
1:2L:12:LYS:NZ	1:2L:64:LYS:HE2	2.23	0.54
1:3A:12:LYS:NZ	1:3A:64:LYS:HE2	2.23	0.54
1:3C:12:LYS:HB2	1:3D:23:MET:CE	2.37	0.54
1:3D:12:LYS:HB2	1:3E:23:MET:CE	2.37	0.54
1:3F:12:LYS:HB2	1:3G:23:MET:CE	2.37	0.54
1:3M:12:LYS:NZ	1:3M:64:LYS:HE2	2.23	0.54
1:3N:12:LYS:NZ	1:3N:64:LYS:HE2	2.23	0.54
1:4G:12:LYS:HB2	1:4H:23:MET:CE	2.37	0.54
1:5A:55:PHE:CD1	2:5A:101:LHG:C21	2.88	0.54
2:1K:101:LHG:H331	1:5J:24:CYS:SG	2.48	0.54
1:1B:12:LYS:HB2	1:1C:23:MET:CE	2.37	0.54
1:2B:12:LYS:HB2	1:2C:23:MET:CE	2.37	0.54
1:2I:12:LYS:NZ	1:2I:64:LYS:HE2	2.23	0.54
1:3C:12:LYS:NZ	1:3C:64:LYS:HE2	2.23	0.54
1:4E:55:PHE:HD1	2:4E:101:LHG:C22	2.18	0.54
1:4I:12:LYS:NZ	1:4I:64:LYS:HE2	2.23	0.54
1:5B:12:LYS:NZ	1:5B:64:LYS:HE2	2.23	0.54
1:5L:12:LYS:NZ	1:5L:64:LYS:HE2	2.23	0.54
1:5M:12:LYS:NZ	1:5M:64:LYS:HE2	2.23	0.54
1:1F:12:LYS:NZ	1:1F:64:LYS:HE2	2.23	0.53
1:2M:55:PHE:HD1	2:2M:101:LHG:C22	2.17	0.53
1:3K:12:LYS:NZ	1:3K:64:LYS:HE2	2.23	0.53
1:3L:12:LYS:NZ	1:3L:64:LYS:HE2	2.23	0.53
1:4F:55:PHE:HD1	2:4F:101:LHG:C22	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4M:55:PHE:CD1	2:4M:101:LHG:C21	2.88	0.53
1:4P:12:LYS:NZ	1:4P:64:LYS:HE2	2.23	0.53
1:5G:12:LYS:NZ	1:5G:64:LYS:HE2	2.23	0.53
1:5P:12:LYS:NZ	1:5P:64:LYS:HE2	2.23	0.53
1:1M:12:LYS:NZ	1:1M:64:LYS:HE2	2.23	0.53
1:2C:12:LYS:HB2	1:2D:23:MET:CE	2.37	0.53
1:2P:12:LYS:NZ	1:2P:64:LYS:HE2	2.23	0.53
1:3D:55:PHE:CD1	2:3D:101:LHG:C21	2.88	0.53
1:4C:12:LYS:NZ	1:4C:64:LYS:HE2	2.23	0.53
1:4E:12:LYS:HB2	1:4F:23:MET:CE	2.37	0.53
1:4N:12:LYS:NZ	1:4N:64:LYS:HE2	2.23	0.53
1:5O:12:LYS:NZ	1:5O:64:LYS:HE2	2.23	0.53
1:1J:12:LYS:NZ	1:1J:64:LYS:HE2	2.23	0.53
1:2E:12:LYS:NZ	1:2E:64:LYS:HE2	2.23	0.53
1:2O:12:LYS:NZ	1:2O:64:LYS:HE2	2.23	0.53
1:3G:12:LYS:NZ	1:3G:64:LYS:HE2	2.23	0.53
1:4F:12:LYS:NZ	1:4F:64:LYS:HE2	2.23	0.53
1:5D:12:LYS:NZ	1:5D:64:LYS:HE2	2.23	0.53
1:5E:12:LYS:NZ	1:5E:64:LYS:HE2	2.23	0.53
1:1D:47:LEU:HD11	1:5C:31:ILE:HD11	1.91	0.53
1:1G:12:LYS:NZ	1:1G:64:LYS:HE2	2.23	0.53
1:3E:12:LYS:HB2	1:3F:23:MET:CE	2.37	0.53
1:3M:55:PHE:HD1	2:3M:101:LHG:C22	2.17	0.53
1:4E:12:LYS:NZ	1:4E:64:LYS:HE2	2.23	0.53
1:4F:12:LYS:HB2	1:4G:23:MET:CE	2.37	0.53
1:3K:20:PHE:HE2	2:4L:101:LHG:C37	2.21	0.53
1:5H:12:LYS:NZ	1:5H:64:LYS:HE2	2.23	0.53
1:4J:20:PHE:CE2	2:5K:101:LHG:H371	2.39	0.53
1:1C:47:LEU:HD11	1:5B:31:ILE:HD11	1.90	0.53
1:4M:12:LYS:NZ	1:4M:64:LYS:HE2	2.23	0.53
1:5E:55:PHE:HD1	2:5E:101:LHG:C22	2.17	0.53
1:4F:20:PHE:HE2	2:5G:101:LHG:H372	1.72	0.53
1:1F:20:PHE:HE2	2:2G:101:LHG:H372	1.72	0.53
1:2N:55:PHE:HD1	2:2N:101:LHG:C22	2.17	0.53
1:4B:12:LYS:NZ	1:4B:64:LYS:HE2	2.23	0.53
1:2M:55:PHE:CD1	2:2M:101:LHG:C21	2.88	0.53
1:3H:12:LYS:NZ	1:3H:64:LYS:HE2	2.23	0.53
1:4C:20:PHE:CE2	2:5D:101:LHG:H371	2.41	0.53
1:4J:12:LYS:NZ	1:4J:64:LYS:HE2	2.23	0.53
1:2C:20:PHE:CE2	2:3D:101:LHG:H371	2.41	0.53
2:5N:101:LHG:C21	2:5N:101:LHG:H372	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5O:55:PHE:CD1	2:5O:101:LHG:C21	2.88	0.53
1:2L:55:PHE:HD1	2:2L:101:LHG:C22	2.17	0.53
1:1K:20:PHE:HE2	2:2L:101:LHG:C37	2.21	0.53
1:2F:20:PHE:CE2	2:3G:101:LHG:C37	2.86	0.53
2:5J:101:LHG:C21	2:5J:101:LHG:H372	2.25	0.53
1:1G:20:PHE:HE2	2:2H:101:LHG:H372	1.73	0.53
2:1M:101:LHG:C21	2:1M:101:LHG:H372	2.25	0.53
2:4K:101:LHG:C21	2:4K:101:LHG:H372	2.25	0.53
1:1I:47:LEU:HD11	1:5H:31:ILE:HD11	1.91	0.53
1:1E:55:PHE:CD1	2:1E:101:LHG:C21	2.88	0.52
2:1G:101:LHG:C37	1:5F:20:PHE:CE2	2.82	0.52
1:3J:20:PHE:CE2	2:4K:101:LHG:H371	2.39	0.52
1:4N:55:PHE:HD1	2:4N:101:LHG:C22	2.17	0.52
2:1J:101:LHG:C37	1:5I:20:PHE:CE2	2.88	0.52
1:1K:55:PHE:CD1	2:1K:101:LHG:C21	2.88	0.52
1:2H:20:PHE:CE2	2:3I:101:LHG:C37	2.87	0.52
1:4B:8:LYS:CD	1:4B:8:LYS:N	2.73	0.52
2:4G:101:LHG:H372	2:4G:101:LHG:C21	2.25	0.52
1:1D:8:LYS:CD	1:1D:8:LYS:N	2.73	0.52
1:1E:8:LYS:N	1:1E:8:LYS:CD	2.73	0.52
1:2H:8:LYS:CD	1:2H:8:LYS:N	2.73	0.52
1:2I:8:LYS:CD	1:2I:8:LYS:N	2.73	0.52
1:2K:20:PHE:HE2	2:3L:101:LHG:C37	2.21	0.52
1:2J:8:LYS:N	1:2J:8:LYS:CD	2.73	0.52
1:3B:20:PHE:CE2	2:4C:101:LHG:H371	2.42	0.52
2:3H:101:LHG:C21	2:3H:101:LHG:H372	2.25	0.52
1:4L:8:LYS:N	1:4L:8:LYS:CD	2.73	0.52
1:1F:55:PHE:HD1	2:1F:101:LHG:C22	2.17	0.52
1:1F:8:LYS:N	1:1F:8:LYS:CD	2.73	0.52
2:2A:101:LHG:H372	2:2A:101:LHG:C21	2.25	0.52
1:2B:20:PHE:CE2	2:3C:101:LHG:H371	2.42	0.52
2:3F:101:LHG:C21	2:3F:101:LHG:C37	2.88	0.52
1:4A:8:LYS:CD	1:4A:8:LYS:N	2.73	0.52
1:4C:8:LYS:N	1:4C:8:LYS:CD	2.73	0.52
1:4E:20:PHE:HE2	2:5F:101:LHG:H372	1.73	0.52
1:4K:8:LYS:N	1:4K:8:LYS:CD	2.73	0.52
1:5O:8:LYS:N	1:5O:8:LYS:CD	2.73	0.52
1:5P:8:LYS:CD	1:5P:8:LYS:N	2.73	0.52
1:1C:8:LYS:CD	1:1C:8:LYS:N	2.73	0.52
2:1N:101:LHG:C21	2:1N:101:LHG:C37	2.88	0.52
2:2M:101:LHG:C37	2:2M:101:LHG:C21	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2N:101:LHG:C21	2:2N:101:LHG:C37	2.88	0.52
2:3D:101:LHG:H372	2:3D:101:LHG:C21	2.25	0.52
1:4M:8:LYS:N	1:4M:8:LYS:CD	2.73	0.52
2:1M:101:LHG:C37	1:5L:20:PHE:HE2	2.23	0.52
1:2A:20:PHE:CE2	2:3B:101:LHG:H371	2.42	0.52
1:2G:8:LYS:CD	1:2G:8:LYS:N	2.73	0.52
1:3H:8:LYS:N	1:3H:8:LYS:CD	2.73	0.52
1:3M:8:LYS:CD	1:3M:8:LYS:N	2.73	0.52
1:3G:15:PHE:CE2	2:4I:101:LHG:H142	2.45	0.52
1:4K:37:TYR:O	1:4K:41:LYS:N	2.40	0.52
1:5A:8:LYS:CD	1:5A:8:LYS:N	2.73	0.52
1:2G:15:PHE:CE2	2:3I:101:LHG:H142	2.45	0.52
1:3I:37:TYR:O	1:3I:41:LYS:N	2.40	0.52
1:3I:8:LYS:N	1:3I:8:LYS:CD	2.73	0.52
2:4E:101:LHG:C37	2:4E:101:LHG:C21	2.88	0.52
2:4F:101:LHG:C37	2:4F:101:LHG:C21	2.88	0.52
1:4J:8:LYS:CD	1:4J:8:LYS:N	2.73	0.52
1:5E:8:LYS:CD	1:5E:8:LYS:N	2.73	0.52
1:1G:8:LYS:CD	1:1G:8:LYS:N	2.73	0.52
2:2E:101:LHG:C37	2:2E:101:LHG:C21	2.88	0.52
2:2E:101:LHG:H372	2:2E:101:LHG:C21	2.25	0.52
1:2K:8:LYS:N	1:2K:8:LYS:CD	2.73	0.52
2:2L:101:LHG:C21	2:2L:101:LHG:C37	2.88	0.52
1:3C:55:PHE:CD1	2:3C:101:LHG:C21	2.88	0.52
1:3G:8:LYS:N	1:3G:8:LYS:CD	2.73	0.52
1:3L:8:LYS:CD	1:3L:8:LYS:N	2.73	0.52
1:3N:8:LYS:CD	1:3N:8:LYS:N	2.73	0.52
1:4G:15:PHE:CE2	2:5I:101:LHG:H142	2.45	0.52
1:4G:20:PHE:HE2	2:5H:101:LHG:H372	1.73	0.52
1:5F:8:LYS:CD	1:5F:8:LYS:N	2.73	0.52
1:1G:20:PHE:CE2	2:2H:101:LHG:C37	2.85	0.51
1:1O:8:LYS:N	1:1O:8:LYS:CD	2.73	0.51
1:1P:8:LYS:CD	1:1P:8:LYS:N	2.73	0.51
2:2O:101:LHG:C37	2:2O:101:LHG:C21	2.88	0.51
1:2F:20:PHE:HE2	2:3G:101:LHG:H372	1.72	0.51
2:4G:101:LHG:C21	2:4G:101:LHG:C37	2.88	0.51
2:4O:101:LHG:C21	2:4O:101:LHG:H372	2.25	0.51
1:4O:37:TYR:O	1:4O:41:LYS:N	2.40	0.51
1:1J:55:PHE:CD1	2:1J:101:LHG:C21	2.88	0.51
1:2G:37:TYR:O	1:2G:41:LYS:N	2.40	0.51
1:3F:20:PHE:HE2	2:4G:101:LHG:H372	1.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3G:101:LHG:C21	2:3G:101:LHG:C37	2.88	0.51
1:4D:8:LYS:N	1:4D:8:LYS:CD	2.73	0.51
1:5D:8:LYS:N	1:5D:8:LYS:CD	2.73	0.51
1:5G:8:LYS:N	1:5G:8:LYS:CD	2.73	0.51
2:5M:101:LHG:C37	2:5M:101:LHG:C21	2.88	0.51
1:5N:8:LYS:N	1:5N:8:LYS:CD	2.73	0.51
2:1B:101:LHG:C21	2:1B:101:LHG:H372	2.25	0.51
1:1B:8:LYS:CD	1:1B:8:LYS:N	2.73	0.51
1:2G:20:PHE:HE2	2:3H:101:LHG:H372	1.73	0.51
1:2K:55:PHE:CD1	2:2K:101:LHG:C21	2.88	0.51
1:3K:8:LYS:N	1:3K:8:LYS:CD	2.73	0.51
2:3L:101:LHG:C21	2:3L:101:LHG:H372	2.25	0.51
2:4D:101:LHG:C37	2:4D:101:LHG:C21	2.88	0.51
2:1B:101:LHG:H371	1:5A:20:PHE:CE2	2.43	0.51
2:1C:101:LHG:C37	2:1C:101:LHG:C21	2.88	0.51
1:1N:8:LYS:CD	1:1N:8:LYS:N	2.73	0.51
2:1O:101:LHG:C21	2:1O:101:LHG:C37	2.88	0.51
1:2F:8:LYS:N	1:2F:8:LYS:CD	2.73	0.51
2:2K:101:LHG:C21	2:2K:101:LHG:C37	2.88	0.51
1:3F:8:LYS:N	1:3F:8:LYS:CD	2.73	0.51
1:3L:55:PHE:HD1	2:3L:101:LHG:C22	2.17	0.51
1:4E:55:PHE:CD1	2:4E:101:LHG:C21	2.88	0.51
2:4H:101:LHG:C21	2:4H:101:LHG:C37	2.87	0.51
1:1E:37:TYR:O	1:1E:41:LYS:N	2.40	0.51
1:1H:55:PHE:CD1	2:1H:101:LHG:C21	2.88	0.51
1:1E:20:PHE:HE2	2:2F:101:LHG:H372	1.73	0.51
1:1H:8:LYS:CD	1:1H:8:LYS:N	2.73	0.51
2:2E:101:LHG:H382	2:2E:101:LHG:H221	1.93	0.51
1:3C:55:PHE:HD1	2:3C:101:LHG:C22	2.18	0.51
1:3D:55:PHE:HD1	2:3D:101:LHG:C22	2.18	0.51
2:3N:101:LHG:H382	2:3N:101:LHG:H221	1.93	0.51
1:3O:8:LYS:CD	1:3O:8:LYS:N	2.73	0.51
2:4D:101:LHG:H221	2:4D:101:LHG:H382	1.93	0.51
1:4I:8:LYS:N	1:4I:8:LYS:CD	2.73	0.51
1:4O:12:LYS:HZ2	1:4O:64:LYS:HE2	1.75	0.51
1:4O:55:PHE:CD1	2:4O:101:LHG:C21	2.88	0.51
1:5H:8:LYS:CD	1:5H:8:LYS:N	2.73	0.51
2:1B:101:LHG:H382	2:1B:101:LHG:H221	1.93	0.51
1:1G:15:PHE:CE2	2:2I:101:LHG:H142	2.45	0.51
2:2D:101:LHG:H382	2:2D:101:LHG:H221	1.93	0.51
1:2L:8:LYS:N	1:2L:8:LYS:CD	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3E:8:LYS:N	1:3E:8:LYS:CD	2.73	0.51
1:4A:55:PHE:CD1	2:4A:101:LHG:C21	2.88	0.51
1:3A:20:PHE:CE2	2:4B:101:LHG:H371	2.42	0.51
1:4P:8:LYS:N	1:4P:8:LYS:CD	2.73	0.51
1:5C:8:LYS:CD	1:5C:8:LYS:N	2.73	0.51
2:1A:101:LHG:H382	2:1A:101:LHG:H221	1.93	0.51
1:1M:8:LYS:CD	1:1M:8:LYS:N	2.73	0.51
2:1N:101:LHG:H221	2:1N:101:LHG:H382	1.93	0.51
2:2A:101:LHG:H382	2:2A:101:LHG:H221	1.93	0.51
1:2A:8:LYS:CD	1:2A:8:LYS:N	2.73	0.51
2:2B:101:LHG:H382	2:2B:101:LHG:H221	1.93	0.51
2:2C:101:LHG:H382	2:2C:101:LHG:H221	1.93	0.51
1:2D:8:LYS:N	1:2D:8:LYS:CD	2.73	0.51
2:2F:101:LHG:C21	2:2F:101:LHG:C37	2.88	0.51
2:2M:101:LHG:H382	2:2M:101:LHG:H221	1.93	0.51
2:2O:101:LHG:H221	2:2O:101:LHG:H382	1.93	0.51
2:3O:101:LHG:C21	2:3O:101:LHG:C37	2.88	0.51
2:4C:101:LHG:C37	2:4C:101:LHG:C21	2.88	0.51
1:4D:55:PHE:CD1	2:4D:101:LHG:C21	2.88	0.51
2:5A:101:LHG:H382	2:5A:101:LHG:H221	1.93	0.51
1:5C:37:TYR:O	1:5C:41:LYS:N	2.40	0.51
1:5D:55:PHE:HD1	2:5D:101:LHG:C22	2.18	0.51
2:1G:101:LHG:H372	1:5F:20:PHE:CE2	2.46	0.51
2:5G:101:LHG:H221	2:5G:101:LHG:H382	1.93	0.51
1:5M:8:LYS:CD	1:5M:8:LYS:N	2.73	0.51
2:1H:101:LHG:H382	2:1H:101:LHG:H221	1.93	0.51
1:1I:8:LYS:CD	1:1I:8:LYS:N	2.73	0.51
2:1J:101:LHG:H221	2:1J:101:LHG:H382	1.93	0.51
1:1J:8:LYS:N	1:1J:8:LYS:CD	2.73	0.51
2:1L:101:LHG:H221	2:1L:101:LHG:H382	1.93	0.51
1:2B:8:LYS:N	1:2B:8:LYS:CD	2.73	0.51
1:2C:8:LYS:N	1:2C:8:LYS:CD	2.73	0.51
1:2E:8:LYS:CD	1:2E:8:LYS:N	2.73	0.51
2:2K:101:LHG:H221	2:2K:101:LHG:H382	1.93	0.51
2:3A:101:LHG:H221	2:3A:101:LHG:H382	1.93	0.51
2:3B:101:LHG:H382	2:3B:101:LHG:H221	1.93	0.51
2:3C:101:LHG:H221	2:3C:101:LHG:H382	1.93	0.51
2:3D:101:LHG:H382	2:3D:101:LHG:H221	1.93	0.51
2:3E:101:LHG:H382	2:3E:101:LHG:H221	1.93	0.51
2:3F:101:LHG:H382	2:3F:101:LHG:H221	1.93	0.51
2:3G:101:LHG:H382	2:3G:101:LHG:H221	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2H:15:PHE:CE2	2:3J:101:LHG:H142	2.46	0.51
1:3L:55:PHE:CD1	2:3L:101:LHG:C21	2.88	0.51
2:3N:101:LHG:C21	2:3N:101:LHG:C37	2.88	0.51
1:3N:37:TYR:O	1:3N:41:LYS:N	2.40	0.51
2:4E:101:LHG:H382	2:4E:101:LHG:H221	1.93	0.51
2:4F:101:LHG:H382	2:4F:101:LHG:H221	1.93	0.51
2:4O:101:LHG:H221	2:4O:101:LHG:H382	1.93	0.51
2:5E:101:LHG:H382	2:5E:101:LHG:H221	1.93	0.51
2:5F:101:LHG:H382	2:5F:101:LHG:H221	1.93	0.51
2:5K:101:LHG:H382	2:5K:101:LHG:H221	1.93	0.51
2:1D:101:LHG:C37	2:1D:101:LHG:C21	2.88	0.51
1:1K:8:LYS:CD	1:1K:8:LYS:N	2.73	0.51
1:1L:8:LYS:N	1:1L:8:LYS:CD	2.73	0.51
2:1O:101:LHG:H221	2:1O:101:LHG:H382	1.93	0.51
1:3A:8:LYS:CD	1:3A:8:LYS:N	2.73	0.51
1:3B:8:LYS:CD	1:3B:8:LYS:N	2.73	0.51
1:3J:8:LYS:N	1:3J:8:LYS:CD	2.73	0.51
1:3P:8:LYS:N	1:3P:8:LYS:CD	2.73	0.51
1:4A:37:TYR:O	1:4A:41:LYS:N	2.40	0.51
2:4B:101:LHG:H382	2:4B:101:LHG:H221	1.93	0.51
2:4C:101:LHG:H382	2:4C:101:LHG:H221	1.93	0.51
1:4E:8:LYS:CD	1:4E:8:LYS:N	2.73	0.51
2:4I:101:LHG:C37	2:4I:101:LHG:C21	2.87	0.51
2:4J:101:LHG:H221	2:4J:101:LHG:H382	1.93	0.51
2:5C:101:LHG:H221	2:5C:101:LHG:H382	1.93	0.51
2:5F:101:LHG:C21	2:5F:101:LHG:C37	2.88	0.51
2:5G:101:LHG:C37	2:5G:101:LHG:C21	2.88	0.51
2:5I:101:LHG:H221	2:5I:101:LHG:H382	1.93	0.51
2:5J:101:LHG:H382	2:5J:101:LHG:H221	1.93	0.51
2:5N:101:LHG:C21	2:5N:101:LHG:C37	2.88	0.51
2:1C:101:LHG:H221	2:1C:101:LHG:H382	1.93	0.50
2:1D:101:LHG:H382	2:1D:101:LHG:H221	1.93	0.50
2:1F:101:LHG:H382	2:1F:101:LHG:H221	1.93	0.50
2:1I:101:LHG:H382	2:1I:101:LHG:H221	1.93	0.50
1:1K:55:PHE:HD1	2:1K:101:LHG:C22	2.17	0.50
2:1M:101:LHG:H221	2:1M:101:LHG:H382	1.93	0.50
2:2L:101:LHG:H382	2:2L:101:LHG:H221	1.93	0.50
1:2L:55:PHE:CD1	2:2L:101:LHG:C21	2.88	0.50
2:2N:101:LHG:H221	2:2N:101:LHG:H382	1.93	0.50
1:3C:8:LYS:CD	1:3C:8:LYS:N	2.73	0.50
1:3D:8:LYS:N	1:3D:8:LYS:CD	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3E:20:PHE:HE2	2:4F:101:LHG:H372	1.73	0.50
2:3H:101:LHG:C21	2:3H:101:LHG:C37	2.88	0.50
1:3H:15:PHE:CE2	2:4J:101:LHG:H142	2.46	0.50
2:3L:101:LHG:H221	2:3L:101:LHG:H382	1.93	0.50
2:3M:101:LHG:C37	2:3M:101:LHG:C21	2.87	0.50
2:3O:101:LHG:H221	2:3O:101:LHG:H382	1.93	0.50
2:4G:101:LHG:H382	2:4G:101:LHG:H221	1.93	0.50
2:4H:101:LHG:H382	2:4H:101:LHG:H221	1.93	0.50
2:4I:101:LHG:H221	2:4I:101:LHG:H382	1.93	0.50
2:4L:101:LHG:C37	2:4L:101:LHG:C21	2.88	0.50
1:4A:20:PHE:CE2	2:5B:101:LHG:H371	2.42	0.50
1:5D:55:PHE:CD1	2:5D:101:LHG:C21	2.88	0.50
1:1H:57:THR:HG21	1:5E:4:LEU:HD11	1.93	0.50
2:5H:101:LHG:C21	2:5H:101:LHG:C37	2.88	0.50
1:5I:8:LYS:CD	1:5I:8:LYS:N	2.73	0.50
1:5K:8:LYS:CD	1:5K:8:LYS:N	2.73	0.50
2:5L:101:LHG:H221	2:5L:101:LHG:H382	1.93	0.50
2:5M:101:LHG:H221	2:5M:101:LHG:H382	1.93	0.50
1:1A:8:LYS:CD	1:1A:8:LYS:N	2.73	0.50
1:1H:15:PHE:CE2	2:2J:101:LHG:H142	2.46	0.50
1:1L:55:PHE:HD1	2:1L:101:LHG:C22	2.17	0.50
2:2J:101:LHG:C37	2:2J:101:LHG:C21	2.88	0.50
1:2P:8:LYS:CD	1:2P:8:LYS:N	2.73	0.50
1:3G:20:PHE:HE2	2:4H:101:LHG:H372	1.73	0.50
2:4N:101:LHG:H382	2:4N:101:LHG:H221	1.93	0.50
1:4O:8:LYS:N	1:4O:8:LYS:CD	2.73	0.50
2:5H:101:LHG:H382	2:5H:101:LHG:H221	1.93	0.50
1:5J:8:LYS:CD	1:5J:8:LYS:N	2.73	0.50
1:4J:24:CYS:SG	2:5K:101:LHG:H331	2.52	0.50
1:5L:8:LYS:CD	1:5L:8:LYS:N	2.73	0.50
2:5N:101:LHG:H221	2:5N:101:LHG:H382	1.93	0.50
2:1K:101:LHG:H221	2:1K:101:LHG:H382	1.93	0.50
1:2D:37:TYR:O	1:2D:41:LYS:N	2.40	0.50
2:2F:101:LHG:H382	2:2F:101:LHG:H221	1.93	0.50
1:2F:15:PHE:CE2	2:3H:101:LHG:H142	2.46	0.50
1:1H:20:PHE:CE2	2:2I:101:LHG:C37	2.87	0.50
1:3F:37:TYR:O	1:3F:41:LYS:N	2.40	0.50
2:3H:101:LHG:H382	2:3H:101:LHG:H221	1.94	0.50
2:4K:101:LHG:H382	2:4K:101:LHG:H221	1.93	0.50
2:5B:101:LHG:H221	2:5B:101:LHG:H382	1.93	0.50
2:5D:101:LHG:H382	2:5D:101:LHG:H221	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5E:101:LHG:C37	2:5E:101:LHG:C21	2.88	0.50
2:1G:101:LHG:H382	2:1G:101:LHG:H221	1.93	0.50
2:2G:101:LHG:H221	2:2G:101:LHG:H382	1.93	0.50
2:2I:101:LHG:H382	2:2I:101:LHG:H221	1.94	0.50
2:2J:101:LHG:H382	2:2J:101:LHG:H221	1.93	0.50
2:3I:101:LHG:H221	2:3I:101:LHG:H382	1.93	0.50
2:3J:101:LHG:H382	2:3J:101:LHG:H221	1.93	0.50
2:3M:101:LHG:H382	2:3M:101:LHG:H221	1.93	0.50
1:4F:15:PHE:CE2	2:5H:101:LHG:H142	2.46	0.50
1:4H:37:TYR:O	1:4H:41:LYS:N	2.40	0.50
1:4H:8:LYS:CD	1:4H:8:LYS:N	2.73	0.50
1:3J:24:CYS:SG	2:4K:101:LHG:H331	2.52	0.50
1:4P:37:TYR:O	1:4P:41:LYS:N	2.40	0.50
2:5I:101:LHG:C37	2:5I:101:LHG:C21	2.87	0.50
2:5O:101:LHG:H221	2:5O:101:LHG:H382	1.93	0.50
2:1A:101:LHG:C37	2:1A:101:LHG:C21	2.88	0.50
2:1E:101:LHG:H382	2:1E:101:LHG:H221	1.93	0.50
1:1J:24:CYS:SG	2:2K:101:LHG:H331	2.52	0.50
1:1P:37:TYR:O	1:1P:41:LYS:N	2.40	0.50
1:1A:20:PHE:CE2	2:2B:101:LHG:H371	2.43	0.50
2:3L:101:LHG:C37	2:3L:101:LHG:C21	2.88	0.50
2:4A:101:LHG:H382	2:4A:101:LHG:H221	1.93	0.50
2:4L:101:LHG:H382	2:4L:101:LHG:H221	1.93	0.50
2:4M:101:LHG:H221	2:4M:101:LHG:H382	1.93	0.50
1:5B:8:LYS:CD	1:5B:8:LYS:N	2.73	0.50
1:1B:37:TYR:O	1:1B:41:LYS:N	2.40	0.50
2:1E:101:LHG:C21	2:1E:101:LHG:C37	2.88	0.50
1:1C:20:PHE:HE2	2:2D:101:LHG:H372	1.77	0.50
1:2M:8:LYS:CD	1:2M:8:LYS:N	2.73	0.50
2:3K:101:LHG:C37	2:3K:101:LHG:C21	2.87	0.50
2:3K:101:LHG:H221	2:3K:101:LHG:H382	1.93	0.50
2:4B:101:LHG:C21	2:4B:101:LHG:C37	2.88	0.50
1:4B:20:PHE:CE2	2:5C:101:LHG:H371	2.42	0.50
1:1F:15:PHE:CE2	2:2H:101:LHG:H142	2.46	0.50
2:2H:101:LHG:H221	2:2H:101:LHG:H382	1.93	0.50
1:2M:37:TYR:O	1:2M:41:LYS:N	2.40	0.50
1:2O:8:LYS:N	1:2O:8:LYS:CD	2.73	0.50
1:3K:55:PHE:CD1	2:3K:101:LHG:C21	2.88	0.50
1:4F:8:LYS:N	1:4F:8:LYS:CD	2.73	0.50
2:4M:101:LHG:C37	2:4M:101:LHG:C21	2.88	0.50
1:4G:20:PHE:CE2	2:5H:101:LHG:C37	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1J:101:LHG:H372	1:5I:20:PHE:HE2	1.74	0.50
1:1F:20:PHE:CE2	2:2G:101:LHG:C37	2.86	0.50
2:2G:101:LHG:C37	2:2G:101:LHG:C21	2.88	0.50
1:3M:12:LYS:HZ2	1:3M:64:LYS:HE2	1.77	0.50
1:4D:20:PHE:HE2	2:5E:101:LHG:H372	1.75	0.50
1:4I:12:LYS:HZ2	1:4I:64:LYS:HE2	1.76	0.50
1:4N:8:LYS:N	1:4N:8:LYS:CD	2.73	0.50
2:5C:101:LHG:C21	2:5C:101:LHG:C37	2.88	0.50
2:5D:101:LHG:C21	2:5D:101:LHG:C37	2.88	0.50
1:1B:20:PHE:CE2	2:2C:101:LHG:H371	2.42	0.50
1:4M:55:PHE:HD1	2:4M:101:LHG:C22	2.17	0.50
1:5J:37:TYR:O	1:5J:41:LYS:N	2.40	0.50
2:5O:101:LHG:C21	2:5O:101:LHG:C37	2.88	0.50
1:1E:55:PHE:HD1	2:1E:101:LHG:C22	2.17	0.49
2:2A:101:LHG:C37	2:2A:101:LHG:C21	2.88	0.49
1:2H:55:PHE:CD1	2:2H:101:LHG:C21	2.88	0.49
1:2E:20:PHE:HE2	2:3F:101:LHG:H372	1.73	0.49
1:4G:8:LYS:N	1:4G:8:LYS:CD	2.73	0.49
1:4F:20:PHE:CE2	2:5G:101:LHG:C37	2.86	0.49
2:5J:101:LHG:C21	2:5J:101:LHG:C37	2.87	0.49
1:5N:37:TYR:O	1:5N:41:LYS:N	2.40	0.49
2:1F:101:LHG:C21	2:1F:101:LHG:C37	2.88	0.49
1:2N:8:LYS:CD	1:2N:8:LYS:N	2.73	0.49
1:3F:15:PHE:CE2	2:4H:101:LHG:H142	2.46	0.49
2:4J:101:LHG:C21	2:4J:101:LHG:C37	2.88	0.49
2:4N:101:LHG:C21	2:4N:101:LHG:C37	2.88	0.49
2:1E:101:LHG:C37	1:5D:20:PHE:CE2	2.89	0.49
1:2J:24:CYS:SG	2:3K:101:LHG:H331	2.52	0.49
1:3M:20:PHE:HE2	2:4N:101:LHG:H371	1.78	0.49
2:4O:101:LHG:C37	2:4O:101:LHG:C21	2.88	0.49
2:1H:101:LHG:H372	1:5G:20:PHE:CE2	2.46	0.49
1:1I:57:THR:HG21	1:5F:4:LEU:HD11	1.95	0.49
1:1B:20:PHE:HE2	2:2C:101:LHG:H372	1.78	0.49
1:2P:12:LYS:HZ1	1:2P:64:LYS:HE2	1.77	0.49
1:3O:37:TYR:O	1:3O:41:LYS:N	2.40	0.49
1:1G:57:THR:HG21	1:5D:4:LEU:HD11	1.94	0.49
2:1G:101:LHG:C37	2:1G:101:LHG:C21	2.88	0.49
1:1L:37:TYR:O	1:1L:41:LYS:N	2.40	0.49
1:1P:47:LEU:HD11	1:5O:31:ILE:HD11	1.94	0.49
2:3I:101:LHG:C21	2:3I:101:LHG:C37	2.87	0.49
1:4H:15:PHE:CE2	2:5J:101:LHG:H142	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4L:37:TYR:O	1:4L:41:LYS:N	2.40	0.49
2:1B:101:LHG:C21	2:1B:101:LHG:C37	2.88	0.49
2:1H:101:LHG:C21	2:1H:101:LHG:C37	2.88	0.49
2:1I:101:LHG:H142	1:5G:15:PHE:CE2	2.47	0.49
1:3J:37:TYR:O	1:3J:41:LYS:N	2.40	0.49
1:3F:20:PHE:CE2	2:4G:101:LHG:C37	2.86	0.49
2:5A:101:LHG:C21	2:5A:101:LHG:C37	2.88	0.49
1:4A:20:PHE:HE2	2:5B:101:LHG:H372	1.77	0.49
2:1F:101:LHG:C37	1:5E:20:PHE:CE2	2.85	0.49
2:2B:101:LHG:C37	2:2B:101:LHG:C21	2.88	0.49
1:3O:55:PHE:CD1	2:3O:101:LHG:C21	2.88	0.49
1:4H:20:PHE:CE2	2:5I:101:LHG:C37	2.87	0.49
2:1I:101:LHG:C37	2:1I:101:LHG:C21	2.87	0.49
1:2H:37:TYR:O	1:2H:41:LYS:N	2.40	0.49
1:2M:20:PHE:HE2	2:3N:101:LHG:H371	1.77	0.49
1:1F:37:TYR:O	1:1F:41:LYS:N	2.40	0.49
2:2H:101:LHG:C21	2:2H:101:LHG:C37	2.88	0.49
1:3D:37:TYR:O	1:3D:41:LYS:N	2.40	0.49
1:4F:37:TYR:O	1:4F:41:LYS:N	2.40	0.49
2:5K:101:LHG:C37	2:5K:101:LHG:C21	2.88	0.49
1:3D:20:PHE:HE2	2:4E:101:LHG:H372	1.75	0.49
1:5D:37:TYR:O	1:5D:41:LYS:N	2.40	0.49
1:1K:37:TYR:O	1:1K:41:LYS:N	2.40	0.48
1:2F:8:LYS:H	1:2F:8:LYS:HD2	1.78	0.48
1:2N:37:TYR:O	1:2N:41:LYS:N	2.40	0.48
1:4B:37:TYR:O	1:4B:41:LYS:N	2.40	0.48
1:4M:20:PHE:HE2	2:5N:101:LHG:H371	1.77	0.48
1:1C:8:LYS:HD2	1:1C:8:LYS:H	1.78	0.48
1:3I:8:LYS:H	1:3I:8:LYS:HD2	1.78	0.48
1:4E:8:LYS:H	1:4E:8:LYS:HD2	1.78	0.48
1:4L:8:LYS:HD2	1:4L:8:LYS:H	1.78	0.48
1:5H:8:LYS:HD2	1:5H:8:LYS:H	1.78	0.48
1:5I:37:TYR:O	1:5I:41:LYS:N	2.40	0.48
2:1J:101:LHG:C37	2:1J:101:LHG:C21	2.88	0.48
2:3A:101:LHG:C21	2:3A:101:LHG:C37	2.88	0.48
1:5O:8:LYS:H	1:5O:8:LYS:HD2	1.78	0.48
1:1K:8:LYS:H	1:1K:8:LYS:HD2	1.78	0.48
2:2C:101:LHG:C21	2:2C:101:LHG:C37	2.88	0.48
1:1H:20:PHE:HE2	2:2I:101:LHG:H372	1.78	0.48
1:3P:37:TYR:O	1:3P:41:LYS:N	2.40	0.48
1:4A:8:LYS:HD2	1:4A:8:LYS:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5C:8:LYS:H	1:5C:8:LYS:HD2	1.78	0.48
2:1O:101:LHG:C37	1:5N:20:PHE:HE2	2.27	0.48
1:2B:37:TYR:O	1:2B:41:LYS:N	2.40	0.48
1:2O:37:TYR:O	1:2O:41:LYS:N	2.40	0.48
1:4H:28:ALA:O	1:4H:32:VAL:HG22	2.14	0.48
2:2I:101:LHG:C37	2:2I:101:LHG:C21	2.87	0.48
1:2M:28:ALA:O	1:2M:32:VAL:HG22	2.14	0.48
1:2N:28:ALA:O	1:2N:32:VAL:HG22	2.14	0.48
1:2N:8:LYS:HD2	1:2N:8:LYS:H	1.78	0.48
2:3B:101:LHG:C21	2:3B:101:LHG:C37	2.88	0.48
1:3B:28:ALA:O	1:3B:32:VAL:HG22	2.14	0.48
1:3H:8:LYS:H	1:3H:8:LYS:HD2	1.78	0.48
1:4C:28:ALA:O	1:4C:32:VAL:HG22	2.14	0.48
1:4E:28:ALA:O	1:4E:32:VAL:HG22	2.14	0.48
1:3E:20:PHE:CE2	2:4F:101:LHG:C37	2.89	0.48
2:4K:101:LHG:C21	2:4K:101:LHG:C37	2.88	0.48
1:5C:55:PHE:HD1	2:5C:101:LHG:C22	2.17	0.48
1:5D:8:LYS:H	1:5D:8:LYS:HD2	1.78	0.48
1:5F:28:ALA:O	1:5F:32:VAL:HG22	2.14	0.48
1:5H:28:ALA:O	1:5H:32:VAL:HG22	2.14	0.48
1:5I:28:ALA:O	1:5I:32:VAL:HG22	2.14	0.48
1:1B:8:LYS:H	1:1B:8:LYS:HD2	1.78	0.48
1:1K:28:ALA:O	1:1K:32:VAL:HG22	2.14	0.48
1:1L:28:ALA:O	1:1L:32:VAL:HG22	2.14	0.48
1:1M:20:PHE:HE2	2:2N:101:LHG:H371	1.77	0.48
1:2A:28:ALA:O	1:2A:32:VAL:HG22	2.14	0.48
1:2G:55:PHE:CD1	2:2G:101:LHG:C21	2.88	0.48
1:3E:28:ALA:O	1:3E:32:VAL:HG22	2.14	0.48
1:3N:28:ALA:O	1:3N:32:VAL:HG22	2.14	0.48
1:4C:20:PHE:HE2	2:5D:101:LHG:H372	1.77	0.48
1:4D:8:LYS:HD2	1:4D:8:LYS:H	1.78	0.48
1:4I:37:TYR:O	1:4I:41:LYS:N	2.40	0.48
1:1F:8:LYS:H	1:1F:8:LYS:HD2	1.78	0.48
1:1G:28:ALA:O	1:1G:32:VAL:HG22	2.14	0.48
1:1J:28:ALA:O	1:1J:32:VAL:HG22	2.14	0.48
2:1K:101:LHG:C37	2:1K:101:LHG:C21	2.88	0.48
1:2O:28:ALA:O	1:2O:32:VAL:HG22	2.14	0.48
1:3A:8:LYS:HD2	1:3A:8:LYS:H	1.78	0.48
1:3B:37:TYR:O	1:3B:41:LYS:N	2.40	0.48
1:3P:28:ALA:O	1:3P:32:VAL:HG22	2.14	0.48
1:4D:28:ALA:O	1:4D:32:VAL:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5G:8:LYS:HD2	1:5G:8:LYS:H	1.78	0.48
1:2B:55:PHE:HD1	2:2B:101:LHG:C22	2.18	0.48
1:2C:28:ALA:O	1:2C:32:VAL:HG22	2.14	0.48
1:2D:28:ALA:O	1:2D:32:VAL:HG22	2.14	0.48
1:2E:15:PHE:CE2	2:3G:101:LHG:H142	2.49	0.48
1:2J:28:ALA:O	1:2J:32:VAL:HG22	2.14	0.48
1:2K:28:ALA:O	1:2K:32:VAL:HG22	2.14	0.48
1:3A:20:PHE:HE2	2:4B:101:LHG:H372	1.77	0.48
1:3A:28:ALA:O	1:3A:32:VAL:HG22	2.14	0.48
1:3D:28:ALA:O	1:3D:32:VAL:HG22	2.14	0.48
1:3G:28:ALA:O	1:3G:32:VAL:HG22	2.14	0.48
1:3G:37:TYR:O	1:3G:41:LYS:N	2.40	0.48
2:3J:101:LHG:C21	2:3J:101:LHG:C37	2.88	0.48
1:4E:37:TYR:O	1:4E:41:LYS:N	2.40	0.48
1:4G:37:TYR:O	1:4G:41:LYS:N	2.40	0.48
1:4K:8:LYS:HD2	1:4K:8:LYS:H	1.78	0.48
1:4O:28:ALA:O	1:4O:32:VAL:HG22	2.14	0.48
1:5D:28:ALA:O	1:5D:32:VAL:HG22	2.14	0.48
1:5G:28:ALA:O	1:5G:32:VAL:HG22	2.14	0.48
1:5K:28:ALA:O	1:5K:32:VAL:HG22	2.14	0.48
2:5L:101:LHG:C37	2:5L:101:LHG:C21	2.88	0.48
1:1G:8:LYS:H	1:1G:8:LYS:HD2	1.78	0.47
1:1I:28:ALA:O	1:1I:32:VAL:HG22	2.14	0.47
1:1J:8:LYS:HD2	1:1J:8:LYS:H	1.78	0.47
1:1M:37:TYR:O	1:1M:41:LYS:N	2.40	0.47
1:2C:8:LYS:H	1:2C:8:LYS:HD2	1.78	0.47
1:1D:20:PHE:HE2	2:2E:101:LHG:H372	1.75	0.47
1:2E:8:LYS:H	1:2E:8:LYS:HD2	1.78	0.47
1:2I:8:LYS:H	1:2I:8:LYS:HD2	1.78	0.47
1:2P:28:ALA:O	1:2P:32:VAL:HG22	2.14	0.47
1:4F:28:ALA:O	1:4F:32:VAL:HG22	2.14	0.47
1:4P:28:ALA:O	1:4P:32:VAL:HG22	2.14	0.47
1:5G:37:TYR:O	1:5G:41:LYS:N	2.40	0.47
1:5K:37:TYR:O	1:5K:41:LYS:N	2.40	0.47
1:1N:28:ALA:O	1:1N:32:VAL:HG22	2.14	0.47
1:1N:12:LYS:HZ2	1:1N:64:LYS:HE2	1.79	0.47
1:2B:8:LYS:H	1:2B:8:LYS:HD2	1.77	0.47
1:2E:37:TYR:O	1:2E:41:LYS:N	2.40	0.47
1:1E:15:PHE:CE2	2:2G:101:LHG:H142	2.49	0.47
1:2H:20:PHE:HE2	2:3I:101:LHG:H372	1.78	0.47
1:3F:28:ALA:O	1:3F:32:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3M:28:ALA:O	1:3M:32:VAL:HG22	2.14	0.47
2:4A:101:LHG:C21	2:4A:101:LHG:C37	2.88	0.47
1:3C:20:PHE:HE2	2:4D:101:LHG:H372	1.77	0.47
1:4E:15:PHE:CE2	2:5G:101:LHG:H142	2.49	0.47
2:5B:101:LHG:C37	2:5B:101:LHG:C21	2.88	0.47
1:5N:8:LYS:H	1:5N:8:LYS:HD2	1.78	0.47
1:1A:28:ALA:O	1:1A:32:VAL:HG22	2.14	0.47
1:2B:28:ALA:O	1:2B:32:VAL:HG22	2.14	0.47
1:2C:55:PHE:HD1	2:2C:101:LHG:C22	2.17	0.47
1:2J:8:LYS:H	1:2J:8:LYS:HD2	1.78	0.47
2:3C:101:LHG:C37	2:3C:101:LHG:C21	2.88	0.47
1:3C:28:ALA:O	1:3C:32:VAL:HG22	2.14	0.47
1:3G:20:PHE:CE2	2:4H:101:LHG:C37	2.85	0.47
1:4J:28:ALA:O	1:4J:32:VAL:HG22	2.14	0.47
1:1E:28:ALA:O	1:1E:32:VAL:HG22	2.14	0.47
1:1H:28:ALA:O	1:1H:32:VAL:HG22	2.14	0.47
1:2H:28:ALA:O	1:2H:32:VAL:HG22	2.14	0.47
1:3D:12:LYS:HZ2	1:3D:64:LYS:HE2	1.77	0.47
1:3L:28:ALA:O	1:3L:32:VAL:HG22	2.14	0.47
1:4A:28:ALA:O	1:4A:32:VAL:HG22	2.14	0.47
1:4K:12:LYS:HZ2	1:4K:64:LYS:HE2	1.79	0.47
1:1C:28:ALA:O	1:1C:32:VAL:HG22	2.14	0.47
1:2C:37:TYR:O	1:2C:41:LYS:N	2.40	0.47
2:2D:101:LHG:C21	2:2D:101:LHG:C37	2.88	0.47
1:2D:20:PHE:HE2	2:3E:101:LHG:H372	1.75	0.47
1:2F:28:ALA:O	1:2F:32:VAL:HG22	2.14	0.47
1:2I:28:ALA:O	1:2I:32:VAL:HG22	2.14	0.47
1:2M:8:LYS:HD2	1:2M:8:LYS:H	1.78	0.47
1:4I:28:ALA:O	1:4I:32:VAL:HG22	2.14	0.47
1:4E:20:PHE:CE2	2:5F:101:LHG:C37	2.89	0.47
2:1J:101:LHG:H142	1:5H:15:PHE:CE2	2.48	0.47
1:5K:8:LYS:H	1:5K:8:LYS:HD2	1.78	0.47
1:5L:8:LYS:HD2	1:5L:8:LYS:H	1.78	0.47
1:5P:28:ALA:O	1:5P:32:VAL:HG22	2.14	0.47
1:1J:47:LEU:HD11	1:5I:31:ILE:HD11	1.97	0.47
2:1L:101:LHG:C37	2:1L:101:LHG:C21	2.88	0.47
1:1M:28:ALA:O	1:1M:32:VAL:HG22	2.14	0.47
1:1N:8:LYS:HD2	1:1N:8:LYS:H	1.78	0.47
1:1O:28:ALA:O	1:1O:32:VAL:HG22	2.14	0.47
1:2J:12:LYS:HZ1	1:2J:64:LYS:HE2	1.79	0.47
1:3I:28:ALA:O	1:3I:32:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3K:28:ALA:O	1:3K:32:VAL:HG22	2.14	0.47
1:4G:28:ALA:O	1:4G:32:VAL:HG22	2.14	0.47
1:5M:28:ALA:O	1:5M:32:VAL:HG22	2.14	0.47
1:1B:28:ALA:O	1:1B:32:VAL:HG22	2.14	0.47
1:1F:28:ALA:O	1:1F:32:VAL:HG22	2.14	0.47
1:1I:37:TYR:O	1:1I:41:LYS:N	2.40	0.47
1:2L:28:ALA:O	1:2L:32:VAL:HG22	2.14	0.47
1:3A:37:TYR:O	1:3A:41:LYS:N	2.40	0.47
1:3B:20:PHE:HE2	2:4C:101:LHG:H372	1.78	0.47
1:3F:8:LYS:H	1:3F:8:LYS:HD2	1.78	0.47
1:3H:12:LYS:HZ2	1:3H:64:LYS:HE2	1.80	0.47
1:4N:28:ALA:O	1:4N:32:VAL:HG22	2.14	0.47
1:1C:37:TYR:O	1:1C:41:LYS:N	2.40	0.47
1:3C:37:TYR:O	1:3C:41:LYS:N	2.40	0.47
1:3L:8:LYS:H	1:3L:8:LYS:HD2	1.78	0.47
1:3P:8:LYS:H	1:3P:8:LYS:HD2	1.78	0.47
1:4B:20:PHE:HE2	2:5C:101:LHG:H372	1.77	0.47
1:4B:28:ALA:O	1:4B:32:VAL:HG22	2.14	0.47
1:5B:28:ALA:O	1:5B:32:VAL:HG22	2.14	0.47
1:5B:8:LYS:HD2	1:5B:8:LYS:H	1.78	0.47
1:5D:12:LYS:HZ2	1:5D:64:LYS:HE2	1.79	0.47
1:2L:37:TYR:O	1:2L:41:LYS:N	2.40	0.47
2:2N:101:LHG:C21	2:2N:101:LHG:H382	2.45	0.47
1:3B:12:LYS:HZ2	1:3B:64:LYS:HE2	1.80	0.47
1:4D:37:TYR:O	1:4D:41:LYS:N	2.40	0.47
1:4H:20:PHE:HE2	2:5I:101:LHG:H372	1.78	0.47
1:4H:8:LYS:H	1:4H:8:LYS:HD2	1.78	0.47
1:4M:28:ALA:O	1:4M:32:VAL:HG22	2.14	0.47
1:5L:28:ALA:O	1:5L:32:VAL:HG22	2.14	0.47
1:1A:37:TYR:O	1:1A:41:LYS:N	2.40	0.47
1:1E:8:LYS:HD2	1:1E:8:LYS:H	1.78	0.47
2:1H:101:LHG:H142	1:5F:15:PHE:CE2	2.49	0.47
1:2H:8:LYS:H	1:2H:8:LYS:HD2	1.78	0.47
1:3E:8:LYS:HD2	1:3E:8:LYS:H	1.78	0.47
1:3M:8:LYS:H	1:3M:8:LYS:HD2	1.78	0.47
1:4L:28:ALA:O	1:4L:32:VAL:HG22	2.14	0.47
1:5C:28:ALA:O	1:5C:32:VAL:HG22	2.14	0.47
1:5N:28:ALA:O	1:5N:32:VAL:HG22	2.14	0.47
2:1E:101:LHG:H382	2:1E:101:LHG:C21	2.45	0.47
1:1F:57:THR:HG21	1:5C:4:LEU:HD11	1.97	0.47
2:1L:101:LHG:H382	2:1L:101:LHG:C21	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1P:28:ALA:O	1:1P:32:VAL:HG22	2.14	0.47
2:2A:101:LHG:H382	2:2A:101:LHG:C21	2.45	0.47
1:2A:20:PHE:HE2	2:3B:101:LHG:H372	1.77	0.47
2:3D:101:LHG:C37	2:3D:101:LHG:C21	2.88	0.47
2:4N:101:LHG:C21	2:4N:101:LHG:H382	2.45	0.47
1:5A:28:ALA:O	1:5A:32:VAL:HG22	2.14	0.47
1:5J:55:PHE:HD1	2:5J:101:LHG:C22	2.17	0.47
2:5N:101:LHG:C21	2:5N:101:LHG:H382	2.45	0.47
1:1D:28:ALA:O	1:1D:32:VAL:HG22	2.14	0.46
1:1J:37:TYR:O	1:1J:41:LYS:N	2.40	0.46
1:1M:12:LYS:HZ1	1:1M:64:LYS:HE2	1.80	0.46
1:2F:31:ILE:HD11	1:3G:47:LEU:HD11	1.98	0.46
2:4B:101:LHG:H382	2:4B:101:LHG:C21	2.45	0.46
1:4C:37:TYR:O	1:4C:41:LYS:N	2.40	0.46
1:3F:31:ILE:HD11	1:4G:47:LEU:HD11	1.98	0.46
2:4M:101:LHG:H382	2:4M:101:LHG:C21	2.45	0.46
1:4O:8:LYS:HD2	1:4O:8:LYS:H	1.78	0.46
2:5C:101:LHG:C21	2:5C:101:LHG:H382	2.45	0.46
1:5E:28:ALA:O	1:5E:32:VAL:HG22	2.14	0.46
2:5J:101:LHG:C21	2:5J:101:LHG:H382	2.45	0.46
1:5J:28:ALA:O	1:5J:32:VAL:HG22	2.14	0.46
2:1N:101:LHG:H371	1:5M:20:PHE:HE2	1.79	0.46
1:5O:28:ALA:O	1:5O:32:VAL:HG22	2.14	0.46
1:5O:12:LYS:HZ1	1:5O:64:LYS:HE2	1.79	0.46
2:1L:101:LHG:H371	1:5K:20:PHE:CE2	2.48	0.46
2:1N:101:LHG:C37	1:5M:20:PHE:HE2	2.28	0.46
2:2C:101:LHG:H382	2:2C:101:LHG:C21	2.45	0.46
1:2E:28:ALA:O	1:2E:32:VAL:HG22	2.14	0.46
2:2G:101:LHG:H382	2:2G:101:LHG:C21	2.45	0.46
2:2H:101:LHG:C21	2:2H:101:LHG:H382	2.45	0.46
2:2I:101:LHG:H382	2:2I:101:LHG:C21	2.45	0.46
2:2M:101:LHG:H382	2:2M:101:LHG:C21	2.45	0.46
1:1N:20:PHE:HE2	2:2O:101:LHG:H371	1.81	0.46
2:3E:101:LHG:H382	2:3E:101:LHG:C21	2.45	0.46
1:3J:28:ALA:O	1:3J:32:VAL:HG22	2.14	0.46
2:3K:101:LHG:H382	2:3K:101:LHG:C21	2.45	0.46
1:3O:28:ALA:O	1:3O:32:VAL:HG22	2.14	0.46
2:4H:101:LHG:C21	2:4H:101:LHG:H382	2.45	0.46
1:4I:8:LYS:H	1:4I:8:LYS:HD2	1.78	0.46
2:4O:101:LHG:C21	2:4O:101:LHG:H382	2.45	0.46
2:5B:101:LHG:H382	2:5B:101:LHG:C21	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5H:12:LYS:HZ1	1:5H:64:LYS:HE2	1.79	0.46
1:1D:55:PHE:CD1	2:1D:101:LHG:C21	2.88	0.46
2:1G:101:LHG:H382	2:1G:101:LHG:C21	2.45	0.46
1:1J:57:THR:HG21	1:5G:4:LEU:HD11	1.98	0.46
2:2B:101:LHG:H382	2:2B:101:LHG:C21	2.45	0.46
1:2G:28:ALA:O	1:2G:32:VAL:HG22	2.14	0.46
1:3E:15:PHE:CE2	2:4G:101:LHG:H142	2.49	0.46
1:3H:28:ALA:O	1:3H:32:VAL:HG22	2.14	0.46
2:3I:101:LHG:C21	2:3I:101:LHG:H382	2.45	0.46
1:3L:20:PHE:HE2	2:4M:101:LHG:C37	2.28	0.46
2:4F:101:LHG:H382	2:4F:101:LHG:C21	2.45	0.46
1:4F:55:PHE:CD1	2:4F:101:LHG:C21	2.88	0.46
2:4L:101:LHG:H382	2:4L:101:LHG:C21	2.45	0.46
1:4P:8:LYS:HD2	1:4P:8:LYS:H	1.78	0.46
2:5A:101:LHG:C21	2:5A:101:LHG:H382	2.45	0.46
1:5O:37:TYR:O	1:5O:41:LYS:N	2.40	0.46
2:1A:101:LHG:H382	2:1A:101:LHG:C21	2.45	0.46
1:1G:37:TYR:O	1:1G:41:LYS:N	2.40	0.46
1:1L:12:LYS:HZ1	1:1L:64:LYS:HE2	1.80	0.46
2:1M:101:LHG:C21	2:1M:101:LHG:C37	2.88	0.46
2:1M:101:LHG:C21	2:1M:101:LHG:H382	2.45	0.46
1:1E:20:PHE:CE2	2:2F:101:LHG:C37	2.89	0.46
1:2I:37:TYR:O	1:2I:41:LYS:N	2.40	0.46
1:1L:20:PHE:HE2	2:2M:101:LHG:C37	2.28	0.46
2:3C:101:LHG:H382	2:3C:101:LHG:C21	2.45	0.46
2:3E:101:LHG:C37	2:3E:101:LHG:C21	2.88	0.46
2:3F:101:LHG:H382	2:3F:101:LHG:C21	2.45	0.46
1:4C:8:LYS:HD2	1:4C:8:LYS:H	1.78	0.46
1:4F:31:ILE:HD11	1:5G:47:LEU:HD11	1.98	0.46
2:4G:101:LHG:H382	2:4G:101:LHG:C21	2.45	0.46
1:4K:28:ALA:O	1:4K:32:VAL:HG22	2.14	0.46
2:5D:101:LHG:C21	2:5D:101:LHG:H382	2.45	0.46
1:5E:37:TYR:O	1:5E:41:LYS:N	2.40	0.46
2:5H:101:LHG:H382	2:5H:101:LHG:C21	2.45	0.46
2:5I:101:LHG:H382	2:5I:101:LHG:C21	2.45	0.46
2:5O:101:LHG:C21	2:5O:101:LHG:H382	2.45	0.46
2:2F:101:LHG:C21	2:2F:101:LHG:H382	2.45	0.46
2:2J:101:LHG:H382	2:2J:101:LHG:C21	2.45	0.46
2:2O:101:LHG:C21	2:2O:101:LHG:H382	2.45	0.46
1:3E:37:TYR:O	1:3E:41:LYS:N	2.40	0.46
1:3I:15:PHE:CE2	2:4K:101:LHG:H142	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3K:37:TYR:O	1:3K:41:LYS:N	2.40	0.46
1:3K:8:LYS:HD2	1:3K:8:LYS:H	1.78	0.46
2:4A:101:LHG:C21	2:4A:101:LHG:H382	2.45	0.46
2:4E:101:LHG:H382	2:4E:101:LHG:C21	2.45	0.46
1:4M:37:TYR:O	1:4M:41:LYS:N	2.40	0.46
1:5A:37:TYR:O	1:5A:41:LYS:N	2.40	0.46
2:5K:101:LHG:H382	2:5K:101:LHG:C21	2.45	0.46
1:5K:55:PHE:HD1	2:5K:101:LHG:C22	2.18	0.46
1:5L:12:LYS:HZ2	1:5L:64:LYS:HE2	1.80	0.46
2:1C:101:LHG:C21	2:1C:101:LHG:H382	2.45	0.46
1:3G:8:LYS:HD2	1:3G:8:LYS:H	1.78	0.46
1:3H:20:PHE:HE2	2:4I:101:LHG:H372	1.78	0.46
2:3L:101:LHG:C21	2:3L:101:LHG:H382	2.45	0.46
2:3M:101:LHG:H382	2:3M:101:LHG:C21	2.45	0.46
2:4K:101:LHG:H382	2:4K:101:LHG:C21	2.45	0.46
1:5F:8:LYS:H	1:5F:8:LYS:HD2	1.78	0.46
2:5G:101:LHG:C21	2:5G:101:LHG:H382	2.45	0.46
1:4L:20:PHE:HE2	2:5M:101:LHG:C37	2.28	0.46
1:1I:8:LYS:H	1:1I:8:LYS:HD2	1.78	0.46
1:1P:8:LYS:H	1:1P:8:LYS:HD2	1.78	0.46
1:2A:8:LYS:H	1:2A:8:LYS:HD2	1.78	0.46
1:1F:31:ILE:HD11	1:2G:47:LEU:HD11	1.98	0.46
1:2L:20:PHE:HE2	2:3M:101:LHG:C37	2.28	0.46
1:2N:55:PHE:CD1	2:2N:101:LHG:C21	2.88	0.46
2:3B:101:LHG:C21	2:3B:101:LHG:H382	2.45	0.46
1:4J:8:LYS:HD2	1:4J:8:LYS:H	1.78	0.46
2:5E:101:LHG:H382	2:5E:101:LHG:C21	2.45	0.46
1:4N:20:PHE:HE2	2:5O:101:LHG:H371	1.81	0.46
2:1K:101:LHG:C21	2:1K:101:LHG:H382	2.45	0.46
2:2D:101:LHG:C21	2:2D:101:LHG:H382	2.45	0.46
1:2D:8:LYS:H	1:2D:8:LYS:HD2	1.78	0.46
2:2K:101:LHG:C21	2:2K:101:LHG:H382	2.45	0.46
1:2P:8:LYS:H	1:2P:8:LYS:HD2	1.78	0.46
2:3J:101:LHG:H382	2:3J:101:LHG:C21	2.45	0.46
2:3N:101:LHG:C21	2:3N:101:LHG:H382	2.45	0.46
2:3O:101:LHG:C21	2:3O:101:LHG:H382	2.45	0.46
2:4D:101:LHG:H382	2:4D:101:LHG:C21	2.45	0.46
1:1A:8:LYS:HD2	1:1A:8:LYS:H	1.78	0.46
2:1D:101:LHG:H382	2:1D:101:LHG:C21	2.45	0.46
2:1F:101:LHG:H382	2:1F:101:LHG:C21	2.45	0.46
1:2E:20:PHE:CE2	2:3F:101:LHG:C37	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3D:20:PHE:CE2	2:4E:101:LHG:C37	2.93	0.46
2:5L:101:LHG:H382	2:5L:101:LHG:C21	2.45	0.46
2:1I:101:LHG:H382	2:1I:101:LHG:C21	2.45	0.46
1:1M:8:LYS:HD2	1:1M:8:LYS:H	1.78	0.46
1:1N:37:TYR:O	1:1N:41:LYS:N	2.40	0.46
2:1O:101:LHG:C21	2:1O:101:LHG:H382	2.45	0.46
1:2A:37:TYR:O	1:2A:41:LYS:N	2.40	0.46
1:2C:20:PHE:HE2	2:3D:101:LHG:H372	1.77	0.46
2:2E:101:LHG:H382	2:2E:101:LHG:C21	2.45	0.46
2:2L:101:LHG:C21	2:2L:101:LHG:H382	2.45	0.46
1:3B:8:LYS:H	1:3B:8:LYS:HD2	1.78	0.46
1:2E:31:ILE:HD11	1:3F:47:LEU:HD11	1.98	0.46
1:3E:31:ILE:HD11	1:4F:47:LEU:HD11	1.98	0.46
2:4J:101:LHG:H382	2:4J:101:LHG:C21	2.45	0.46
2:5F:101:LHG:C21	2:5F:101:LHG:H382	2.45	0.46
1:5H:37:TYR:O	1:5H:41:LYS:N	2.40	0.46
1:1G:14:THR:HG21	1:2I:54:VAL:HG11	1.97	0.45
1:1I:15:PHE:CE2	2:2K:101:LHG:H142	2.51	0.45
1:1J:54:VAL:O	1:1J:58:VAL:HG22	2.17	0.45
1:2B:20:PHE:HE2	2:3C:101:LHG:H372	1.78	0.45
1:2B:54:VAL:O	1:2B:58:VAL:HG22	2.17	0.45
1:2D:54:VAL:O	1:2D:58:VAL:HG22	2.16	0.45
1:2K:37:TYR:O	1:2K:41:LYS:N	2.40	0.45
1:2L:8:LYS:H	1:2L:8:LYS:HD2	1.78	0.45
1:2P:37:TYR:O	1:2P:41:LYS:N	2.40	0.45
2:3A:101:LHG:C21	2:3A:101:LHG:H382	2.45	0.45
2:3D:101:LHG:H382	2:3D:101:LHG:C21	2.45	0.45
1:3E:54:VAL:O	1:3E:58:VAL:HG22	2.16	0.45
1:3F:54:VAL:O	1:3F:58:VAL:HG22	2.17	0.45
1:4G:14:THR:HG21	1:5I:54:VAL:HG11	1.97	0.45
1:4I:15:PHE:CE2	2:5K:101:LHG:H142	2.51	0.45
1:4I:54:VAL:O	1:4I:58:VAL:HG22	2.17	0.45
1:4N:8:LYS:H	1:4N:8:LYS:HD2	1.78	0.45
1:3N:20:PHE:HE2	2:4O:101:LHG:H371	1.80	0.45
1:5M:8:LYS:H	1:5M:8:LYS:HD2	1.78	0.45
2:1B:101:LHG:C21	2:1B:101:LHG:H382	2.45	0.45
1:1G:12:LYS:HZ2	1:1G:64:LYS:HE2	1.80	0.45
1:1I:54:VAL:O	1:1I:58:VAL:HG22	2.17	0.45
1:3D:8:LYS:H	1:3D:8:LYS:HD2	1.78	0.45
1:3P:54:VAL:O	1:3P:58:VAL:HG22	2.17	0.45
1:4D:54:VAL:O	1:4D:58:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3G:31:ILE:HD11	1:4H:47:LEU:HD11	1.99	0.45
1:4J:54:VAL:O	1:4J:58:VAL:HG22	2.17	0.45
1:4N:12:LYS:HZ1	1:4N:64:LYS:HE2	1.80	0.45
1:5F:54:VAL:O	1:5F:58:VAL:HG22	2.16	0.45
1:5G:54:VAL:O	1:5G:58:VAL:HG22	2.17	0.45
1:5L:37:TYR:O	1:5L:41:LYS:N	2.40	0.45
1:5L:54:VAL:O	1:5L:58:VAL:HG22	2.17	0.45
1:1A:54:VAL:O	1:1A:58:VAL:HG22	2.17	0.45
2:1J:101:LHG:C21	2:1J:101:LHG:H382	2.45	0.45
1:1M:54:VAL:O	1:1M:58:VAL:HG22	2.17	0.45
2:1N:101:LHG:C21	2:1N:101:LHG:H382	2.45	0.45
1:1O:54:VAL:O	1:1O:58:VAL:HG22	2.17	0.45
1:1P:54:VAL:O	1:1P:58:VAL:HG22	2.17	0.45
1:2C:54:VAL:O	1:2C:58:VAL:HG22	2.17	0.45
1:1E:31:ILE:HD11	1:2F:47:LEU:HD11	1.99	0.45
1:2M:54:VAL:O	1:2M:58:VAL:HG22	2.17	0.45
1:2P:54:VAL:O	1:2P:58:VAL:HG22	2.17	0.45
1:3C:54:VAL:O	1:3C:58:VAL:HG22	2.17	0.45
2:3G:101:LHG:C21	2:3G:101:LHG:H382	2.45	0.45
1:3H:14:THR:HG21	1:4J:54:VAL:HG11	1.98	0.45
1:4B:12:LYS:HZ1	1:4B:64:LYS:HE2	1.81	0.45
2:4C:101:LHG:H382	2:4C:101:LHG:C21	2.45	0.45
1:4F:54:VAL:O	1:4F:58:VAL:HG22	2.17	0.45
1:4H:54:VAL:O	1:4H:58:VAL:HG22	2.17	0.45
1:5A:54:VAL:O	1:5A:58:VAL:HG22	2.17	0.45
1:5F:12:LYS:HZ2	1:5F:64:LYS:HE2	1.81	0.45
1:4G:31:ILE:HD11	1:5H:47:LEU:HD11	1.99	0.45
1:5J:8:LYS:H	1:5J:8:LYS:HD2	1.78	0.45
1:1D:15:PHE:CE2	2:2F:101:LHG:H142	2.52	0.45
1:1D:54:VAL:O	1:1D:58:VAL:HG22	2.17	0.45
1:1E:54:VAL:O	1:1E:58:VAL:HG22	2.16	0.45
1:1K:54:VAL:O	1:1K:58:VAL:HG22	2.17	0.45
1:2A:54:VAL:O	1:2A:58:VAL:HG22	2.17	0.45
1:2E:12:LYS:HZ2	1:2E:64:LYS:HE2	1.81	0.45
1:2H:14:THR:HG21	1:3J:54:VAL:HG11	1.98	0.45
1:2L:54:VAL:O	1:2L:58:VAL:HG22	2.17	0.45
1:2N:54:VAL:O	1:2N:58:VAL:HG22	2.17	0.45
1:3G:14:THR:HG21	1:4I:54:VAL:HG11	1.97	0.45
1:3G:54:VAL:O	1:3G:58:VAL:HG22	2.17	0.45
2:3H:101:LHG:H382	2:3H:101:LHG:C21	2.45	0.45
1:2N:20:PHE:HE2	2:3O:101:LHG:H371	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4C:54:VAL:O	1:4C:58:VAL:HG22	2.17	0.45
1:4E:31:ILE:HD11	1:5F:47:LEU:HD11	1.98	0.45
1:4E:12:LYS:HZ1	1:4E:64:LYS:HE2	1.79	0.45
1:4G:8:LYS:H	1:4G:8:LYS:HD2	1.78	0.45
1:5B:54:VAL:O	1:5B:58:VAL:HG22	2.17	0.45
1:5F:37:TYR:O	1:5F:41:LYS:N	2.40	0.45
1:5J:54:VAL:O	1:5J:58:VAL:HG22	2.17	0.45
2:5M:101:LHG:H382	2:5M:101:LHG:C21	2.45	0.45
1:5M:54:VAL:O	1:5M:58:VAL:HG22	2.17	0.45
2:1H:101:LHG:H382	2:1H:101:LHG:C21	2.45	0.45
1:2G:31:ILE:HD11	1:3H:47:LEU:HD11	1.99	0.45
1:2H:54:VAL:O	1:2H:58:VAL:HG22	2.17	0.45
1:3D:54:VAL:O	1:3D:58:VAL:HG22	2.17	0.45
1:3O:54:VAL:O	1:3O:58:VAL:HG22	2.17	0.45
1:2G:54:VAL:O	1:2G:58:VAL:HG22	2.17	0.45
1:3A:54:VAL:O	1:3A:58:VAL:HG22	2.17	0.45
1:2A:31:ILE:HD11	1:3B:47:LEU:HD11	1.99	0.45
1:3K:54:VAL:O	1:3K:58:VAL:HG22	2.17	0.45
1:3O:8:LYS:HD2	1:3O:8:LYS:H	1.78	0.45
1:4A:12:LYS:HZ2	1:4A:64:LYS:HE2	1.80	0.45
1:5B:55:PHE:HD1	2:5B:101:LHG:C22	2.18	0.45
1:5I:54:VAL:O	1:5I:58:VAL:HG22	2.17	0.45
1:5K:54:VAL:O	1:5K:58:VAL:HG22	2.17	0.45
1:1C:54:VAL:O	1:1C:58:VAL:HG22	2.17	0.45
1:1N:54:VAL:O	1:1N:58:VAL:HG22	2.17	0.45
1:1O:8:LYS:H	1:1O:8:LYS:HD2	1.78	0.45
1:3G:12:LYS:HZ2	1:3G:64:LYS:HE2	1.82	0.45
1:4G:54:VAL:O	1:4G:58:VAL:HG22	2.17	0.45
2:4I:101:LHG:C21	2:4I:101:LHG:H382	2.45	0.45
1:5G:12:LYS:HZ2	1:5G:64:LYS:HE2	1.81	0.45
1:5H:54:VAL:O	1:5H:58:VAL:HG22	2.17	0.45
2:5I:101:LHG:C38	2:5I:101:LHG:H212	2.47	0.45
1:1A:20:PHE:HE2	2:2B:101:LHG:H372	1.77	0.45
1:1H:37:TYR:O	1:1H:41:LYS:N	2.40	0.45
1:2C:12:LYS:HZ2	1:2C:64:LYS:HE2	1.82	0.45
2:2N:101:LHG:C38	2:2N:101:LHG:H212	2.47	0.45
1:3H:54:VAL:O	1:3H:58:VAL:HG22	2.17	0.45
1:3J:54:VAL:O	1:3J:58:VAL:HG22	2.17	0.45
1:4E:54:VAL:O	1:4E:58:VAL:HG22	2.16	0.45
1:4J:37:TYR:O	1:4J:41:LYS:N	2.40	0.45
1:4K:54:VAL:O	1:4K:58:VAL:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4N:54:VAL:O	1:4N:58:VAL:HG22	2.17	0.45
1:4A:31:ILE:HD11	1:5B:47:LEU:HD11	1.99	0.45
1:5E:54:VAL:O	1:5E:58:VAL:HG22	2.16	0.45
1:5N:54:VAL:O	1:5N:58:VAL:HG22	2.17	0.45
1:1H:54:VAL:O	1:1H:58:VAL:HG22	2.17	0.45
2:2B:101:LHG:H212	2:2B:101:LHG:C38	2.47	0.45
2:2O:101:LHG:C38	2:2O:101:LHG:H212	2.47	0.45
2:3D:101:LHG:C38	2:3D:101:LHG:H212	2.47	0.45
1:2G:14:THR:HG21	1:3I:54:VAL:HG11	1.97	0.45
1:3L:54:VAL:O	1:3L:58:VAL:HG22	2.17	0.45
1:4B:54:VAL:O	1:4B:58:VAL:HG22	2.17	0.45
2:4H:101:LHG:H212	2:4H:101:LHG:C38	2.47	0.45
1:4O:54:VAL:O	1:4O:58:VAL:HG22	2.17	0.45
2:1L:101:LHG:H331	1:5K:24:CYS:SG	2.57	0.45
1:1F:54:VAL:O	1:1F:58:VAL:HG22	2.16	0.45
2:1J:101:LHG:C38	2:1J:101:LHG:H212	2.47	0.45
1:1A:31:ILE:HD11	1:2B:47:LEU:HD11	1.99	0.45
1:2D:15:PHE:CE2	2:3F:101:LHG:H142	2.52	0.45
1:2I:54:VAL:O	1:2I:58:VAL:HG22	2.17	0.45
1:2K:54:VAL:O	1:2K:58:VAL:HG22	2.17	0.45
1:3A:31:ILE:HD11	1:4B:47:LEU:HD11	1.99	0.45
1:5C:54:VAL:O	1:5C:58:VAL:HG22	2.17	0.45
1:1D:8:LYS:H	1:1D:8:LYS:HD2	1.78	0.44
2:2C:101:LHG:H212	2:2C:101:LHG:C38	2.47	0.44
1:2E:54:VAL:O	1:2E:58:VAL:HG22	2.16	0.44
1:2F:54:VAL:O	1:2F:58:VAL:HG22	2.17	0.44
2:2H:101:LHG:C38	2:2H:101:LHG:H212	2.47	0.44
1:2J:37:TYR:O	1:2J:41:LYS:N	2.40	0.44
1:1N:20:PHE:HE2	2:2O:101:LHG:C37	2.31	0.44
1:2O:54:VAL:O	1:2O:58:VAL:HG22	2.17	0.44
2:3C:101:LHG:H212	2:3C:101:LHG:C38	2.47	0.44
1:3H:20:PHE:CE2	2:4I:101:LHG:C37	2.87	0.44
2:4M:101:LHG:C38	2:4M:101:LHG:H212	2.47	0.44
1:4M:54:VAL:O	1:4M:58:VAL:HG22	2.17	0.44
1:5A:8:LYS:H	1:5A:8:LYS:HD2	1.78	0.44
2:5J:101:LHG:H212	2:5J:101:LHG:C38	2.47	0.44
1:1H:14:THR:HG21	1:2J:54:VAL:HG11	1.98	0.44
1:1L:54:VAL:O	1:1L:58:VAL:HG22	2.17	0.44
2:1M:101:LHG:C38	2:1M:101:LHG:H212	2.47	0.44
2:1N:101:LHG:C38	2:1N:101:LHG:H212	2.47	0.44
2:2I:101:LHG:H212	2:2I:101:LHG:C38	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3B:54:VAL:O	1:3B:58:VAL:HG22	2.17	0.44
1:3D:15:PHE:HB2	1:3E:27:ILE:HD11	2.00	0.44
2:3O:101:LHG:H212	2:3O:101:LHG:C38	2.47	0.44
2:4E:101:LHG:C38	2:4E:101:LHG:H212	2.47	0.44
1:4G:15:PHE:HB2	1:4H:27:ILE:HD11	1.99	0.44
1:4H:12:LYS:HZ1	1:4H:64:LYS:HE2	1.81	0.44
2:4L:101:LHG:C38	2:4L:101:LHG:H212	2.47	0.44
1:3K:20:PHE:CE2	2:4L:101:LHG:H371	2.49	0.44
2:4N:101:LHG:H212	2:4N:101:LHG:C38	2.47	0.44
2:5H:101:LHG:H212	2:5H:101:LHG:C38	2.47	0.44
1:1G:31:ILE:HD11	1:2H:47:LEU:HD11	1.99	0.44
2:1I:101:LHG:H372	1:5H:20:PHE:CE2	2.49	0.44
2:1K:101:LHG:C38	2:1K:101:LHG:H212	2.47	0.44
1:1M:15:PHE:HB2	1:1N:27:ILE:HD11	1.99	0.44
1:1O:37:TYR:O	1:1O:41:LYS:N	2.40	0.44
1:2F:14:THR:HG21	1:3H:54:VAL:HG11	1.99	0.44
1:3D:15:PHE:CE2	2:4F:101:LHG:H142	2.52	0.44
1:3I:54:VAL:O	1:3I:58:VAL:HG22	2.17	0.44
1:3J:49:LEU:O	1:3J:53:ILE:HG12	2.18	0.44
1:3N:54:VAL:O	1:3N:58:VAL:HG22	2.17	0.44
2:4I:101:LHG:C38	2:4I:101:LHG:H212	2.47	0.44
1:4M:49:LEU:O	1:4M:53:ILE:HG12	2.18	0.44
2:5C:101:LHG:H212	2:5C:101:LHG:C38	2.47	0.44
1:4I:20:PHE:CE2	2:5J:101:LHG:C37	2.93	0.44
1:5P:54:VAL:O	1:5P:58:VAL:HG22	2.17	0.44
2:1A:101:LHG:C38	2:1A:101:LHG:H212	2.47	0.44
1:1D:49:LEU:O	1:1D:53:ILE:HG12	2.18	0.44
1:1O:49:LEU:O	1:1O:53:ILE:HG12	2.18	0.44
1:2A:15:PHE:HB2	1:2B:27:ILE:HD11	2.00	0.44
2:2G:101:LHG:H212	2:2G:101:LHG:C38	2.47	0.44
1:2I:15:PHE:CE2	2:3K:101:LHG:H142	2.51	0.44
2:3G:101:LHG:H212	2:3G:101:LHG:C38	2.47	0.44
2:4D:101:LHG:C38	2:4D:101:LHG:H212	2.47	0.44
1:4D:15:PHE:CE2	2:5F:101:LHG:H142	2.52	0.44
1:4F:14:THR:HG21	1:5H:54:VAL:HG11	1.99	0.44
2:4G:101:LHG:H212	2:4G:101:LHG:C38	2.47	0.44
1:3E:4:LEU:HD11	1:4H:57:THR:HG21	2.00	0.44
1:4H:15:PHE:HB2	1:4I:27:ILE:HD11	1.99	0.44
1:4P:54:VAL:O	1:4P:58:VAL:HG22	2.17	0.44
2:5B:101:LHG:C38	2:5B:101:LHG:H212	2.47	0.44
1:5J:15:PHE:HB2	1:5K:27:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5K:15:PHE:HB2	1:5L:27:ILE:HD11	1.99	0.44
1:5L:49:LEU:O	1:5L:53:ILE:HG12	2.18	0.44
1:1B:55:PHE:HD1	2:1B:101:LHG:C22	2.17	0.44
2:1I:101:LHG:H212	2:1I:101:LHG:C38	2.47	0.44
1:1N:15:PHE:HB2	1:1O:27:ILE:HD11	1.99	0.44
1:2A:8:LYS:CD	1:2A:8:LYS:H	2.31	0.44
1:2G:49:LEU:O	1:2G:53:ILE:HG12	2.18	0.44
1:2G:8:LYS:H	1:2G:8:LYS:HD2	1.78	0.44
2:2J:101:LHG:C38	2:2J:101:LHG:H212	2.47	0.44
1:2O:12:LYS:HZ2	1:2O:64:LYS:HE2	1.82	0.44
1:3H:37:TYR:O	1:3H:41:LYS:N	2.40	0.44
1:4H:14:THR:HG21	1:5J:54:VAL:HG11	1.98	0.44
1:4I:49:LEU:O	1:4I:53:ILE:HG12	2.18	0.44
2:4O:101:LHG:H212	2:4O:101:LHG:C38	2.47	0.44
1:5A:49:LEU:O	1:5A:53:ILE:HG12	2.18	0.44
2:5D:101:LHG:H212	2:5D:101:LHG:C38	2.47	0.44
1:5O:49:LEU:O	1:5O:53:ILE:HG12	2.18	0.44
1:5P:49:LEU:O	1:5P:53:ILE:HG12	2.18	0.44
2:1B:101:LHG:C38	2:1B:101:LHG:H212	2.47	0.44
1:1B:54:VAL:O	1:1B:58:VAL:HG22	2.17	0.44
1:1P:49:LEU:O	1:1P:53:ILE:HG12	2.18	0.44
1:2B:15:PHE:HB2	1:2C:27:ILE:HD11	1.99	0.44
2:2F:101:LHG:H212	2:2F:101:LHG:C38	2.47	0.44
2:2K:101:LHG:C38	2:2K:101:LHG:H212	2.47	0.44
1:2D:31:ILE:HD11	1:3E:47:LEU:HD11	2.00	0.44
1:3E:15:PHE:HB2	1:3F:27:ILE:HD11	2.00	0.44
1:3O:15:PHE:HB2	1:3P:27:ILE:HD11	1.99	0.44
2:4A:101:LHG:H212	2:4A:101:LHG:C38	2.47	0.44
1:4B:8:LYS:H	1:4B:8:LYS:HD2	1.77	0.44
1:4F:15:PHE:HB2	1:4G:27:ILE:HD11	1.99	0.44
2:4K:101:LHG:H212	2:4K:101:LHG:C38	2.47	0.44
1:4K:49:LEU:O	1:4K:53:ILE:HG12	2.18	0.44
1:4L:49:LEU:O	1:4L:53:ILE:HG12	2.18	0.44
2:5A:101:LHG:H212	2:5A:101:LHG:C38	2.47	0.44
1:5M:49:LEU:O	1:5M:53:ILE:HG12	2.18	0.44
2:2A:101:LHG:C38	2:2A:101:LHG:H212	2.47	0.44
1:2E:49:LEU:O	1:2E:53:ILE:HG12	2.18	0.44
2:2L:101:LHG:H212	2:2L:101:LHG:C38	2.47	0.44
1:3B:8:LYS:H	1:3B:8:LYS:CD	2.31	0.44
1:3C:8:LYS:H	1:3C:8:LYS:CD	2.31	0.44
1:3H:49:LEU:O	1:3H:53:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3J:8:LYS:HD2	1:3J:8:LYS:H	1.78	0.44
1:3K:49:LEU:O	1:3K:53:ILE:HG12	2.18	0.44
1:3M:54:VAL:O	1:3M:58:VAL:HG22	2.17	0.44
1:3D:31:ILE:HD11	1:4E:47:LEU:HD11	2.00	0.44
1:4G:8:LYS:H	1:4G:8:LYS:CD	2.31	0.44
1:4H:8:LYS:H	1:4H:8:LYS:CD	2.31	0.44
2:4J:101:LHG:C38	2:4J:101:LHG:H212	2.47	0.44
1:4J:49:LEU:O	1:4J:53:ILE:HG12	2.18	0.44
2:5F:101:LHG:C38	2:5F:101:LHG:H212	2.47	0.44
1:5I:8:LYS:CD	1:5I:8:LYS:H	2.31	0.44
2:5L:101:LHG:H212	2:5L:101:LHG:C38	2.47	0.44
1:4K:20:PHE:CE2	2:5L:101:LHG:H371	2.49	0.44
2:1O:101:LHG:H371	1:5N:20:PHE:HE2	1.83	0.44
2:5O:101:LHG:C38	2:5O:101:LHG:H212	2.47	0.44
1:1C:49:LEU:O	1:1C:53:ILE:HG12	2.18	0.44
1:1D:31:ILE:HD11	1:2E:47:LEU:HD11	2.00	0.44
1:1G:54:VAL:O	1:1G:58:VAL:HG22	2.17	0.44
1:1J:8:LYS:H	1:1J:8:LYS:CD	2.31	0.44
1:2C:49:LEU:O	1:2C:53:ILE:HG12	2.18	0.44
1:2J:54:VAL:O	1:2J:58:VAL:HG22	2.17	0.44
2:2M:101:LHG:H212	2:2M:101:LHG:C38	2.47	0.44
1:2M:15:PHE:HB2	1:2N:27:ILE:HD11	1.99	0.44
1:2L:15:PHE:HB2	1:2M:27:ILE:HD11	1.99	0.44
1:3C:15:PHE:HB2	1:3D:27:ILE:HD11	2.00	0.44
1:2D:20:PHE:CE2	2:3E:101:LHG:C37	2.93	0.44
2:3E:101:LHG:H212	2:3E:101:LHG:C38	2.47	0.44
1:3F:49:LEU:O	1:3F:53:ILE:HG12	2.18	0.44
1:3I:49:LEU:O	1:3I:53:ILE:HG12	2.18	0.44
2:4B:101:LHG:C38	2:4B:101:LHG:H212	2.47	0.44
1:3N:20:PHE:HE2	2:4O:101:LHG:C37	2.30	0.44
1:5H:8:LYS:CD	1:5H:8:LYS:H	2.31	0.44
1:5I:12:LYS:HZ2	1:5I:64:LYS:HE2	1.81	0.44
1:5I:15:PHE:HB2	1:5J:27:ILE:HD11	2.00	0.44
1:1A:55:PHE:HD1	2:1A:101:LHG:C22	2.17	0.44
1:1B:15:PHE:HB2	1:1C:27:ILE:HD11	1.99	0.44
1:1E:12:LYS:HZ2	1:1E:64:LYS:HE2	1.83	0.44
2:1L:101:LHG:C38	2:1L:101:LHG:H212	2.47	0.44
1:1L:15:PHE:HB2	1:1M:27:ILE:HD11	2.00	0.44
2:1O:101:LHG:C38	2:1O:101:LHG:H212	2.47	0.44
1:1O:12:LYS:HZ2	1:1O:64:LYS:HE2	1.83	0.44
1:2B:8:LYS:H	1:2B:8:LYS:CD	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2D:101:LHG:H212	2:2D:101:LHG:C38	2.47	0.44
1:2F:37:TYR:O	1:2F:41:LYS:N	2.40	0.44
1:2F:49:LEU:O	1:2F:53:ILE:HG12	2.18	0.44
2:3B:101:LHG:H212	2:3B:101:LHG:C38	2.47	0.44
2:3F:101:LHG:H212	2:3F:101:LHG:C38	2.47	0.44
1:2N:20:PHE:HE2	2:3O:101:LHG:C37	2.31	0.44
2:4F:101:LHG:C38	2:4F:101:LHG:H212	2.47	0.44
1:4L:54:VAL:O	1:4L:58:VAL:HG22	2.17	0.44
1:5D:54:VAL:O	1:5D:58:VAL:HG22	2.17	0.44
2:5E:101:LHG:C38	2:5E:101:LHG:H212	2.47	0.44
2:5M:101:LHG:C38	2:5M:101:LHG:H212	2.47	0.44
1:1A:49:LEU:O	1:1A:53:ILE:HG12	2.18	0.43
1:1K:8:LYS:CD	1:1K:8:LYS:H	2.31	0.43
1:1N:49:LEU:O	1:1N:53:ILE:HG12	2.18	0.43
1:2D:49:LEU:O	1:2D:53:ILE:HG12	2.18	0.43
2:2M:101:LHG:H271	2:2M:101:LHG:H301	1.93	0.43
1:2N:8:LYS:CD	1:2N:8:LYS:H	2.31	0.43
1:2O:8:LYS:H	1:2O:8:LYS:CD	2.31	0.43
1:2O:15:PHE:HB2	1:2P:27:ILE:HD11	1.99	0.43
1:3G:49:LEU:O	1:3G:53:ILE:HG12	2.18	0.43
2:3H:101:LHG:H212	2:3H:101:LHG:C38	2.47	0.43
1:3L:37:TYR:O	1:3L:41:LYS:N	2.40	0.43
1:4A:49:LEU:O	1:4A:53:ILE:HG12	2.18	0.43
1:4A:54:VAL:O	1:4A:58:VAL:HG22	2.17	0.43
2:4C:101:LHG:H212	2:4C:101:LHG:C38	2.47	0.43
1:4D:31:ILE:HD11	1:5E:47:LEU:HD11	2.00	0.43
1:5C:49:LEU:O	1:5C:53:ILE:HG12	2.18	0.43
1:4D:20:PHE:CE2	2:5E:101:LHG:C37	2.93	0.43
1:5K:49:LEU:O	1:5K:53:ILE:HG12	2.18	0.43
2:5N:101:LHG:C38	2:5N:101:LHG:H212	2.47	0.43
1:4N:20:PHE:HE2	2:5O:101:LHG:C37	2.31	0.43
1:1B:49:LEU:O	1:1B:53:ILE:HG12	2.18	0.43
1:1D:8:LYS:H	1:1D:8:LYS:CD	2.31	0.43
1:1E:49:LEU:O	1:1E:53:ILE:HG12	2.18	0.43
1:1J:15:PHE:HB2	1:1K:27:ILE:HD11	1.99	0.43
1:1L:8:LYS:H	1:1L:8:LYS:CD	2.31	0.43
2:2E:101:LHG:H212	2:2E:101:LHG:C38	2.47	0.43
1:2H:49:LEU:O	1:2H:53:ILE:HG12	2.18	0.43
2:2J:101:LHG:H301	2:2J:101:LHG:H271	1.93	0.43
1:2P:49:LEU:O	1:2P:53:ILE:HG12	2.18	0.43
2:3A:101:LHG:H212	2:3A:101:LHG:C38	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3I:101:LHG:C21	2:3I:101:LHG:C38	2.97	0.43
1:3K:15:PHE:HB2	1:3L:27:ILE:HD11	1.99	0.43
1:3M:37:TYR:O	1:3M:41:LYS:N	2.40	0.43
2:3N:101:LHG:H212	2:3N:101:LHG:C38	2.47	0.43
1:3P:8:LYS:CD	1:3P:8:LYS:H	2.31	0.43
1:4B:49:LEU:O	1:4B:53:ILE:HG12	2.18	0.43
1:3D:4:LEU:HD11	1:4G:57:THR:HG21	2.00	0.43
1:4M:8:LYS:CD	1:4M:8:LYS:H	2.31	0.43
1:4N:49:LEU:O	1:4N:53:ILE:HG12	2.18	0.43
1:4N:15:PHE:HB2	1:4O:27:ILE:HD11	1.99	0.43
1:5B:49:LEU:O	1:5B:53:ILE:HG12	2.18	0.43
1:5C:8:LYS:H	1:5C:8:LYS:CD	2.31	0.43
1:5D:49:LEU:O	1:5D:53:ILE:HG12	2.18	0.43
2:5K:101:LHG:C38	2:5K:101:LHG:H212	2.47	0.43
1:5O:54:VAL:O	1:5O:58:VAL:HG22	2.17	0.43
1:5O:15:PHE:HB2	1:5P:27:ILE:HD11	1.99	0.43
1:1A:15:PHE:HB2	1:1B:27:ILE:HD11	2.00	0.43
2:1E:101:LHG:C38	2:1E:101:LHG:H212	2.47	0.43
2:1F:101:LHG:H212	2:1F:101:LHG:C38	2.47	0.43
1:1I:15:PHE:HB2	1:1J:27:ILE:HD11	2.00	0.43
1:1M:49:LEU:O	1:1M:53:ILE:HG12	2.18	0.43
1:1P:12:LYS:HZ2	1:1P:64:LYS:HE2	1.83	0.43
1:2E:15:PHE:HB2	1:2F:27:ILE:HD11	2.00	0.43
1:2H:15:PHE:HB2	1:2I:27:ILE:HD11	1.99	0.43
1:1I:20:PHE:CE2	2:2J:101:LHG:C37	2.93	0.43
1:2M:8:LYS:CD	1:2M:8:LYS:H	2.31	0.43
1:2O:49:LEU:O	1:2O:53:ILE:HG12	2.18	0.43
1:3F:8:LYS:CD	1:3F:8:LYS:H	2.31	0.43
2:3M:101:LHG:C21	2:3M:101:LHG:C38	2.97	0.43
1:3N:15:PHE:HB2	1:3O:27:ILE:HD11	1.99	0.43
1:4A:15:PHE:HB2	1:4B:27:ILE:HD11	2.00	0.43
1:5E:49:LEU:O	1:5E:53:ILE:HG12	2.18	0.43
1:5N:49:LEU:O	1:5N:53:ILE:HG12	2.18	0.43
2:1C:101:LHG:C21	2:1C:101:LHG:C38	2.97	0.43
2:1D:101:LHG:H212	2:1D:101:LHG:C38	2.47	0.43
1:1C:15:PHE:HB2	1:1D:27:ILE:HD11	1.99	0.43
1:1E:15:PHE:HB2	1:1F:27:ILE:HD11	2.00	0.43
1:1F:15:PHE:HB2	1:1G:27:ILE:HD11	2.00	0.43
1:1G:49:LEU:O	1:1G:53:ILE:HG12	2.18	0.43
1:1G:15:PHE:HB2	1:1H:27:ILE:HD11	1.99	0.43
1:1I:8:LYS:H	1:1I:8:LYS:CD	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1K:101:LHG:H142	1:5I:15:PHE:CE2	2.53	0.43
1:1L:49:LEU:O	1:1L:53:ILE:HG12	2.18	0.43
1:1O:15:PHE:HB2	1:1P:27:ILE:HD11	1.99	0.43
1:2B:31:ILE:HD11	1:3C:47:LEU:HD11	2.01	0.43
2:2F:101:LHG:C21	2:2F:101:LHG:C38	2.97	0.43
1:2J:49:LEU:O	1:2J:53:ILE:HG12	2.18	0.43
1:2P:8:LYS:H	1:2P:8:LYS:CD	2.31	0.43
2:3A:101:LHG:C38	2:3A:101:LHG:C21	2.97	0.43
1:3J:8:LYS:H	1:3J:8:LYS:CD	2.31	0.43
1:3K:8:LYS:H	1:3K:8:LYS:CD	2.31	0.43
2:3M:101:LHG:H212	2:3M:101:LHG:C38	2.47	0.43
1:4D:8:LYS:H	1:4D:8:LYS:CD	2.31	0.43
1:4H:49:LEU:O	1:4H:53:ILE:HG12	2.18	0.43
1:4I:15:PHE:HB2	1:4J:27:ILE:HD11	1.99	0.43
2:4L:101:LHG:C38	2:4L:101:LHG:C21	2.97	0.43
1:4L:8:LYS:CD	1:4L:8:LYS:H	2.31	0.43
1:4M:8:LYS:HD2	1:4M:8:LYS:H	1.78	0.43
1:5B:15:PHE:HB2	1:5C:27:ILE:HD11	1.99	0.43
1:5D:15:PHE:HB2	1:5E:27:ILE:HD11	2.00	0.43
2:5G:101:LHG:H212	2:5G:101:LHG:C38	2.47	0.43
1:5F:15:PHE:HB2	1:5G:27:ILE:HD11	1.99	0.43
1:5G:15:PHE:HB2	1:5H:27:ILE:HD11	2.00	0.43
1:5J:8:LYS:H	1:5J:8:LYS:CD	2.31	0.43
1:5K:8:LYS:CD	1:5K:8:LYS:H	2.31	0.43
1:5M:12:LYS:HZ1	1:5M:64:LYS:HE2	1.82	0.43
2:5O:101:LHG:C21	2:5O:101:LHG:C38	2.97	0.43
2:1F:101:LHG:H372	1:5E:20:PHE:CE2	2.48	0.43
1:1F:14:THR:HG21	1:2H:54:VAL:HG11	1.99	0.43
2:1G:101:LHG:C38	2:1G:101:LHG:C21	2.97	0.43
2:1G:101:LHG:C38	2:1G:101:LHG:H212	2.47	0.43
2:1H:101:LHG:H212	2:1H:101:LHG:C38	2.47	0.43
1:1M:8:LYS:H	1:1M:8:LYS:CD	2.31	0.43
1:2D:15:PHE:HB2	1:2E:27:ILE:HD11	2.00	0.43
1:2H:8:LYS:H	1:2H:8:LYS:CD	2.31	0.43
2:2J:101:LHG:C21	2:2J:101:LHG:C38	2.97	0.43
1:2I:15:PHE:HB2	1:2J:27:ILE:HD11	2.00	0.43
1:2J:15:PHE:HB2	1:2K:27:ILE:HD11	1.99	0.43
1:2K:49:LEU:O	1:2K:53:ILE:HG12	2.18	0.43
2:2L:101:LHG:H301	2:2L:101:LHG:H271	1.94	0.43
1:2L:8:LYS:H	1:2L:8:LYS:CD	2.31	0.43
1:2N:49:LEU:O	1:2N:53:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2O:8:LYS:H	1:2O:8:LYS:HD2	1.78	0.43
2:3B:101:LHG:C21	2:3B:101:LHG:C38	2.97	0.43
1:3E:49:LEU:O	1:3E:53:ILE:HG12	2.18	0.43
1:3F:15:PHE:HB2	1:3G:27:ILE:HD11	1.99	0.43
2:3J:101:LHG:H212	2:3J:101:LHG:C38	2.47	0.43
2:3K:101:LHG:H301	2:3K:101:LHG:H271	1.94	0.43
1:3J:15:PHE:HB2	1:3K:27:ILE:HD11	1.99	0.43
1:3O:8:LYS:CD	1:3O:8:LYS:H	2.31	0.43
2:4D:101:LHG:C38	2:4D:101:LHG:C21	2.97	0.43
1:4F:8:LYS:H	1:4F:8:LYS:CD	2.31	0.43
1:4J:55:PHE:HD1	2:4J:101:LHG:C22	2.17	0.43
1:5C:15:PHE:HB2	1:5D:27:ILE:HD11	2.00	0.43
1:1I:54:VAL:HG11	1:5G:14:THR:HG21	2.00	0.43
1:5G:8:LYS:H	1:5G:8:LYS:CD	2.31	0.43
1:5L:24:CYS:HA	1:5L:27:ILE:HG22	2.00	0.43
1:5L:15:PHE:HB2	1:5M:27:ILE:HD11	2.00	0.43
1:5N:8:LYS:CD	1:5N:8:LYS:H	2.31	0.43
2:1B:101:LHG:C38	2:1B:101:LHG:C21	2.97	0.43
1:1D:4:LEU:HD11	1:2G:57:THR:HG21	2.01	0.43
1:1H:49:LEU:O	1:1H:53:ILE:HG12	2.18	0.43
1:1H:15:PHE:HB2	1:1I:27:ILE:HD11	1.99	0.43
1:1K:49:LEU:O	1:1K:53:ILE:HG12	2.18	0.43
1:1L:8:LYS:H	1:1L:8:LYS:HD2	1.78	0.43
1:2B:49:LEU:O	1:2B:53:ILE:HG12	2.18	0.43
1:2F:15:PHE:HB2	1:2G:27:ILE:HD11	1.99	0.43
2:2K:101:LHG:H271	2:2K:101:LHG:H301	1.93	0.43
1:2K:15:PHE:HB2	1:2L:27:ILE:HD11	2.00	0.43
1:3A:8:LYS:CD	1:3A:8:LYS:H	2.31	0.43
2:3H:101:LHG:C21	2:3H:101:LHG:C38	2.97	0.43
1:3H:15:PHE:HB2	1:3I:27:ILE:HD11	2.00	0.43
1:3I:8:LYS:H	1:3I:8:LYS:CD	2.31	0.43
2:3K:101:LHG:C38	2:3K:101:LHG:H212	2.47	0.43
2:3L:101:LHG:C21	2:3L:101:LHG:C38	2.97	0.43
1:3L:15:PHE:HB2	1:3M:27:ILE:HD11	2.00	0.43
1:3M:49:LEU:O	1:3M:53:ILE:HG12	2.18	0.43
1:2M:20:PHE:HE2	2:3N:101:LHG:C37	2.32	0.43
1:3O:49:LEU:O	1:3O:53:ILE:HG12	2.18	0.43
2:4A:101:LHG:C21	2:4A:101:LHG:C38	2.97	0.43
1:4B:15:PHE:HB2	1:4C:27:ILE:HD11	2.00	0.43
1:4B:8:LYS:H	1:4B:8:LYS:CD	2.31	0.43
1:4D:49:LEU:O	1:4D:53:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4E:101:LHG:C38	2:4E:101:LHG:C21	2.97	0.43
1:4G:12:LYS:HZ1	1:4G:64:LYS:HE2	1.82	0.43
1:4K:24:CYS:HA	1:4K:27:ILE:HG22	2.01	0.43
2:4M:101:LHG:C38	2:4M:101:LHG:C21	2.97	0.43
1:4L:15:PHE:HB2	1:4M:27:ILE:HD11	2.00	0.43
1:3M:20:PHE:HE2	2:4N:101:LHG:C37	2.32	0.43
1:4M:15:PHE:HB2	1:4N:27:ILE:HD11	2.00	0.43
2:4O:101:LHG:C21	2:4O:101:LHG:C38	2.97	0.43
1:4O:15:PHE:HB2	1:4P:27:ILE:HD11	1.99	0.43
2:5A:101:LHG:C21	2:5A:101:LHG:C38	2.97	0.43
2:5D:101:LHG:C21	2:5D:101:LHG:C38	2.97	0.43
2:5G:101:LHG:C21	2:5G:101:LHG:C38	2.97	0.43
2:1C:101:LHG:H212	2:1C:101:LHG:C38	2.47	0.43
1:1C:15:PHE:CE2	2:2E:101:LHG:H142	2.54	0.43
1:1C:24:CYS:HA	1:1C:27:ILE:HG22	2.01	0.43
2:1D:101:LHG:C21	2:1D:101:LHG:C38	2.97	0.43
1:1D:37:TYR:O	1:1D:41:LYS:N	2.40	0.43
1:1D:15:PHE:HB2	1:1E:27:ILE:HD11	1.99	0.43
2:1F:101:LHG:C21	2:1F:101:LHG:C38	2.97	0.43
1:1H:8:LYS:H	1:1H:8:LYS:HD2	1.78	0.43
1:1J:54:VAL:HG11	1:5H:14:THR:HG21	2.00	0.43
1:2A:12:LYS:HZ1	1:2A:64:LYS:HE2	1.82	0.43
2:2E:101:LHG:C38	2:2E:101:LHG:C21	2.97	0.43
2:2G:101:LHG:C38	2:2G:101:LHG:C21	2.97	0.43
1:2G:15:PHE:HB2	1:2H:27:ILE:HD11	1.99	0.43
2:2I:101:LHG:C21	2:2I:101:LHG:C38	2.97	0.43
1:2I:8:LYS:CD	1:2I:8:LYS:H	2.31	0.43
2:2K:101:LHG:C38	2:2K:101:LHG:C21	2.97	0.43
1:2N:15:PHE:HB2	1:2O:27:ILE:HD11	2.00	0.43
1:3B:31:ILE:HD11	1:4C:47:LEU:HD11	2.01	0.43
1:3C:49:LEU:O	1:3C:53:ILE:HG12	2.18	0.43
1:3E:8:LYS:CD	1:3E:8:LYS:H	2.31	0.43
2:3I:101:LHG:H212	2:3I:101:LHG:C38	2.47	0.43
1:3I:24:CYS:HA	1:3I:27:ILE:HG22	2.01	0.43
2:3J:101:LHG:C21	2:3J:101:LHG:C38	2.97	0.43
2:3L:101:LHG:H212	2:3L:101:LHG:C38	2.47	0.43
2:3N:101:LHG:C21	2:3N:101:LHG:C38	2.97	0.43
1:3N:49:LEU:O	1:3N:53:ILE:HG12	2.18	0.43
1:3N:8:LYS:CD	1:3N:8:LYS:H	2.31	0.43
1:4I:8:LYS:CD	1:4I:8:LYS:H	2.31	0.43
1:4J:24:CYS:HA	1:4J:27:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4K:101:LHG:C38	2:4K:101:LHG:C21	2.97	0.43
1:4K:8:LYS:H	1:4K:8:LYS:CD	2.31	0.43
2:5C:101:LHG:C21	2:5C:101:LHG:C38	2.97	0.43
1:5E:8:LYS:HD2	1:5E:8:LYS:H	1.78	0.43
2:5H:101:LHG:C38	2:5H:101:LHG:C21	2.97	0.43
1:5I:49:LEU:O	1:5I:53:ILE:HG12	2.18	0.43
2:5N:101:LHG:C38	2:5N:101:LHG:C21	2.97	0.43
1:1A:8:LYS:CD	1:1A:8:LYS:H	2.31	0.43
1:1F:49:LEU:O	1:1F:53:ILE:HG12	2.18	0.43
2:1J:101:LHG:C21	2:1J:101:LHG:C38	2.97	0.43
1:1J:49:LEU:O	1:1J:53:ILE:HG12	2.18	0.43
2:1K:101:LHG:C21	2:1K:101:LHG:C38	2.97	0.43
2:1N:101:LHG:C21	2:1N:101:LHG:C38	2.97	0.43
1:1N:8:LYS:CD	1:1N:8:LYS:H	2.31	0.43
2:1O:101:LHG:C21	2:1O:101:LHG:C38	2.97	0.43
1:1O:24:CYS:HA	1:1O:27:ILE:HG22	2.01	0.43
1:2E:24:CYS:HA	1:2E:27:ILE:HG22	2.01	0.43
1:2F:24:CYS:HA	1:2F:27:ILE:HG22	2.01	0.43
1:2I:12:LYS:HZ2	1:2I:64:LYS:HE2	1.83	0.43
1:2K:12:LYS:HZ2	1:2K:64:LYS:HE2	1.83	0.43
1:2K:8:LYS:H	1:2K:8:LYS:CD	2.31	0.43
1:2C:31:ILE:HD11	1:3D:47:LEU:HD11	2.01	0.43
1:3G:15:PHE:HB2	1:3H:27:ILE:HD11	1.99	0.43
1:3H:24:CYS:HA	1:3H:27:ILE:HG22	2.01	0.43
1:3I:15:PHE:HB2	1:3J:27:ILE:HD11	2.00	0.43
1:3L:8:LYS:H	1:3L:8:LYS:CD	2.31	0.43
1:3M:15:PHE:HB2	1:3N:27:ILE:HD11	1.99	0.43
1:3P:12:LYS:HZ1	1:3P:64:LYS:HE2	1.83	0.43
1:4A:15:PHE:CE2	2:5C:101:LHG:H142	2.54	0.43
1:4C:8:LYS:CD	1:4C:8:LYS:H	2.31	0.43
1:3C:31:ILE:HD11	1:4D:47:LEU:HD11	2.01	0.43
1:4D:15:PHE:HB2	1:4E:27:ILE:HD11	1.99	0.43
2:4F:101:LHG:C38	2:4F:101:LHG:C21	2.97	0.43
1:4I:24:CYS:HA	1:4I:27:ILE:HG22	2.01	0.43
1:4M:20:PHE:HE2	2:5N:101:LHG:C37	2.32	0.43
1:1E:57:THR:HG21	1:5B:4:LEU:HD11	2.00	0.43
1:4B:31:ILE:HD11	1:5C:47:LEU:HD11	2.01	0.43
1:5G:49:LEU:O	1:5G:53:ILE:HG12	2.18	0.43
1:5N:24:CYS:HA	1:5N:27:ILE:HG22	2.01	0.43
1:5P:8:LYS:HD2	1:5P:8:LYS:H	1.78	0.43
1:1B:15:PHE:CE2	2:2D:101:LHG:H142	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1B:31:ILE:HD11	1:2C:47:LEU:HD11	2.01	0.43
1:1E:4:LEU:HD11	1:2H:57:THR:HG21	2.00	0.43
2:1H:101:LHG:C21	2:1H:101:LHG:C38	2.97	0.43
2:1L:101:LHG:C38	2:1L:101:LHG:C21	2.97	0.43
2:1M:101:LHG:C38	2:1M:101:LHG:C21	2.97	0.43
1:2C:15:PHE:HB2	1:2D:27:ILE:HD11	2.00	0.43
1:2G:8:LYS:CD	1:2G:8:LYS:H	2.31	0.43
1:2J:8:LYS:CD	1:2J:8:LYS:H	2.31	0.43
2:2N:101:LHG:C21	2:2N:101:LHG:C38	2.97	0.43
1:3B:49:LEU:O	1:3B:53:ILE:HG12	2.18	0.43
2:3C:101:LHG:C21	2:3C:101:LHG:C38	2.97	0.43
1:3C:8:LYS:HD2	1:3C:8:LYS:H	1.77	0.43
1:3F:14:THR:HG21	1:4H:54:VAL:HG11	1.99	0.43
1:3G:24:CYS:HA	1:3G:27:ILE:HG22	2.01	0.43
1:3J:24:CYS:HA	1:3J:27:ILE:HG22	2.00	0.43
2:4C:101:LHG:C21	2:4C:101:LHG:C38	2.97	0.43
1:4C:15:PHE:HB2	1:4D:27:ILE:HD11	2.00	0.43
1:4F:49:LEU:O	1:4F:53:ILE:HG12	2.18	0.43
1:4F:8:LYS:HD2	1:4F:8:LYS:H	1.78	0.43
1:4L:24:CYS:HA	1:4L:27:ILE:HG22	2.00	0.43
1:5A:15:PHE:HB2	1:5B:27:ILE:HD11	1.99	0.43
1:5H:49:LEU:O	1:5H:53:ILE:HG12	2.18	0.43
2:5I:101:LHG:C21	2:5I:101:LHG:C38	2.97	0.43
1:5M:24:CYS:HA	1:5M:27:ILE:HG22	2.00	0.43
2:1A:101:LHG:C38	2:1A:101:LHG:C21	2.97	0.43
1:1A:15:PHE:CE2	2:2C:101:LHG:H142	2.54	0.43
1:1A:24:CYS:HA	1:1A:27:ILE:HG22	2.01	0.43
1:1C:31:ILE:HD11	1:2D:47:LEU:HD11	2.01	0.43
1:1D:24:CYS:HA	1:1D:27:ILE:HG22	2.01	0.43
2:1E:101:LHG:H372	1:5D:20:PHE:CE2	2.50	0.43
1:1H:8:LYS:CD	1:1H:8:LYS:H	2.31	0.43
1:1K:15:PHE:HB2	1:1L:27:ILE:HD11	1.99	0.43
1:2D:24:CYS:HA	1:2D:27:ILE:HG22	2.01	0.43
1:1G:20:PHE:CE2	2:2H:101:LHG:H372	2.54	0.43
2:2M:101:LHG:C38	2:2M:101:LHG:C21	2.97	0.43
1:1M:20:PHE:HE2	2:2N:101:LHG:C37	2.32	0.43
2:2O:101:LHG:C38	2:2O:101:LHG:C21	2.97	0.43
1:3B:15:PHE:HB2	1:3C:27:ILE:HD11	1.99	0.43
1:3G:8:LYS:CD	1:3G:8:LYS:H	2.31	0.43
1:3H:8:LYS:H	1:3H:8:LYS:CD	2.31	0.43
1:3N:8:LYS:HD2	1:3N:8:LYS:H	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4B:101:LHG:C38	2:4B:101:LHG:C21	2.97	0.43
1:4D:24:CYS:HA	1:4D:27:ILE:HG22	2.01	0.43
1:4E:24:CYS:HA	1:4E:27:ILE:HG22	2.01	0.43
1:4E:49:LEU:O	1:4E:53:ILE:HG12	2.18	0.43
1:4E:8:LYS:H	1:4E:8:LYS:CD	2.31	0.43
1:4J:8:LYS:CD	1:4J:8:LYS:H	2.31	0.43
1:4K:15:PHE:HB2	1:4L:27:ILE:HD11	1.99	0.43
1:4O:49:LEU:O	1:4O:53:ILE:HG12	2.18	0.43
1:4P:49:LEU:O	1:4P:53:ILE:HG12	2.18	0.43
1:4P:8:LYS:CD	1:4P:8:LYS:H	2.31	0.43
1:5A:24:CYS:HA	1:5A:27:ILE:HG22	2.00	0.43
1:5A:12:LYS:HZ2	1:5A:64:LYS:HE2	1.84	0.43
1:5B:24:CYS:HA	1:5B:27:ILE:HG22	2.01	0.43
2:5E:101:LHG:C21	2:5E:101:LHG:C38	2.97	0.43
1:5E:15:PHE:HB2	1:5F:27:ILE:HD11	2.00	0.43
2:5F:101:LHG:C21	2:5F:101:LHG:C38	2.97	0.43
1:5I:8:LYS:HD2	1:5I:8:LYS:H	1.78	0.43
2:5J:101:LHG:C38	2:5J:101:LHG:C21	2.97	0.43
1:5J:49:LEU:O	1:5J:53:ILE:HG12	2.18	0.43
2:5K:101:LHG:C38	2:5K:101:LHG:C21	2.97	0.43
1:5L:8:LYS:H	1:5L:8:LYS:CD	2.31	0.43
2:5N:101:LHG:H301	2:5N:101:LHG:H271	1.93	0.43
1:5N:15:PHE:HB2	1:5O:27:ILE:HD11	1.99	0.43
1:1B:24:CYS:HA	1:1B:27:ILE:HG22	2.01	0.42
2:1G:101:LHG:H142	1:5E:15:PHE:CE2	2.52	0.42
1:1J:24:CYS:HA	1:1J:27:ILE:HG22	2.01	0.42
1:1N:24:CYS:HA	1:1N:27:ILE:HG22	2.01	0.42
1:1P:24:CYS:HA	1:1P:27:ILE:HG22	2.01	0.42
1:2L:49:LEU:O	1:2L:53:ILE:HG12	2.18	0.42
1:2P:24:CYS:HA	1:2P:27:ILE:HG22	2.01	0.42
1:3A:49:LEU:O	1:3A:53:ILE:HG12	2.18	0.42
1:3D:8:LYS:H	1:3D:8:LYS:CD	2.31	0.42
1:3J:12:LYS:HZ1	1:3J:64:LYS:HE2	1.82	0.42
1:3M:8:LYS:H	1:3M:8:LYS:CD	2.31	0.42
1:4E:15:PHE:HB2	1:4F:27:ILE:HD11	2.00	0.42
1:4N:37:TYR:O	1:4N:41:LYS:N	2.40	0.42
1:5B:8:LYS:CD	1:5B:8:LYS:H	2.31	0.42
1:5F:8:LYS:CD	1:5F:8:LYS:H	2.31	0.42
1:4E:4:LEU:HD11	1:5H:57:THR:HG21	2.00	0.42
1:5K:24:CYS:HA	1:5K:27:ILE:HG22	2.00	0.42
2:5L:101:LHG:C38	2:5L:101:LHG:C21	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5P:37:TYR:O	1:5P:41:LYS:N	2.40	0.42
1:1E:24:CYS:HA	1:1E:27:ILE:HG22	2.01	0.42
1:1F:8:LYS:H	1:1F:8:LYS:CD	2.31	0.42
1:1G:8:LYS:H	1:1G:8:LYS:CD	2.31	0.42
2:1I:101:LHG:C38	2:1I:101:LHG:C21	2.97	0.42
1:1I:24:CYS:HA	1:1I:27:ILE:HG22	2.01	0.42
1:1M:24:CYS:HA	1:1M:27:ILE:HG22	2.01	0.42
1:1O:8:LYS:H	1:1O:8:LYS:CD	2.31	0.42
2:2D:101:LHG:C21	2:2D:101:LHG:C38	2.97	0.42
1:2F:8:LYS:H	1:2F:8:LYS:CD	2.31	0.42
1:2G:24:CYS:HA	1:2G:27:ILE:HG22	2.01	0.42
1:2H:24:CYS:HA	1:2H:27:ILE:HG22	2.00	0.42
1:2C:20:PHE:CE2	2:3D:101:LHG:C37	2.95	0.42
1:3F:24:CYS:HA	1:3F:27:ILE:HG22	2.01	0.42
1:2D:4:LEU:HD11	1:3G:57:THR:HG21	2.00	0.42
1:4M:24:CYS:HA	1:4M:27:ILE:HG22	2.01	0.42
1:5B:37:TYR:O	1:5B:41:LYS:N	2.40	0.42
1:5E:12:LYS:HZ1	1:5E:64:LYS:HE2	1.82	0.42
1:4G:20:PHE:CE2	2:5H:101:LHG:H372	2.54	0.42
1:5H:15:PHE:HB2	1:5I:27:ILE:HD11	2.00	0.42
1:1A:12:LYS:HZ2	1:1A:64:LYS:HE2	1.84	0.42
1:1E:8:LYS:CD	1:1E:8:LYS:H	2.31	0.42
1:1H:24:CYS:HA	1:1H:27:ILE:HG22	2.01	0.42
1:1D:20:PHE:CE2	2:2E:101:LHG:C37	2.93	0.42
1:2I:49:LEU:O	1:2I:53:ILE:HG12	2.18	0.42
1:2M:49:LEU:O	1:2M:53:ILE:HG12	2.18	0.42
1:3A:15:PHE:HB2	1:3B:27:ILE:HD11	1.99	0.42
1:3C:15:PHE:CE2	2:4E:101:LHG:H142	2.54	0.42
2:3G:101:LHG:C21	2:3G:101:LHG:C38	2.97	0.42
2:3L:101:LHG:H301	2:3L:101:LHG:H271	1.93	0.42
1:3L:49:LEU:O	1:3L:53:ILE:HG12	2.18	0.42
1:3L:56:THR:O	1:3L:60:LEU:HG	2.20	0.42
1:4A:8:LYS:CD	1:4A:8:LYS:H	2.31	0.42
1:4C:15:PHE:CE2	2:5E:101:LHG:H142	2.54	0.42
1:4C:24:CYS:HA	1:4C:27:ILE:HG22	2.01	0.42
1:4C:49:LEU:O	1:4C:53:ILE:HG12	2.18	0.42
2:4G:101:LHG:C38	2:4G:101:LHG:C21	2.97	0.42
1:4H:24:CYS:HA	1:4H:27:ILE:HG22	2.00	0.42
1:4I:55:PHE:HD1	2:4I:101:LHG:C22	2.18	0.42
1:4J:15:PHE:HB2	1:4K:27:ILE:HD11	1.99	0.42
1:4P:24:CYS:HA	1:4P:27:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4C:31:ILE:HD11	1:5D:47:LEU:HD11	2.01	0.42
1:4D:4:LEU:HD11	1:5G:57:THR:HG21	2.00	0.42
1:5M:15:PHE:HB2	1:5N:27:ILE:HD11	1.99	0.42
1:5O:24:CYS:HA	1:5O:27:ILE:HG22	2.01	0.42
1:5P:56:THR:O	1:5P:60:LEU:HG	2.20	0.42
2:1E:101:LHG:C38	2:1E:101:LHG:C21	2.97	0.42
1:1G:56:THR:O	1:1G:60:LEU:HG	2.20	0.42
2:2A:101:LHG:C38	2:2A:101:LHG:C21	2.97	0.42
1:2E:8:LYS:CD	1:2E:8:LYS:H	2.31	0.42
1:2G:56:THR:O	1:2G:60:LEU:HG	2.20	0.42
1:2K:24:CYS:HA	1:2K:27:ILE:HG22	2.00	0.42
1:2K:8:LYS:HD2	1:2K:8:LYS:H	1.78	0.42
1:2L:24:CYS:HA	1:2L:27:ILE:HG22	2.01	0.42
2:3D:101:LHG:C38	2:3D:101:LHG:C21	2.97	0.42
1:3K:56:THR:O	1:3K:60:LEU:HG	2.20	0.42
1:3N:24:CYS:HA	1:3N:27:ILE:HG22	2.00	0.42
2:3O:101:LHG:C21	2:3O:101:LHG:C38	2.97	0.42
1:4C:12:LYS:HZ1	1:4C:64:LYS:HE2	1.82	0.42
2:4H:101:LHG:C21	2:4H:101:LHG:C38	2.97	0.42
1:4K:56:THR:O	1:4K:60:LEU:HG	2.20	0.42
1:5F:49:LEU:O	1:5F:53:ILE:HG12	2.18	0.42
1:5J:24:CYS:HA	1:5J:27:ILE:HG22	2.01	0.42
2:5M:101:LHG:C38	2:5M:101:LHG:C21	2.97	0.42
1:5M:37:TYR:O	1:5M:41:LYS:N	2.40	0.42
1:5M:8:LYS:CD	1:5M:8:LYS:H	2.31	0.42
1:1C:8:LYS:H	1:1C:8:LYS:CD	2.31	0.42
1:1H:56:THR:O	1:1H:60:LEU:HG	2.20	0.42
1:1I:49:LEU:O	1:1I:53:ILE:HG12	2.18	0.42
1:1K:57:THR:HG21	1:5H:4:LEU:HD11	2.02	0.42
1:2C:24:CYS:HA	1:2C:27:ILE:HG22	2.01	0.42
1:2D:8:LYS:H	1:2D:8:LYS:CD	2.31	0.42
1:2F:56:THR:O	1:2F:60:LEU:HG	2.20	0.42
2:2H:101:LHG:C38	2:2H:101:LHG:C21	2.97	0.42
2:2L:101:LHG:C21	2:2L:101:LHG:C38	2.97	0.42
1:2C:15:PHE:CE2	2:3E:101:LHG:H142	2.54	0.42
1:3E:24:CYS:HA	1:3E:27:ILE:HG22	2.01	0.42
2:3K:101:LHG:C38	2:3K:101:LHG:C21	2.97	0.42
1:3K:24:CYS:HA	1:3K:27:ILE:HG22	2.00	0.42
1:4F:24:CYS:HA	1:4F:27:ILE:HG22	2.01	0.42
2:4J:101:LHG:C38	2:4J:101:LHG:C21	2.97	0.42
1:4L:56:THR:O	1:4L:60:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4N:101:LHG:C21	2:4N:101:LHG:C38	2.97	0.42
1:4O:8:LYS:CD	1:4O:8:LYS:H	2.31	0.42
2:5B:101:LHG:C38	2:5B:101:LHG:C21	2.97	0.42
1:5B:56:THR:O	1:5B:60:LEU:HG	2.20	0.42
1:5P:24:CYS:HA	1:5P:27:ILE:HG22	2.01	0.42
2:1D:101:LHG:H372	1:5C:20:PHE:CE2	2.52	0.42
1:1I:14:THR:HG21	1:2K:54:VAL:HG11	2.01	0.42
1:1K:24:CYS:HA	1:1K:27:ILE:HG22	2.01	0.42
1:1P:56:THR:O	1:1P:60:LEU:HG	2.20	0.42
1:2A:24:CYS:HA	1:2A:27:ILE:HG22	2.01	0.42
1:2C:8:LYS:H	1:2C:8:LYS:CD	2.31	0.42
1:2H:56:THR:O	1:2H:60:LEU:HG	2.20	0.42
1:2E:4:LEU:HD11	1:3H:57:THR:HG21	2.00	0.42
1:4A:24:CYS:HA	1:4A:27:ILE:HG22	2.01	0.42
1:4B:24:CYS:HA	1:4B:27:ILE:HG22	2.01	0.42
1:4G:49:LEU:O	1:4G:53:ILE:HG12	2.18	0.42
2:4I:101:LHG:C38	2:4I:101:LHG:C21	2.97	0.42
1:3F:4:LEU:HD11	1:4I:57:THR:HG21	2.02	0.42
2:4M:101:LHG:H301	2:4M:101:LHG:H271	1.94	0.42
1:5C:56:THR:O	1:5C:60:LEU:HG	2.20	0.42
1:4B:15:PHE:CE2	2:5D:101:LHG:H142	2.54	0.42
1:5D:8:LYS:H	1:5D:8:LYS:CD	2.31	0.42
1:5O:56:THR:O	1:5O:60:LEU:HG	2.20	0.42
1:1F:24:CYS:HA	1:1F:27:ILE:HG22	2.01	0.42
1:1O:56:THR:O	1:1O:60:LEU:HG	2.20	0.42
1:1P:57:THR:HG21	1:5M:4:LEU:HD11	2.01	0.42
1:1P:8:LYS:CD	1:1P:8:LYS:H	2.31	0.42
1:2A:49:LEU:O	1:2A:53:ILE:HG12	2.18	0.42
1:2B:24:CYS:HA	1:2B:27:ILE:HG22	2.01	0.42
2:2C:101:LHG:C21	2:2C:101:LHG:C38	2.97	0.42
1:2I:24:CYS:HA	1:2I:27:ILE:HG22	2.00	0.42
1:2J:24:CYS:HA	1:2J:27:ILE:HG22	2.00	0.42
1:2M:24:CYS:HA	1:2M:27:ILE:HG22	2.01	0.42
1:3D:49:LEU:O	1:3D:53:ILE:HG12	2.18	0.42
1:3M:56:THR:O	1:3M:60:LEU:HG	2.20	0.42
1:3P:49:LEU:O	1:3P:53:ILE:HG12	2.18	0.42
1:4G:24:CYS:HA	1:4G:27:ILE:HG22	2.01	0.42
1:4J:12:LYS:HZ2	1:4J:64:LYS:HE2	1.83	0.42
1:4L:12:LYS:HZ1	1:4L:64:LYS:HE2	1.82	0.42
1:4O:24:CYS:HA	1:4O:27:ILE:HG22	2.01	0.42
1:4H:31:ILE:HD11	1:5I:47:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:24:CYS:HA	1:1G:27:ILE:HG22	2.01	0.42
1:2A:15:PHE:CE2	2:3C:101:LHG:H142	2.54	0.42
1:2B:15:PHE:CE2	2:3D:101:LHG:H142	2.54	0.42
2:3E:101:LHG:C21	2:3E:101:LHG:C38	2.97	0.42
1:3M:24:CYS:HA	1:3M:27:ILE:HG22	2.01	0.42
1:3O:24:CYS:HA	1:3O:27:ILE:HG22	2.01	0.42
1:4B:56:THR:O	1:4B:60:LEU:HG	2.20	0.42
1:4C:56:THR:O	1:4C:60:LEU:HG	2.20	0.42
1:3H:31:ILE:HD11	1:4I:47:LEU:HD11	2.02	0.42
1:4N:8:LYS:H	1:4N:8:LYS:CD	2.31	0.42
1:4P:56:THR:O	1:4P:60:LEU:HG	2.20	0.42
1:5C:24:CYS:HA	1:5C:27:ILE:HG22	2.01	0.42
1:5E:8:LYS:CD	1:5E:8:LYS:H	2.31	0.42
1:1F:56:THR:O	1:1F:60:LEU:HG	2.20	0.42
1:1I:56:THR:O	1:1I:60:LEU:HG	2.20	0.42
1:1L:24:CYS:HA	1:1L:27:ILE:HG22	2.00	0.42
1:3A:15:PHE:CE2	2:4C:101:LHG:H142	2.54	0.42
2:3M:101:LHG:H271	2:3M:101:LHG:H301	1.93	0.42
2:3O:101:LHG:H301	2:3O:101:LHG:H271	1.94	0.42
1:4D:56:THR:O	1:4D:60:LEU:HG	2.20	0.42
1:5A:56:THR:O	1:5A:60:LEU:HG	2.20	0.42
2:2B:101:LHG:C21	2:2B:101:LHG:C38	2.97	0.42
1:2M:12:LYS:HZ1	1:2M:64:LYS:HE2	1.84	0.42
2:3F:101:LHG:C21	2:3F:101:LHG:C38	2.97	0.42
1:3N:56:THR:O	1:3N:60:LEU:HG	2.20	0.42
1:3P:24:CYS:HA	1:3P:27:ILE:HG22	2.01	0.42
1:4J:56:THR:O	1:4J:60:LEU:HG	2.20	0.42
1:4M:56:THR:O	1:4M:60:LEU:HG	2.20	0.42
1:5D:56:THR:O	1:5D:60:LEU:HG	2.20	0.42
1:5O:8:LYS:H	1:5O:8:LYS:CD	2.31	0.42
1:1M:56:THR:O	1:1M:60:LEU:HG	2.20	0.41
1:1N:56:THR:O	1:1N:60:LEU:HG	2.20	0.41
1:2E:56:THR:O	1:2E:60:LEU:HG	2.20	0.41
1:2G:12:LYS:HZ1	1:2G:64:LYS:HE2	1.83	0.41
1:2N:24:CYS:HA	1:2N:27:ILE:HG22	2.01	0.41
1:2O:24:CYS:HA	1:2O:27:ILE:HG22	2.01	0.41
1:3J:56:THR:O	1:3J:60:LEU:HG	2.20	0.41
1:3L:24:CYS:HA	1:3L:27:ILE:HG22	2.01	0.41
1:4H:56:THR:O	1:4H:60:LEU:HG	2.20	0.41
1:4N:24:CYS:HA	1:4N:27:ILE:HG22	2.01	0.41
1:4O:56:THR:O	1:4O:60:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5C:12:LYS:HZ2	1:5C:64:LYS:HE2	1.84	0.41
1:5F:24:CYS:HA	1:5F:27:ILE:HG22	2.01	0.41
1:5G:24:CYS:HA	1:5G:27:ILE:HG22	2.01	0.41
1:5I:24:CYS:HA	1:5I:27:ILE:HG22	2.01	0.41
1:5P:8:LYS:CD	1:5P:8:LYS:H	2.31	0.41
2:1F:101:LHG:H142	1:5D:15:PHE:CE2	2.55	0.41
1:1K:56:THR:O	1:1K:60:LEU:HG	2.20	0.41
1:2I:56:THR:O	1:2I:60:LEU:HG	2.20	0.41
1:2N:56:THR:O	1:2N:60:LEU:HG	2.20	0.41
2:3N:101:LHG:H301	2:3N:101:LHG:H271	1.93	0.41
1:3A:20:PHE:CE2	2:4B:101:LHG:C37	2.97	0.41
1:4F:56:THR:O	1:4F:60:LEU:HG	2.20	0.41
1:5D:24:CYS:HA	1:5D:27:ILE:HG22	2.01	0.41
1:1B:56:THR:O	1:1B:60:LEU:HG	2.20	0.41
1:1C:56:THR:O	1:1C:60:LEU:HG	2.20	0.41
1:2L:12:LYS:HZ2	1:2L:64:LYS:HE2	1.83	0.41
1:3E:12:LYS:HZ1	1:3E:64:LYS:HE2	1.83	0.41
1:3L:12:LYS:HZ2	1:3L:64:LYS:HE2	1.83	0.41
1:3P:56:THR:O	1:3P:60:LEU:HG	2.20	0.41
1:4D:12:LYS:HZ2	1:4D:64:LYS:HE2	1.84	0.41
1:5N:56:THR:O	1:5N:60:LEU:HG	2.20	0.41
1:1B:8:LYS:CD	1:1B:8:LYS:H	2.31	0.41
1:1J:56:THR:O	1:1J:60:LEU:HG	2.20	0.41
1:2A:56:THR:O	1:2A:60:LEU:HG	2.20	0.41
1:2C:56:THR:O	1:2C:60:LEU:HG	2.20	0.41
1:2D:22:MET:HA	1:2D:25:ILE:HG22	2.03	0.41
1:2K:56:THR:O	1:2K:60:LEU:HG	2.20	0.41
1:2L:56:THR:O	1:2L:60:LEU:HG	2.20	0.41
1:3I:22:MET:HA	1:3I:25:ILE:HG22	2.03	0.41
1:4A:56:THR:O	1:4A:60:LEU:HG	2.20	0.41
1:4I:56:THR:O	1:4I:60:LEU:HG	2.20	0.41
1:5A:8:LYS:CD	1:5A:8:LYS:H	2.31	0.41
1:5E:24:CYS:HA	1:5E:27:ILE:HG22	2.01	0.41
1:5H:24:CYS:HA	1:5H:27:ILE:HG22	2.01	0.41
1:1F:12:LYS:HZ2	1:1F:64:LYS:HE2	1.84	0.41
1:2C:22:MET:HA	1:2C:25:ILE:HG22	2.03	0.41
1:1C:4:LEU:HD11	1:2F:57:THR:HG21	2.03	0.41
1:2N:12:LYS:HZ2	1:2N:64:LYS:HE2	1.83	0.41
1:2P:56:THR:O	1:2P:60:LEU:HG	2.20	0.41
1:3E:56:THR:O	1:3E:60:LEU:HG	2.20	0.41
1:3G:56:THR:O	1:3G:60:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3H:22:MET:HA	1:3H:25:ILE:HG22	2.03	0.41
1:3H:56:THR:O	1:3H:60:LEU:HG	2.20	0.41
1:2H:31:ILE:HD11	1:3I:47:LEU:HD11	2.02	0.41
1:3J:22:MET:HA	1:3J:25:ILE:HG22	2.03	0.41
1:4E:56:THR:O	1:4E:60:LEU:HG	2.20	0.41
1:5I:56:THR:O	1:5I:60:LEU:HG	2.20	0.41
1:5J:56:THR:O	1:5J:60:LEU:HG	2.20	0.41
2:5O:101:LHG:H271	2:5O:101:LHG:H301	1.94	0.41
1:1B:22:MET:HA	1:1B:25:ILE:HG22	2.03	0.41
1:1C:22:MET:HA	1:1C:25:ILE:HG22	2.03	0.41
1:1N:22:MET:HA	1:1N:25:ILE:HG22	2.03	0.41
1:2E:22:MET:HA	1:2E:25:ILE:HG22	2.03	0.41
1:2G:22:MET:HA	1:2G:25:ILE:HG22	2.03	0.41
1:2H:22:MET:HA	1:2H:25:ILE:HG22	2.03	0.41
1:3C:4:LEU:HD11	1:4F:57:THR:HG21	2.03	0.41
1:3D:24:CYS:HA	1:3D:27:ILE:HG22	2.01	0.41
1:3E:22:MET:HA	1:3E:25:ILE:HG22	2.03	0.41
1:3K:22:MET:HA	1:3K:25:ILE:HG22	2.03	0.41
1:3F:20:PHE:CE2	2:4G:101:LHG:H372	2.54	0.41
1:4J:22:MET:HA	1:4J:25:ILE:HG22	2.03	0.41
1:4K:22:MET:HA	1:4K:25:ILE:HG22	2.03	0.41
1:4L:22:MET:HA	1:4L:25:ILE:HG22	2.03	0.41
1:5A:22:MET:HA	1:5A:25:ILE:HG22	2.03	0.41
1:5L:22:MET:HA	1:5L:25:ILE:HG22	2.03	0.41
1:1A:22:MET:HA	1:1A:25:ILE:HG22	2.03	0.41
1:1D:22:MET:HA	1:1D:25:ILE:HG22	2.03	0.41
1:1E:56:THR:O	1:1E:60:LEU:HG	2.20	0.41
1:1M:22:MET:HA	1:1M:25:ILE:HG22	2.03	0.41
1:1O:22:MET:HA	1:1O:25:ILE:HG22	2.03	0.41
1:2D:56:THR:O	1:2D:60:LEU:HG	2.20	0.41
1:2I:14:THR:HG21	1:3K:54:VAL:HG11	2.01	0.41
1:1K:24:CYS:SG	2:2L:101:LHG:H331	2.61	0.41
1:3C:24:CYS:HA	1:3C:27:ILE:HG22	2.01	0.41
1:2G:20:PHE:CE2	2:3H:101:LHG:H372	2.54	0.41
1:3O:56:THR:O	1:3O:60:LEU:HG	2.20	0.41
1:4I:14:THR:HG21	1:5K:54:VAL:HG11	2.01	0.41
1:4K:24:CYS:SG	2:5L:101:LHG:H331	2.61	0.41
1:4M:22:MET:HA	1:4M:25:ILE:HG22	2.03	0.41
2:4N:101:LHG:H301	2:4N:101:LHG:H271	1.94	0.41
1:1H:54:VAL:HG11	1:5F:14:THR:HG21	2.02	0.41
1:5M:22:MET:HA	1:5M:25:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:56:THR:O	1:1A:60:LEU:HG	2.20	0.41
1:1B:12:LYS:HZ2	1:1B:64:LYS:HE2	1.86	0.41
1:1D:56:THR:O	1:1D:60:LEU:HG	2.20	0.41
1:1F:22:MET:HA	1:1F:25:ILE:HG22	2.03	0.41
1:2I:22:MET:HA	1:2I:25:ILE:HG22	2.03	0.41
1:2O:22:MET:HA	1:2O:25:ILE:HG22	2.03	0.41
1:2P:22:MET:HA	1:2P:25:ILE:HG22	2.03	0.41
1:3D:56:THR:O	1:3D:60:LEU:HG	2.20	0.41
1:3F:22:MET:HA	1:3F:25:ILE:HG22	2.03	0.41
1:3G:22:MET:HA	1:3G:25:ILE:HG22	2.03	0.41
1:3N:12:LYS:HZ2	1:3N:64:LYS:HE2	1.85	0.41
1:4A:22:MET:HA	1:4A:25:ILE:HG22	2.03	0.41
1:4I:22:MET:HA	1:4I:25:ILE:HG22	2.03	0.41
1:4N:56:THR:O	1:4N:60:LEU:HG	2.20	0.41
1:5B:22:MET:HA	1:5B:25:ILE:HG22	2.03	0.41
1:5C:22:MET:HA	1:5C:25:ILE:HG22	2.03	0.41
1:5E:56:THR:O	1:5E:60:LEU:HG	2.20	0.41
1:5F:56:THR:O	1:5F:60:LEU:HG	2.20	0.41
1:5K:22:MET:HA	1:5K:25:ILE:HG22	2.03	0.41
1:5N:22:MET:HA	1:5N:25:ILE:HG22	2.03	0.41
2:1D:101:LHG:C37	1:5C:20:PHE:CE2	2.92	0.41
1:1E:22:MET:HA	1:1E:25:ILE:HG22	2.03	0.41
1:1L:22:MET:HA	1:1L:25:ILE:HG22	2.03	0.41
1:1L:56:THR:O	1:1L:60:LEU:HG	2.20	0.41
1:2B:22:MET:HA	1:2B:25:ILE:HG22	2.03	0.41
1:2F:22:MET:HA	1:2F:25:ILE:HG22	2.03	0.41
1:2I:20:PHE:HE2	2:3J:101:LHG:H372	1.85	0.41
1:2M:56:THR:O	1:2M:60:LEU:HG	2.20	0.41
1:2O:56:THR:O	1:2O:60:LEU:HG	2.20	0.41
1:3A:24:CYS:HA	1:3A:27:ILE:HG22	2.01	0.41
1:3B:15:PHE:CE2	2:4D:101:LHG:H142	2.54	0.41
1:3E:20:PHE:CE2	2:4F:101:LHG:H372	2.55	0.41
1:4H:22:MET:HA	1:4H:25:ILE:HG22	2.03	0.41
1:3K:24:CYS:SG	2:4L:101:LHG:H331	2.61	0.41
1:5G:56:THR:O	1:5G:60:LEU:HG	2.20	0.41
1:4F:4:LEU:HD11	1:5I:57:THR:HG21	2.02	0.41
1:5K:56:THR:O	1:5K:60:LEU:HG	2.20	0.41
1:5M:56:THR:O	1:5M:60:LEU:HG	2.20	0.41
1:5O:22:MET:HA	1:5O:25:ILE:HG22	2.03	0.41
1:1G:22:MET:HA	1:1G:25:ILE:HG22	2.03	0.41
1:1P:22:MET:HA	1:1P:25:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2J:22:MET:HA	1:2J:25:ILE:HG22	2.03	0.41
1:2J:56:THR:O	1:2J:60:LEU:HG	2.20	0.41
1:3A:56:THR:O	1:3A:60:LEU:HG	2.20	0.41
1:3B:24:CYS:HA	1:3B:27:ILE:HG22	2.01	0.41
1:3D:22:MET:HA	1:3D:25:ILE:HG22	2.03	0.41
1:3I:56:THR:O	1:3I:60:LEU:HG	2.20	0.41
1:3L:22:MET:HA	1:3L:25:ILE:HG22	2.03	0.41
1:4G:22:MET:HA	1:4G:25:ILE:HG22	2.03	0.41
1:4G:56:THR:O	1:4G:60:LEU:HG	2.20	0.41
1:5J:22:MET:HA	1:5J:25:ILE:HG22	2.03	0.41
1:5P:22:MET:HA	1:5P:25:ILE:HG22	2.03	0.41
1:1F:4:LEU:HD11	1:2I:57:THR:HG21	2.02	0.41
1:1K:47:LEU:HD11	1:5J:31:ILE:HD11	2.03	0.41
1:2B:56:THR:O	1:2B:60:LEU:HG	2.20	0.41
1:2F:4:LEU:HD11	1:3I:57:THR:HG21	2.02	0.41
1:2N:22:MET:HA	1:2N:25:ILE:HG22	2.03	0.41
1:4E:14:THR:HG21	1:5G:54:VAL:HG11	2.03	0.41
1:5I:22:MET:HA	1:5I:25:ILE:HG22	2.03	0.41
1:1K:54:VAL:HG11	1:5I:14:THR:HG21	2.03	0.40
1:2A:22:MET:HA	1:2A:25:ILE:HG22	2.03	0.40
1:3C:22:MET:HA	1:3C:25:ILE:HG22	2.03	0.40
1:3C:56:THR:O	1:3C:60:LEU:HG	2.20	0.40
1:3F:56:THR:O	1:3F:60:LEU:HG	2.20	0.40
1:3O:12:LYS:HZ2	1:3O:64:LYS:HE2	1.84	0.40
1:4N:22:MET:HA	1:4N:25:ILE:HG22	2.03	0.40
1:5H:56:THR:O	1:5H:60:LEU:HG	2.20	0.40
1:5L:56:THR:O	1:5L:60:LEU:HG	2.20	0.40
1:1H:22:MET:HA	1:1H:25:ILE:HG22	2.03	0.40
1:1K:22:MET:HA	1:1K:25:ILE:HG22	2.03	0.40
1:1O:55:PHE:HD1	2:1O:101:LHG:C22	2.17	0.40
1:1H:31:ILE:HD11	1:2I:47:LEU:HD11	2.02	0.40
1:3B:56:THR:O	1:3B:60:LEU:HG	2.20	0.40
1:4B:22:MET:HA	1:4B:25:ILE:HG22	2.03	0.40
1:4F:22:MET:HA	1:4F:25:ILE:HG22	2.03	0.40
1:5D:22:MET:HA	1:5D:25:ILE:HG22	2.03	0.40
2:1K:101:LHG:H372	1:5J:20:PHE:HE2	1.83	0.40
1:5M:55:PHE:HD1	2:5M:101:LHG:C22	2.17	0.40
1:5P:12:LYS:HZ1	1:5P:64:LYS:HE2	1.84	0.40
1:1I:22:MET:HA	1:1I:25:ILE:HG22	2.03	0.40
1:1I:12:LYS:HZ1	1:1I:64:LYS:HE2	1.83	0.40
1:2K:22:MET:HA	1:2K:25:ILE:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2M:22:MET:HA	1:2M:25:ILE:HG22	2.03	0.40
1:3A:22:MET:HA	1:3A:25:ILE:HG22	2.03	0.40
1:3I:29:GLU:OE1	1:3J:38:ILE:HG12	2.22	0.40
1:2K:24:CYS:SG	2:3L:101:LHG:H331	2.61	0.40
1:3M:22:MET:HA	1:3M:25:ILE:HG22	2.03	0.40
1:4C:22:MET:HA	1:4C:25:ILE:HG22	2.03	0.40
1:4O:22:MET:HA	1:4O:25:ILE:HG22	2.03	0.40
1:5E:22:MET:HA	1:5E:25:ILE:HG22	2.03	0.40
1:5N:55:PHE:HD1	2:5N:101:LHG:C22	2.17	0.40
1:1I:29:GLU:OE1	1:1J:38:ILE:HG12	2.22	0.40
1:1J:29:GLU:OE1	1:1K:38:ILE:HG12	2.22	0.40
1:3H:29:GLU:OE1	1:3I:38:ILE:HG12	2.22	0.40
1:3G:29:GLU:OE1	1:3H:38:ILE:HG12	2.22	0.40
1:3P:22:MET:HA	1:3P:25:ILE:HG22	2.03	0.40
1:4C:4:LEU:HD11	1:5F:57:THR:HG21	2.03	0.40
1:4E:29:GLU:OE1	1:4F:38:ILE:HG12	2.22	0.40
1:4F:29:GLU:OE1	1:4G:38:ILE:HG12	2.22	0.40
2:4O:101:LHG:H271	2:4O:101:LHG:H301	1.94	0.40
1:4P:12:LYS:HZ2	1:4P:64:LYS:HE2	1.85	0.40
1:5K:29:GLU:OE1	1:5L:38:ILE:HG12	2.22	0.40
1:5L:29:GLU:OE1	1:5M:38:ILE:HG12	2.22	0.40
1:1J:22:MET:HA	1:1J:25:ILE:HG22	2.03	0.40
1:2A:29:GLU:OE1	1:2B:38:ILE:HG12	2.22	0.40
1:2B:29:GLU:OE1	1:2C:38:ILE:HG12	2.22	0.40
1:2L:22:MET:HA	1:2L:25:ILE:HG22	2.03	0.40
1:3B:22:MET:HA	1:3B:25:ILE:HG22	2.03	0.40
1:3A:29:GLU:OE1	1:3B:38:ILE:HG12	2.22	0.40
1:3F:29:GLU:OE1	1:3G:38:ILE:HG12	2.22	0.40
1:3J:29:GLU:OE1	1:3K:38:ILE:HG12	2.22	0.40
1:3K:29:GLU:OE1	1:3L:38:ILE:HG12	2.22	0.40
1:3M:29:GLU:OE1	1:3N:38:ILE:HG12	2.22	0.40
1:3O:22:MET:HA	1:3O:25:ILE:HG22	2.03	0.40
1:3N:29:GLU:OE1	1:3O:38:ILE:HG12	2.22	0.40
1:4E:22:MET:HA	1:4E:25:ILE:HG22	2.03	0.40
1:4C:20:PHE:CE2	2:5D:101:LHG:C37	2.95	0.40
1:5E:29:GLU:OE1	1:5F:38:ILE:HG12	2.22	0.40
1:5N:29:GLU:OE1	1:5O:38:ILE:HG12	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1B	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1C	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1D	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1E	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1F	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1G	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1H	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1I	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1J	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1K	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1L	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1M	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1N	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1O	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1P	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2A	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2B	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2C	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2D	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2E	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2F	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2G	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2H	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2I	61/63 (97%)	56 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2J	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2K	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2L	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2M	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2N	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2O	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2P	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3A	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3B	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3C	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3D	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3E	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3F	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3G	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3H	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3I	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3J	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3K	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3L	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3M	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3N	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3O	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3P	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4A	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4B	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4C	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4D	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4E	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4F	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4G	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4H	61/63 (97%)	56 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4I	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4J	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4K	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4L	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4M	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4N	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4O	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4P	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5A	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5B	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5C	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5D	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5E	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5F	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5G	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5H	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5I	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5J	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5K	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5L	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5M	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5N	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5O	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5P	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
All	All	4880/5040 (97%)	4480 (92%)	400 (8%)	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	52/52 (100%)	52 (100%)	0	100	100
1	1B	52/52 (100%)	52 (100%)	0	100	100
1	1C	52/52 (100%)	52 (100%)	0	100	100
1	1D	52/52 (100%)	52 (100%)	0	100	100
1	1E	52/52 (100%)	52 (100%)	0	100	100
1	1F	52/52 (100%)	52 (100%)	0	100	100
1	1G	52/52 (100%)	52 (100%)	0	100	100
1	1H	52/52 (100%)	52 (100%)	0	100	100
1	1I	52/52 (100%)	52 (100%)	0	100	100
1	1J	52/52 (100%)	52 (100%)	0	100	100
1	1K	52/52 (100%)	52 (100%)	0	100	100
1	1L	52/52 (100%)	52 (100%)	0	100	100
1	1M	52/52 (100%)	52 (100%)	0	100	100
1	1N	52/52 (100%)	52 (100%)	0	100	100
1	1O	52/52 (100%)	52 (100%)	0	100	100
1	1P	52/52 (100%)	52 (100%)	0	100	100
1	2A	52/52 (100%)	52 (100%)	0	100	100
1	2B	52/52 (100%)	52 (100%)	0	100	100
1	2C	52/52 (100%)	52 (100%)	0	100	100
1	2D	52/52 (100%)	52 (100%)	0	100	100
1	2E	52/52 (100%)	52 (100%)	0	100	100
1	2F	52/52 (100%)	52 (100%)	0	100	100
1	2G	52/52 (100%)	52 (100%)	0	100	100
1	2H	52/52 (100%)	52 (100%)	0	100	100
1	2I	52/52 (100%)	52 (100%)	0	100	100
1	2J	52/52 (100%)	52 (100%)	0	100	100
1	2K	52/52 (100%)	52 (100%)	0	100	100
1	2L	52/52 (100%)	52 (100%)	0	100	100
1	2M	52/52 (100%)	52 (100%)	0	100	100
1	2N	52/52 (100%)	52 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2O	52/52 (100%)	52 (100%)	0	100	100
1	2P	52/52 (100%)	52 (100%)	0	100	100
1	3A	52/52 (100%)	52 (100%)	0	100	100
1	3B	52/52 (100%)	52 (100%)	0	100	100
1	3C	52/52 (100%)	52 (100%)	0	100	100
1	3D	52/52 (100%)	52 (100%)	0	100	100
1	3E	52/52 (100%)	52 (100%)	0	100	100
1	3F	52/52 (100%)	52 (100%)	0	100	100
1	3G	52/52 (100%)	52 (100%)	0	100	100
1	3H	52/52 (100%)	52 (100%)	0	100	100
1	3I	52/52 (100%)	52 (100%)	0	100	100
1	3J	52/52 (100%)	52 (100%)	0	100	100
1	3K	52/52 (100%)	52 (100%)	0	100	100
1	3L	52/52 (100%)	52 (100%)	0	100	100
1	3M	52/52 (100%)	52 (100%)	0	100	100
1	3N	52/52 (100%)	52 (100%)	0	100	100
1	3O	52/52 (100%)	52 (100%)	0	100	100
1	3P	52/52 (100%)	52 (100%)	0	100	100
1	4A	52/52 (100%)	52 (100%)	0	100	100
1	4B	52/52 (100%)	52 (100%)	0	100	100
1	4C	52/52 (100%)	52 (100%)	0	100	100
1	4D	52/52 (100%)	52 (100%)	0	100	100
1	4E	52/52 (100%)	52 (100%)	0	100	100
1	4F	52/52 (100%)	52 (100%)	0	100	100
1	4G	52/52 (100%)	52 (100%)	0	100	100
1	4H	52/52 (100%)	52 (100%)	0	100	100
1	4I	52/52 (100%)	52 (100%)	0	100	100
1	4J	52/52 (100%)	52 (100%)	0	100	100
1	4K	52/52 (100%)	52 (100%)	0	100	100
1	4L	52/52 (100%)	52 (100%)	0	100	100
1	4M	52/52 (100%)	52 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4N	52/52 (100%)	52 (100%)	0	100	100
1	4O	52/52 (100%)	52 (100%)	0	100	100
1	4P	52/52 (100%)	52 (100%)	0	100	100
1	5A	52/52 (100%)	52 (100%)	0	100	100
1	5B	52/52 (100%)	52 (100%)	0	100	100
1	5C	52/52 (100%)	52 (100%)	0	100	100
1	5D	52/52 (100%)	52 (100%)	0	100	100
1	5E	52/52 (100%)	52 (100%)	0	100	100
1	5F	52/52 (100%)	52 (100%)	0	100	100
1	5G	52/52 (100%)	52 (100%)	0	100	100
1	5H	52/52 (100%)	52 (100%)	0	100	100
1	5I	52/52 (100%)	52 (100%)	0	100	100
1	5J	52/52 (100%)	52 (100%)	0	100	100
1	5K	52/52 (100%)	52 (100%)	0	100	100
1	5L	52/52 (100%)	52 (100%)	0	100	100
1	5M	52/52 (100%)	52 (100%)	0	100	100
1	5N	52/52 (100%)	52 (100%)	0	100	100
1	5O	52/52 (100%)	52 (100%)	0	100	100
1	5P	52/52 (100%)	52 (100%)	0	100	100
All	All	4160/4160 (100%)	4160 (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 ⓘ

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	LHG	1A	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	1B	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	1C	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	1D	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	1E	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	1F	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	1G	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	1H	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	1I	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	1J	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	1K	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	1L	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	1M	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	1N	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	1O	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	2A	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	2B	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	2C	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	2D	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	2E	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	2F	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	2G	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	LHG	2H	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	2I	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	2J	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	2K	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	2L	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	2M	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	2N	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	2O	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	3A	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	3B	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	3C	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	3D	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	3E	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	3F	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	3G	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	3H	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	3I	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	3J	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	3K	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	3L	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	3M	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	3N	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	3O	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	4A	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	4B	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	4C	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	4D	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	4E	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	4F	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	4G	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	4H	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	4I	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	4J	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	4K	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	4L	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	LHG	4M	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	4N	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	4O	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	5A	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	5B	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	5C	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	5D	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	5E	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	5F	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	5G	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	5H	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	5I	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	5J	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	5K	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	5L	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	5M	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	5N	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)
2	LHG	5O	101	-	48,48,48	0.60	1 (2%)	49,54,54	0.58	2 (4%)

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	LHG	1A	101	-	-	1/53/53/53	0/0/0/0
2	LHG	1B	101	-	-	1/53/53/53	0/0/0/0
2	LHG	1C	101	-	-	1/53/53/53	0/0/0/0
2	LHG	1D	101	-	-	1/53/53/53	0/0/0/0
2	LHG	1E	101	-	-	1/53/53/53	0/0/0/0
2	LHG	1F	101	-	-	1/53/53/53	0/0/0/0
2	LHG	1G	101	-	-	1/53/53/53	0/0/0/0
2	LHG	1H	101	-	-	1/53/53/53	0/0/0/0
2	LHG	1I	101	-	-	1/53/53/53	0/0/0/0
2	LHG	1J	101	-	-	1/53/53/53	0/0/0/0
2	LHG	1K	101	-	-	1/53/53/53	0/0/0/0
2	LHG	1L	101	-	-	1/53/53/53	0/0/0/0
2	LHG	1M	101	-	-	1/53/53/53	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LHG	1N	101	-	-	1/53/53/53	0/0/0/0
2	LHG	1O	101	-	-	1/53/53/53	0/0/0/0
2	LHG	2A	101	-	-	1/53/53/53	0/0/0/0
2	LHG	2B	101	-	-	1/53/53/53	0/0/0/0
2	LHG	2C	101	-	-	1/53/53/53	0/0/0/0
2	LHG	2D	101	-	-	1/53/53/53	0/0/0/0
2	LHG	2E	101	-	-	1/53/53/53	0/0/0/0
2	LHG	2F	101	-	-	1/53/53/53	0/0/0/0
2	LHG	2G	101	-	-	1/53/53/53	0/0/0/0
2	LHG	2H	101	-	-	1/53/53/53	0/0/0/0
2	LHG	2I	101	-	-	1/53/53/53	0/0/0/0
2	LHG	2J	101	-	-	1/53/53/53	0/0/0/0
2	LHG	2K	101	-	-	1/53/53/53	0/0/0/0
2	LHG	2L	101	-	-	1/53/53/53	0/0/0/0
2	LHG	2M	101	-	-	1/53/53/53	0/0/0/0
2	LHG	2N	101	-	-	1/53/53/53	0/0/0/0
2	LHG	2O	101	-	-	1/53/53/53	0/0/0/0
2	LHG	3A	101	-	-	1/53/53/53	0/0/0/0
2	LHG	3B	101	-	-	1/53/53/53	0/0/0/0
2	LHG	3C	101	-	-	1/53/53/53	0/0/0/0
2	LHG	3D	101	-	-	1/53/53/53	0/0/0/0
2	LHG	3E	101	-	-	1/53/53/53	0/0/0/0
2	LHG	3F	101	-	-	1/53/53/53	0/0/0/0
2	LHG	3G	101	-	-	1/53/53/53	0/0/0/0
2	LHG	3H	101	-	-	1/53/53/53	0/0/0/0
2	LHG	3I	101	-	-	1/53/53/53	0/0/0/0
2	LHG	3J	101	-	-	1/53/53/53	0/0/0/0
2	LHG	3K	101	-	-	1/53/53/53	0/0/0/0
2	LHG	3L	101	-	-	1/53/53/53	0/0/0/0
2	LHG	3M	101	-	-	1/53/53/53	0/0/0/0
2	LHG	3N	101	-	-	1/53/53/53	0/0/0/0
2	LHG	3O	101	-	-	1/53/53/53	0/0/0/0
2	LHG	4A	101	-	-	1/53/53/53	0/0/0/0
2	LHG	4B	101	-	-	1/53/53/53	0/0/0/0
2	LHG	4C	101	-	-	1/53/53/53	0/0/0/0
2	LHG	4D	101	-	-	1/53/53/53	0/0/0/0
2	LHG	4E	101	-	-	1/53/53/53	0/0/0/0
2	LHG	4F	101	-	-	1/53/53/53	0/0/0/0
2	LHG	4G	101	-	-	1/53/53/53	0/0/0/0
2	LHG	4H	101	-	-	1/53/53/53	0/0/0/0
2	LHG	4I	101	-	-	1/53/53/53	0/0/0/0
2	LHG	4J	101	-	-	1/53/53/53	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LHG	4K	101	-	-	1/53/53/53	0/0/0/0
2	LHG	4L	101	-	-	1/53/53/53	0/0/0/0
2	LHG	4M	101	-	-	1/53/53/53	0/0/0/0
2	LHG	4N	101	-	-	1/53/53/53	0/0/0/0
2	LHG	4O	101	-	-	1/53/53/53	0/0/0/0
2	LHG	5A	101	-	-	1/53/53/53	0/0/0/0
2	LHG	5B	101	-	-	1/53/53/53	0/0/0/0
2	LHG	5C	101	-	-	1/53/53/53	0/0/0/0
2	LHG	5D	101	-	-	1/53/53/53	0/0/0/0
2	LHG	5E	101	-	-	1/53/53/53	0/0/0/0
2	LHG	5F	101	-	-	1/53/53/53	0/0/0/0
2	LHG	5G	101	-	-	1/53/53/53	0/0/0/0
2	LHG	5H	101	-	-	1/53/53/53	0/0/0/0
2	LHG	5I	101	-	-	1/53/53/53	0/0/0/0
2	LHG	5J	101	-	-	1/53/53/53	0/0/0/0
2	LHG	5K	101	-	-	1/53/53/53	0/0/0/0
2	LHG	5L	101	-	-	1/53/53/53	0/0/0/0
2	LHG	5M	101	-	-	1/53/53/53	0/0/0/0
2	LHG	5N	101	-	-	1/53/53/53	0/0/0/0
2	LHG	5O	101	-	-	1/53/53/53	0/0/0/0

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4J	101	LHG	C16-C15	-3.43	1.32	1.51
2	2L	101	LHG	C16-C15	-3.43	1.32	1.51
2	4I	101	LHG	C16-C15	-3.43	1.32	1.51
2	3J	101	LHG	C16-C15	-3.42	1.32	1.51
2	5J	101	LHG	C16-C15	-3.42	1.32	1.51
2	1I	101	LHG	C16-C15	-3.42	1.32	1.51
2	1J	101	LHG	C16-C15	-3.42	1.32	1.51
2	2D	101	LHG	C16-C15	-3.42	1.32	1.51
2	3B	101	LHG	C16-C15	-3.42	1.32	1.51
2	1C	101	LHG	C16-C15	-3.42	1.32	1.51
2	5C	101	LHG	C16-C15	-3.42	1.32	1.51
2	3K	101	LHG	C16-C15	-3.42	1.32	1.51
2	3C	101	LHG	C16-C15	-3.42	1.32	1.51
2	2I	101	LHG	C16-C15	-3.42	1.32	1.51
2	2C	101	LHG	C16-C15	-3.42	1.32	1.51
2	5K	101	LHG	C16-C15	-3.42	1.32	1.51
2	2H	101	LHG	C16-C15	-3.42	1.32	1.51
2	3H	101	LHG	C16-C15	-3.42	1.32	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5B	101	LHG	C16-C15	-3.42	1.32	1.51
2	4C	101	LHG	C16-C15	-3.42	1.32	1.51
2	1K	101	LHG	C16-C15	-3.42	1.32	1.51
2	5I	101	LHG	C16-C15	-3.42	1.32	1.51
2	4K	101	LHG	C16-C15	-3.42	1.32	1.51
2	2K	101	LHG	C16-C15	-3.42	1.32	1.51
2	4M	101	LHG	C16-C15	-3.42	1.32	1.51
2	3I	101	LHG	C16-C15	-3.42	1.32	1.51
2	1L	101	LHG	C16-C15	-3.42	1.32	1.51
2	3F	101	LHG	C16-C15	-3.41	1.32	1.51
2	2J	101	LHG	C16-C15	-3.41	1.32	1.51
2	1D	101	LHG	C16-C15	-3.41	1.32	1.51
2	1H	101	LHG	C16-C15	-3.41	1.32	1.51
2	5H	101	LHG	C16-C15	-3.41	1.32	1.51
2	2B	101	LHG	C16-C15	-3.41	1.32	1.51
2	3D	101	LHG	C16-C15	-3.41	1.32	1.51
2	4D	101	LHG	C16-C15	-3.41	1.32	1.51
2	5L	101	LHG	C16-C15	-3.41	1.32	1.51
2	3N	101	LHG	C16-C15	-3.41	1.32	1.51
2	2G	101	LHG	C16-C15	-3.41	1.32	1.51
2	3M	101	LHG	C16-C15	-3.41	1.32	1.51
2	1B	101	LHG	C16-C15	-3.41	1.32	1.51
2	3L	101	LHG	C16-C15	-3.41	1.32	1.51
2	1M	101	LHG	C16-C15	-3.41	1.32	1.51
2	1F	101	LHG	C16-C15	-3.41	1.32	1.51
2	1E	101	LHG	C16-C15	-3.41	1.32	1.51
2	5M	101	LHG	C16-C15	-3.41	1.32	1.51
2	1N	101	LHG	C16-C15	-3.41	1.32	1.51
2	2A	101	LHG	C16-C15	-3.41	1.32	1.51
2	4F	101	LHG	C16-C15	-3.41	1.32	1.51
2	5D	101	LHG	C16-C15	-3.41	1.32	1.51
2	2E	101	LHG	C16-C15	-3.41	1.32	1.51
2	5F	101	LHG	C16-C15	-3.41	1.32	1.51
2	5E	101	LHG	C16-C15	-3.41	1.32	1.51
2	5G	101	LHG	C16-C15	-3.41	1.32	1.51
2	2N	101	LHG	C16-C15	-3.40	1.32	1.51
2	1A	101	LHG	C16-C15	-3.40	1.32	1.51
2	4E	101	LHG	C16-C15	-3.40	1.32	1.51
2	4L	101	LHG	C16-C15	-3.40	1.32	1.51
2	1G	101	LHG	C16-C15	-3.40	1.32	1.51
2	5O	101	LHG	C16-C15	-3.40	1.32	1.51
2	5N	101	LHG	C16-C15	-3.40	1.32	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2M	101	LHG	C16-C15	-3.40	1.32	1.51
2	3G	101	LHG	C16-C15	-3.40	1.32	1.51
2	5A	101	LHG	C16-C15	-3.40	1.32	1.51
2	4B	101	LHG	C16-C15	-3.40	1.32	1.51
2	4G	101	LHG	C16-C15	-3.40	1.32	1.51
2	2O	101	LHG	C16-C15	-3.40	1.32	1.51
2	4N	101	LHG	C16-C15	-3.40	1.32	1.51
2	3O	101	LHG	C16-C15	-3.40	1.32	1.51
2	1O	101	LHG	C16-C15	-3.40	1.32	1.51
2	2F	101	LHG	C16-C15	-3.40	1.32	1.51
2	3E	101	LHG	C16-C15	-3.40	1.32	1.51
2	4O	101	LHG	C16-C15	-3.40	1.32	1.51
2	3A	101	LHG	C16-C15	-3.39	1.32	1.51
2	4H	101	LHG	C16-C15	-3.39	1.32	1.51
2	4A	101	LHG	C16-C15	-3.39	1.32	1.51

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4F	101	LHG	C16-C15-C14	2.21	126.00	114.54
2	3G	101	LHG	C16-C15-C14	2.21	126.01	114.54
2	2E	101	LHG	C16-C15-C14	2.21	126.02	114.54
2	4A	101	LHG	C16-C15-C14	2.21	126.03	114.54
2	2G	101	LHG	C16-C15-C14	2.21	126.03	114.54
2	3O	101	LHG	C17-C16-C15	2.21	126.03	114.54
2	3A	101	LHG	C16-C15-C14	2.21	126.03	114.54
2	2F	101	LHG	C16-C15-C14	2.21	126.04	114.54
2	5G	101	LHG	C16-C15-C14	2.21	126.04	114.54
2	1G	101	LHG	C16-C15-C14	2.21	126.04	114.54
2	2A	101	LHG	C16-C15-C14	2.21	126.04	114.54
2	2D	101	LHG	C16-C15-C14	2.21	126.04	114.54
2	5N	101	LHG	C17-C16-C15	2.21	126.04	114.54
2	2O	101	LHG	C17-C16-C15	2.21	126.05	114.54
2	5H	101	LHG	C16-C15-C14	2.21	126.05	114.54
2	3F	101	LHG	C16-C15-C14	2.22	126.05	114.54
2	4H	101	LHG	C16-C15-C14	2.22	126.05	114.54
2	4G	101	LHG	C16-C15-C14	2.22	126.05	114.54
2	5F	101	LHG	C16-C15-C14	2.22	126.05	114.54
2	2A	101	LHG	C17-C16-C15	2.22	126.05	114.54
2	1A	101	LHG	C16-C15-C14	2.22	126.05	114.54
2	2H	101	LHG	C16-C15-C14	2.22	126.05	114.54
2	5O	101	LHG	C17-C16-C15	2.22	126.06	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2C	101	LHG	C16-C15-C14	2.22	126.06	114.54
2	1F	101	LHG	C16-C15-C14	2.22	126.06	114.54
2	5A	101	LHG	C16-C15-C14	2.22	126.06	114.54
2	3E	101	LHG	C16-C15-C14	2.22	126.06	114.54
2	4A	101	LHG	C17-C16-C15	2.22	126.06	114.54
2	4I	101	LHG	C16-C15-C14	2.22	126.06	114.54
2	1D	101	LHG	C16-C15-C14	2.22	126.06	114.54
2	2N	101	LHG	C17-C16-C15	2.22	126.06	114.54
2	1O	101	LHG	C17-C16-C15	2.22	126.07	114.54
2	4B	101	LHG	C16-C15-C14	2.22	126.07	114.54
2	1H	101	LHG	C16-C15-C14	2.22	126.07	114.54
2	4C	101	LHG	C16-C15-C14	2.22	126.07	114.54
2	3A	101	LHG	C17-C16-C15	2.22	126.07	114.54
2	1E	101	LHG	C16-C15-C14	2.22	126.07	114.54
2	4E	101	LHG	C16-C15-C14	2.22	126.07	114.54
2	1C	101	LHG	C16-C15-C14	2.22	126.08	114.54
2	2I	101	LHG	C16-C15-C14	2.22	126.08	114.54
2	3I	101	LHG	C16-C15-C14	2.22	126.08	114.54
2	4N	101	LHG	C17-C16-C15	2.22	126.08	114.54
2	5N	101	LHG	C16-C15-C14	2.22	126.08	114.54
2	1I	101	LHG	C16-C15-C14	2.22	126.08	114.54
2	2J	101	LHG	C16-C15-C14	2.22	126.09	114.54
2	1A	101	LHG	C17-C16-C15	2.22	126.09	114.54
2	5E	101	LHG	C16-C15-C14	2.22	126.09	114.54
2	5I	101	LHG	C16-C15-C14	2.22	126.09	114.54
2	1B	101	LHG	C16-C15-C14	2.22	126.09	114.54
2	3C	101	LHG	C16-C15-C14	2.22	126.09	114.54
2	3D	101	LHG	C16-C15-C14	2.22	126.09	114.54
2	2N	101	LHG	C16-C15-C14	2.22	126.09	114.54
2	5J	101	LHG	C16-C15-C14	2.22	126.09	114.54
2	4O	101	LHG	C17-C16-C15	2.22	126.09	114.54
2	4D	101	LHG	C16-C15-C14	2.22	126.10	114.54
2	3H	101	LHG	C16-C15-C14	2.22	126.10	114.54
2	1N	101	LHG	C17-C16-C15	2.23	126.10	114.54
2	5A	101	LHG	C17-C16-C15	2.23	126.10	114.54
2	4N	101	LHG	C16-C15-C14	2.23	126.10	114.54
2	1J	101	LHG	C16-C15-C14	2.23	126.10	114.54
2	2E	101	LHG	C17-C16-C15	2.23	126.10	114.54
2	5D	101	LHG	C16-C15-C14	2.23	126.10	114.54
2	2G	101	LHG	C17-C16-C15	2.23	126.11	114.54
2	5B	101	LHG	C16-C15-C14	2.23	126.11	114.54
2	5M	101	LHG	C16-C15-C14	2.23	126.11	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5G	101	LHG	C17-C16-C15	2.23	126.11	114.54
2	3M	101	LHG	C16-C15-C14	2.23	126.11	114.54
2	3G	101	LHG	C17-C16-C15	2.23	126.11	114.54
2	5H	101	LHG	C17-C16-C15	2.23	126.11	114.54
2	5F	101	LHG	C17-C16-C15	2.23	126.11	114.54
2	2F	101	LHG	C17-C16-C15	2.23	126.12	114.54
2	3J	101	LHG	C16-C15-C14	2.23	126.12	114.54
2	3N	101	LHG	C17-C16-C15	2.23	126.12	114.54
2	4G	101	LHG	C17-C16-C15	2.23	126.12	114.54
2	5B	101	LHG	C17-C16-C15	2.23	126.12	114.54
2	2B	101	LHG	C16-C15-C14	2.23	126.12	114.54
2	3K	101	LHG	C16-C15-C14	2.23	126.12	114.54
2	1G	101	LHG	C17-C16-C15	2.23	126.13	114.54
2	3D	101	LHG	C17-C16-C15	2.23	126.13	114.54
2	4E	101	LHG	C17-C16-C15	2.23	126.13	114.54
2	2M	101	LHG	C16-C15-C14	2.23	126.13	114.54
2	5M	101	LHG	C17-C16-C15	2.23	126.13	114.54
2	5D	101	LHG	C17-C16-C15	2.23	126.13	114.54
2	1K	101	LHG	C16-C15-C14	2.23	126.13	114.54
2	4F	101	LHG	C17-C16-C15	2.23	126.13	114.54
2	2D	101	LHG	C17-C16-C15	2.23	126.13	114.54
2	1N	101	LHG	C16-C15-C14	2.23	126.14	114.54
2	3B	101	LHG	C16-C15-C14	2.23	126.14	114.54
2	3O	101	LHG	C16-C15-C14	2.23	126.14	114.54
2	1O	101	LHG	C16-C15-C14	2.23	126.14	114.54
2	5O	101	LHG	C16-C15-C14	2.23	126.14	114.54
2	5C	101	LHG	C16-C15-C14	2.23	126.14	114.54
2	4J	101	LHG	C16-C15-C14	2.23	126.14	114.54
2	4B	101	LHG	C17-C16-C15	2.23	126.14	114.54
2	1B	101	LHG	C17-C16-C15	2.23	126.14	114.54
2	3H	101	LHG	C17-C16-C15	2.23	126.15	114.54
2	3M	101	LHG	C17-C16-C15	2.23	126.15	114.54
2	4C	101	LHG	C17-C16-C15	2.23	126.15	114.54
2	3L	101	LHG	C16-C15-C14	2.23	126.15	114.54
2	4H	101	LHG	C17-C16-C15	2.23	126.15	114.54
2	2H	101	LHG	C17-C16-C15	2.23	126.15	114.54
2	3J	101	LHG	C17-C16-C15	2.24	126.15	114.54
2	4O	101	LHG	C16-C15-C14	2.24	126.15	114.54
2	1D	101	LHG	C17-C16-C15	2.24	126.15	114.54
2	1E	101	LHG	C17-C16-C15	2.24	126.16	114.54
2	2M	101	LHG	C17-C16-C15	2.24	126.16	114.54
2	1F	101	LHG	C17-C16-C15	2.24	126.16	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1H	101	LHG	C17-C16-C15	2.24	126.16	114.54
2	1I	101	LHG	C17-C16-C15	2.24	126.16	114.54
2	4M	101	LHG	C16-C15-C14	2.24	126.16	114.54
2	5I	101	LHG	C17-C16-C15	2.24	126.17	114.54
2	4L	101	LHG	C16-C15-C14	2.24	126.17	114.54
2	2O	101	LHG	C16-C15-C14	2.24	126.17	114.54
2	1C	101	LHG	C17-C16-C15	2.24	126.17	114.54
2	2K	101	LHG	C16-C15-C14	2.24	126.17	114.54
2	3E	101	LHG	C17-C16-C15	2.24	126.17	114.54
2	4D	101	LHG	C17-C16-C15	2.24	126.17	114.54
2	1L	101	LHG	C16-C15-C14	2.24	126.17	114.54
2	5E	101	LHG	C17-C16-C15	2.24	126.17	114.54
2	3I	101	LHG	C17-C16-C15	2.24	126.17	114.54
2	3B	101	LHG	C17-C16-C15	2.24	126.17	114.54
2	2I	101	LHG	C17-C16-C15	2.24	126.18	114.54
2	3C	101	LHG	C17-C16-C15	2.24	126.18	114.54
2	2C	101	LHG	C17-C16-C15	2.24	126.18	114.54
2	1J	101	LHG	C17-C16-C15	2.24	126.18	114.54
2	3F	101	LHG	C17-C16-C15	2.24	126.18	114.54
2	3N	101	LHG	C16-C15-C14	2.24	126.18	114.54
2	1M	101	LHG	C16-C15-C14	2.24	126.18	114.54
2	4K	101	LHG	C16-C15-C14	2.24	126.18	114.54
2	4I	101	LHG	C17-C16-C15	2.24	126.18	114.54
2	2B	101	LHG	C17-C16-C15	2.24	126.18	114.54
2	3L	101	LHG	C17-C16-C15	2.24	126.19	114.54
2	5K	101	LHG	C16-C15-C14	2.24	126.19	114.54
2	3K	101	LHG	C17-C16-C15	2.24	126.19	114.54
2	5L	101	LHG	C16-C15-C14	2.24	126.20	114.54
2	4L	101	LHG	C17-C16-C15	2.24	126.20	114.54
2	5J	101	LHG	C17-C16-C15	2.24	126.20	114.54
2	1M	101	LHG	C17-C16-C15	2.24	126.20	114.54
2	5C	101	LHG	C17-C16-C15	2.24	126.20	114.54
2	2J	101	LHG	C17-C16-C15	2.25	126.20	114.54
2	2L	101	LHG	C16-C15-C14	2.25	126.21	114.54
2	4J	101	LHG	C17-C16-C15	2.25	126.21	114.54
2	4M	101	LHG	C17-C16-C15	2.25	126.21	114.54
2	1L	101	LHG	C17-C16-C15	2.25	126.23	114.54
2	1K	101	LHG	C17-C16-C15	2.25	126.24	114.54
2	5K	101	LHG	C17-C16-C15	2.25	126.24	114.54
2	2L	101	LHG	C17-C16-C15	2.25	126.25	114.54
2	2K	101	LHG	C17-C16-C15	2.26	126.27	114.54
2	4K	101	LHG	C17-C16-C15	2.26	126.28	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5L	101	LHG	C17-C16-C15	2.26	126.29	114.54

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	5F	101	LHG	C5-O7-C7-C8
2	3E	101	LHG	C5-O7-C7-C8
2	2H	101	LHG	C5-O7-C7-C8
2	4I	101	LHG	C5-O7-C7-C8
2	4J	101	LHG	C5-O7-C7-C8
2	5H	101	LHG	C5-O7-C7-C8
2	5I	101	LHG	C5-O7-C7-C8
2	4B	101	LHG	C5-O7-C7-C8
2	2F	101	LHG	C5-O7-C7-C8
2	3J	101	LHG	C5-O7-C7-C8
2	5E	101	LHG	C5-O7-C7-C8
2	4K	101	LHG	C5-O7-C7-C8
2	3C	101	LHG	C5-O7-C7-C8
2	1J	101	LHG	C5-O7-C7-C8
2	1K	101	LHG	C5-O7-C7-C8
2	5J	101	LHG	C5-O7-C7-C8
2	4E	101	LHG	C5-O7-C7-C8
2	4G	101	LHG	C5-O7-C7-C8
2	3O	101	LHG	C5-O7-C7-C8
2	1E	101	LHG	C5-O7-C7-C8
2	2O	101	LHG	C5-O7-C7-C8
2	5K	101	LHG	C5-O7-C7-C8
2	3F	101	LHG	C5-O7-C7-C8
2	5L	101	LHG	C5-O7-C7-C8
2	3B	101	LHG	C5-O7-C7-C8
2	2E	101	LHG	C5-O7-C7-C8
2	4N	101	LHG	C5-O7-C7-C8
2	1I	101	LHG	C5-O7-C7-C8
2	3A	101	LHG	C5-O7-C7-C8
2	2C	101	LHG	C5-O7-C7-C8
2	1B	101	LHG	C5-O7-C7-C8
2	1F	101	LHG	C5-O7-C7-C8
2	5O	101	LHG	C5-O7-C7-C8
2	2D	101	LHG	C5-O7-C7-C8
2	5N	101	LHG	C5-O7-C7-C8
2	1D	101	LHG	C5-O7-C7-C8

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Mol	Chain	Res	Type	Atoms
2	3I	101	LHG	C5-O7-C7-C8
2	1N	101	LHG	C5-O7-C7-C8
2	3G	101	LHG	C5-O7-C7-C8
2	5C	101	LHG	C5-O7-C7-C8
2	2I	101	LHG	C5-O7-C7-C8
2	2A	101	LHG	C5-O7-C7-C8
2	3L	101	LHG	C5-O7-C7-C8
2	1H	101	LHG	C5-O7-C7-C8
2	5D	101	LHG	C5-O7-C7-C8
2	2K	101	LHG	C5-O7-C7-C8
2	1O	101	LHG	C5-O7-C7-C8
2	4D	101	LHG	C5-O7-C7-C8
2	3H	101	LHG	C5-O7-C7-C8
2	1A	101	LHG	C5-O7-C7-C8
2	3D	101	LHG	C5-O7-C7-C8
2	2J	101	LHG	C5-O7-C7-C8
2	4A	101	LHG	C5-O7-C7-C8
2	1C	101	LHG	C5-O7-C7-C8
2	4C	101	LHG	C5-O7-C7-C8
2	4F	101	LHG	C5-O7-C7-C8
2	3M	101	LHG	C5-O7-C7-C8
2	3N	101	LHG	C5-O7-C7-C8
2	4H	101	LHG	C5-O7-C7-C8
2	1G	101	LHG	C5-O7-C7-C8
2	1M	101	LHG	C5-O7-C7-C8
2	5A	101	LHG	C5-O7-C7-C8
2	5G	101	LHG	C5-O7-C7-C8
2	2B	101	LHG	C5-O7-C7-C8
2	2L	101	LHG	C5-O7-C7-C8
2	4O	101	LHG	C5-O7-C7-C8
2	4M	101	LHG	C5-O7-C7-C8
2	5B	101	LHG	C5-O7-C7-C8
2	4L	101	LHG	C5-O7-C7-C8
2	1L	101	LHG	C5-O7-C7-C8
2	2N	101	LHG	C5-O7-C7-C8
2	3K	101	LHG	C5-O7-C7-C8
2	5M	101	LHG	C5-O7-C7-C8
2	2M	101	LHG	C5-O7-C7-C8
2	2G	101	LHG	C5-O7-C7-C8

There are no ring outliers.

75 monomers are involved in 2082 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1A	101	LHG	23	0
2	1B	101	LHG	28	0
2	1C	101	LHG	28	0
2	1D	101	LHG	30	0
2	1E	101	LHG	30	0
2	1F	101	LHG	31	0
2	1G	101	LHG	31	0
2	1H	101	LHG	30	0
2	1I	101	LHG	30	0
2	1J	101	LHG	29	0
2	1K	101	LHG	29	0
2	1L	101	LHG	27	0
2	1M	101	LHG	24	0
2	1N	101	LHG	25	0
2	1O	101	LHG	25	0
2	2A	101	LHG	22	0
2	2B	101	LHG	28	0
2	2C	101	LHG	29	0
2	2D	101	LHG	28	0
2	2E	101	LHG	29	0
2	2F	101	LHG	29	0
2	2G	101	LHG	29	0
2	2H	101	LHG	30	0
2	2I	101	LHG	29	0
2	2J	101	LHG	29	0
2	2K	101	LHG	28	0
2	2L	101	LHG	27	0
2	2M	101	LHG	26	0
2	2N	101	LHG	25	0
2	2O	101	LHG	24	0
2	3A	101	LHG	22	0
2	3B	101	LHG	27	0
2	3C	101	LHG	29	0
2	3D	101	LHG	30	0
2	3E	101	LHG	29	0
2	3F	101	LHG	29	0
2	3G	101	LHG	29	0
2	3H	101	LHG	30	0
2	3I	101	LHG	29	0
2	3J	101	LHG	28	0
2	3K	101	LHG	28	0
2	3L	101	LHG	27	0
2	3M	101	LHG	26	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	3N	101	LHG	26	0
2	3O	101	LHG	26	0
2	4A	101	LHG	22	0
2	4B	101	LHG	28	0
2	4C	101	LHG	28	0
2	4D	101	LHG	28	0
2	4E	101	LHG	30	0
2	4F	101	LHG	31	0
2	4G	101	LHG	30	0
2	4H	101	LHG	29	0
2	4I	101	LHG	30	0
2	4J	101	LHG	28	0
2	4K	101	LHG	28	0
2	4L	101	LHG	27	0
2	4M	101	LHG	26	0
2	4N	101	LHG	26	0
2	4O	101	LHG	26	0
2	5A	101	LHG	22	0
2	5B	101	LHG	28	0
2	5C	101	LHG	29	0
2	5D	101	LHG	30	0
2	5E	101	LHG	30	0
2	5F	101	LHG	30	0
2	5G	101	LHG	30	0
2	5H	101	LHG	30	0
2	5I	101	LHG	29	0
2	5J	101	LHG	29	0
2	5K	101	LHG	28	0
2	5L	101	LHG	27	0
2	5M	101	LHG	25	0
2	5N	101	LHG	26	0
2	5O	101	LHG	25	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.