



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 11:32 PM EDT

PDB ID : 6YFO  
Title : Virus-like particle of bacteriophage GQ-907  
Authors : Rumnieks, J.; Kalnins, G.; Sisovs, M.; Lieknina, I.; Tars, K.  
Deposited on : 2020-03-26  
Resolution : 3.48 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

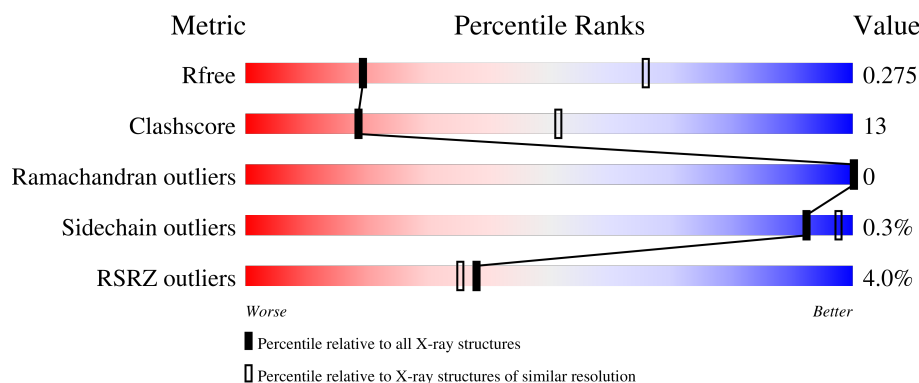
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.48 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	131	<div> <div>3%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
1	AB	131	<div> <div>2%</div> <div>68%</div> <div>32%</div> </div>
1	AC	131	<div> <div>7%</div> <div>74%</div> <div>26%</div> </div>
1	AD	131	<div> <div>4%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>
1	AE	131	<div> <div>2%</div> <div>69%</div> <div>31%</div> </div>

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Mol	Chain	Length	Quality of chain
1	AF	131	
1	AG	131	
1	AH	131	
1	AI	131	
1	AJ	131	
1	AK	131	
1	AL	131	
1	AM	131	
1	AN	131	
1	AO	131	
1	AP	131	
1	AQ	131	
1	AR	131	
1	AS	131	
1	AT	131	
1	AU	131	
1	AV	131	
1	AW	131	
1	AX	131	
1	AY	131	
1	AZ	131	
1	BA	131	
1	BB	131	
1	BC	131	
1	BD	131	

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Mol	Chain	Length	Quality of chain
1	BE	131	
1	BF	131	
1	BG	131	
1	BH	131	
1	BI	131	
1	BJ	131	
1	BK	131	
1	BL	131	
1	BM	131	
1	BN	131	
1	BO	131	
1	BP	131	
1	BQ	131	
1	BR	131	
1	BS	131	
1	BT	131	
1	BU	131	
1	BV	131	
1	BW	131	
1	BX	131	
1	BY	131	
1	BZ	131	
1	CA	131	
1	CB	131	
1	CC	131	

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Mol	Chain	Length	Quality of chain
1	CD	131	<div> <div>3%</div> <div>66%</div> <div>34%</div> </div>
1	CE	131	<div> <div>6%</div> <div>69%</div> <div>31%</div> </div>
1	CF	131	<div> <div>5%</div> <div>80%</div> <div>19%</div> </div>
1	CG	131	<div> <div>5%</div> <div>69%</div> <div>31%</div> </div>
1	CH	131	<div> <div>4%</div> <div>79%</div> <div>21%</div> </div>
1	CI	131	<div> <div>5%</div> <div>77%</div> <div>22%</div> </div>
1	CJ	131	<div> <div>2%</div> <div>69%</div> <div>31%</div> </div>
1	CK	131	<div> <div>6%</div> <div>75%</div> <div>25%</div> </div>
1	CL	131	<div> <div>8%</div> <div>80%</div> <div>19%</div> </div>
1	CM	131	<div> <div>3%</div> <div>70%</div> <div>30%</div> </div>
1	CN	131	<div> <div>%</div> <div>76%</div> <div>24%</div> </div>
1	CO	131	<div> <div>2%</div> <div>83%</div> <div>16%</div> </div>
1	CP	131	<div> <div>2%</div> <div>70%</div> <div>30%</div> </div>
1	CQ	131	<div> <div>2%</div> <div>81%</div> <div>19%</div> </div>
1	CR	131	<div> <div>5%</div> <div>81%</div> <div>18%</div> </div>
1	CS	131	<div> <div>4%</div> <div>70%</div> <div>30%</div> </div>
1	CT	131	<div> <div>12%</div> <div>74%</div> <div>26%</div> </div>
1	CU	131	<div> <div>3%</div> <div>80%</div> <div>19%</div> </div>
1	CV	131	<div> <div>4%</div> <div>69%</div> <div>31%</div> </div>
1	CW	131	<div> <div>13%</div> <div>76%</div> <div>24%</div> </div>
1	CX	131	<div> <div>3%</div> <div>80%</div> <div>19%</div> </div>
1	CY	131	<div> <div>%</div> <div>72%</div> <div>28%</div> </div>
1	CZ	131	<div> <div>3%</div> <div>76%</div> <div>24%</div> </div>
1	DA	131	<div> <div>2%</div> <div>79%</div> <div>20%</div> </div>
1	DB	131	<div> <div>6%</div> <div>69%</div> <div>31%</div> </div>

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Mol	Chain	Length	Quality of chain
1	DC	131	
1	DD	131	
1	DE	131	
1	DF	131	
1	DG	131	
1	DH	131	
1	DI	131	
1	DJ	131	
1	DK	131	
1	DL	131	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 87480 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			
1	AB	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			
1	AC	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			
1	AD	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			
1	AE	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			
1	AF	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			
1	AG	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			
1	AH	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			
1	AI	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			
1	AJ	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			
1	AK	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			
1	AL	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			
1	AM	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			
1	AN	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			
1	AO	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			
1	AP	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AQ	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	AR	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	AS	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	AT	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	AU	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	AV	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	AW	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	AX	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	AY	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	AZ	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	BA	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	BB	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	BC	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	BD	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	BE	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	BF	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	BG	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	BH	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	BI	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	BJ	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	BK	131	Total 972	C 607	N 166	O 198	S 1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BL	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	BM	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	BN	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	BO	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	BP	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	BQ	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	BR	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	BS	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	BT	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	BU	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	BV	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	BW	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	BX	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	BY	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	BZ	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	CA	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	CB	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	CC	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	CD	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	CE	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	CF	131	Total 972	C 607	N 166	O 198	S 1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CG	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	CH	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	CI	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	CJ	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	CK	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	CL	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	CM	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	CN	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	CO	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	CP	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	CQ	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	CR	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	CS	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	CT	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	CU	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	CV	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	CW	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	CX	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	CY	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	CZ	131	Total 972	C 607	N 166	O 198	S 1	0	0	0
1	DA	131	Total 972	C 607	N 166	O 198	S 1	0	0	0

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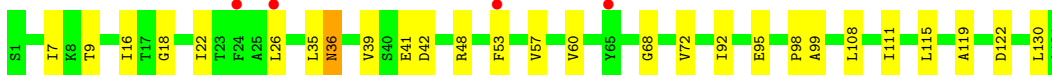
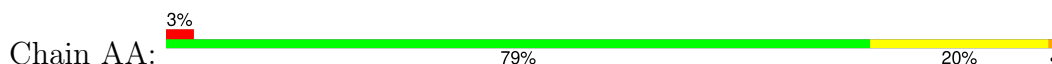
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	DB	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			
1	DC	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			
1	DD	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			
1	DE	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			
1	DF	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			
1	DG	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			
1	DH	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			
1	DI	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			
1	DJ	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			
1	DK	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			
1	DL	131	Total	C	N	O	S	0	0	0
			972	607	166	198	1			

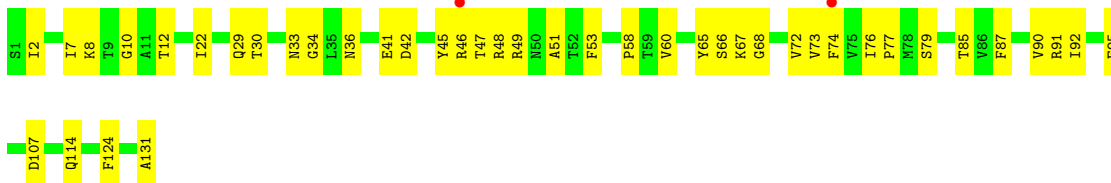
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

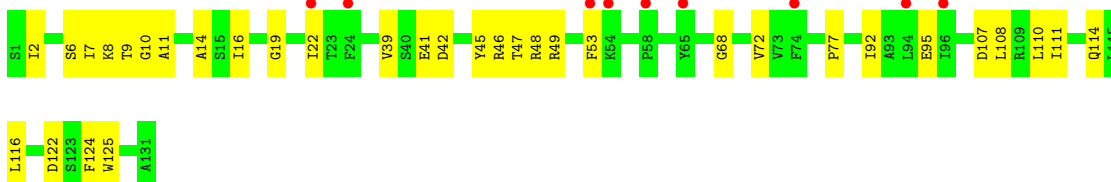
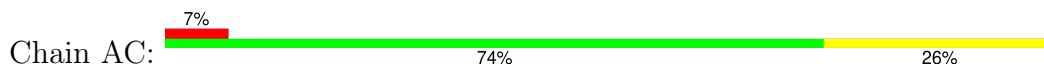
- Molecule 1: coat protein



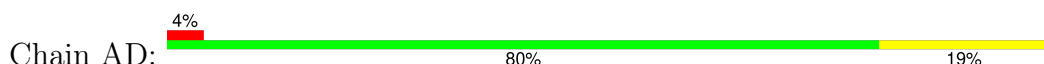
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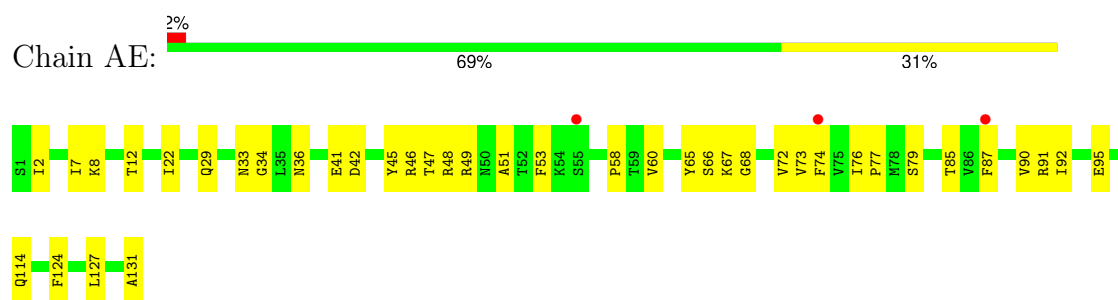
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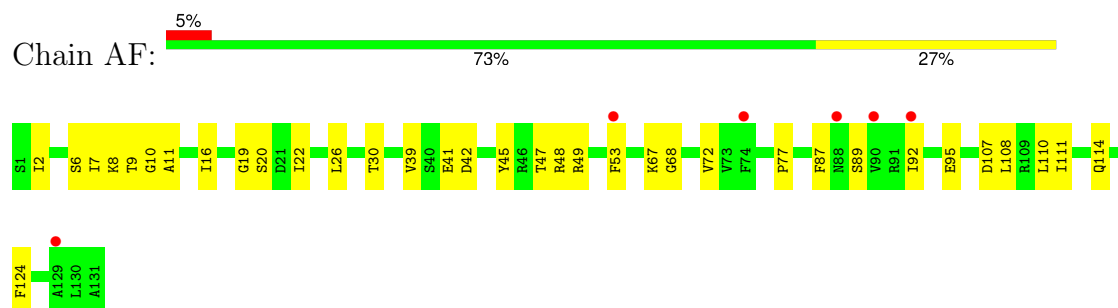
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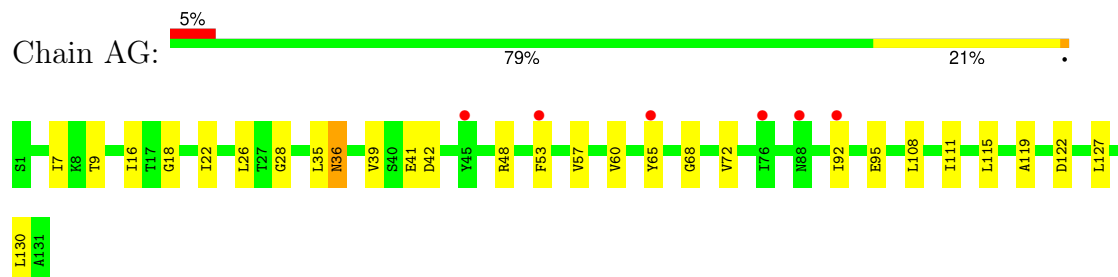
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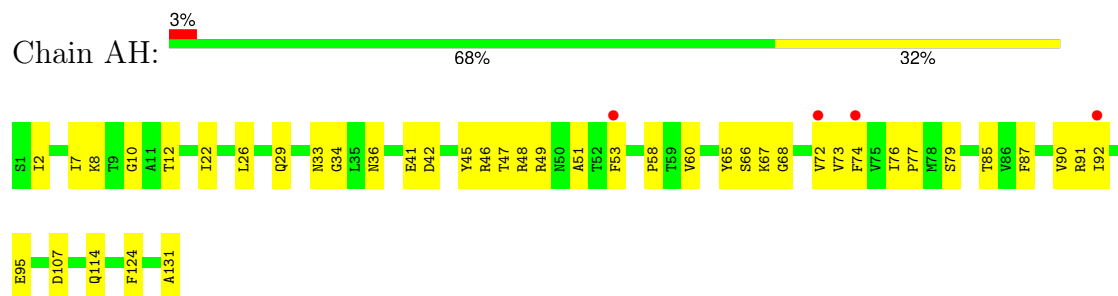
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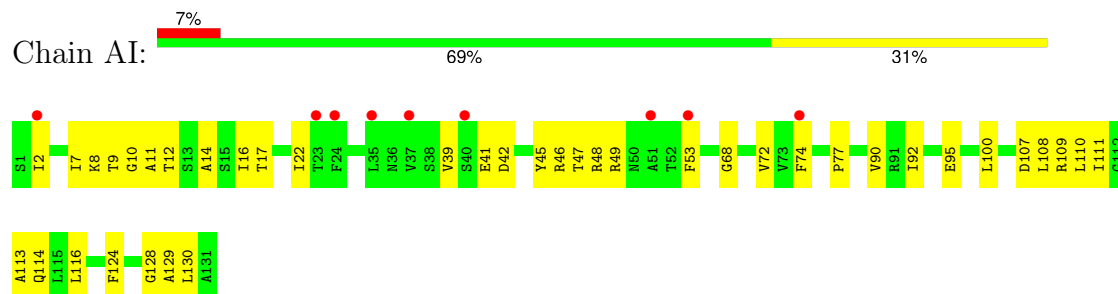
- Molecule 1: coat protein



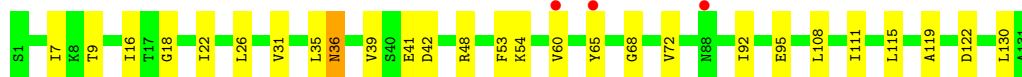
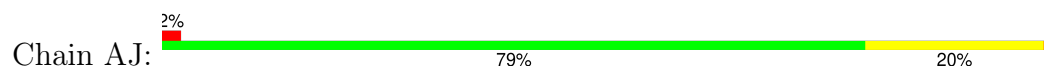
- Molecule 1: coat protein



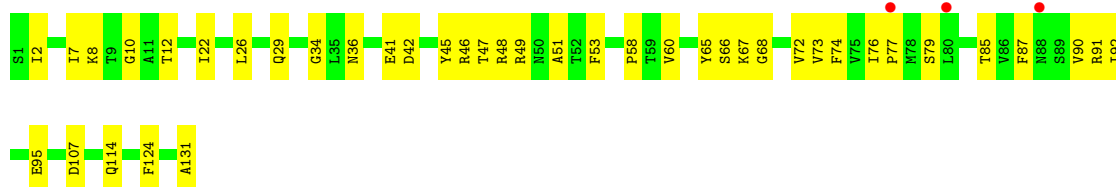
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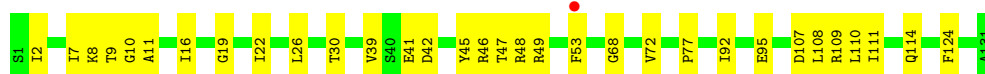
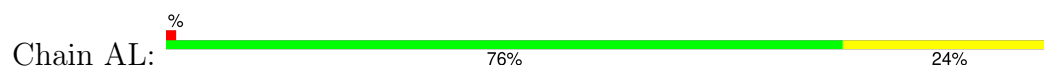
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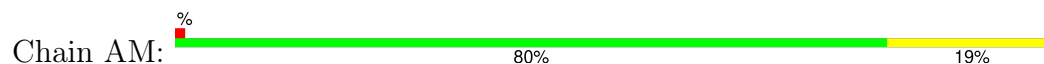
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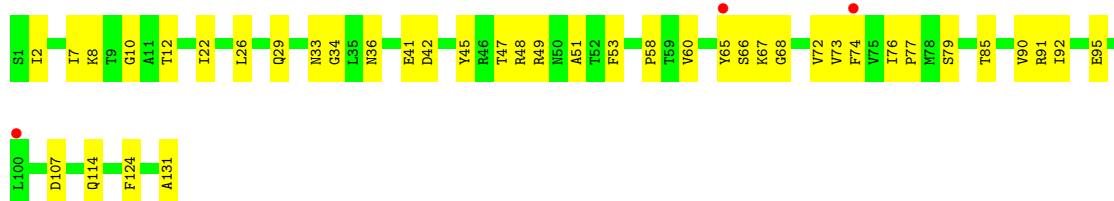
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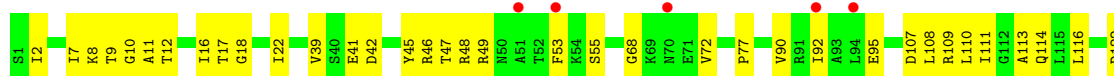
- Molecule 1: coat protein

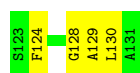


- Molecule 1: coat protein

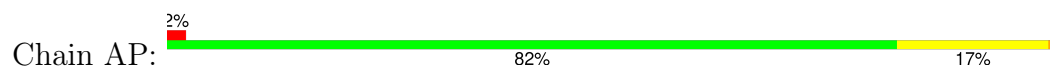


- Molecule 1: coat protein

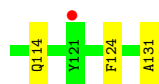
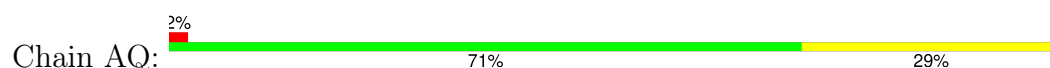




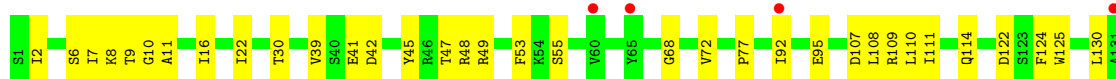
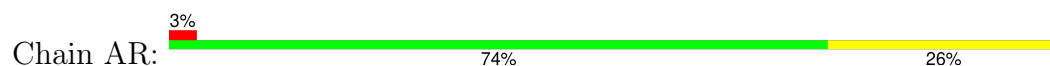
- Molecule 1: coat protein



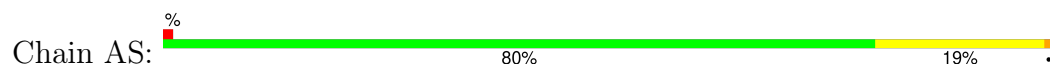
- Molecule 1: coat protein



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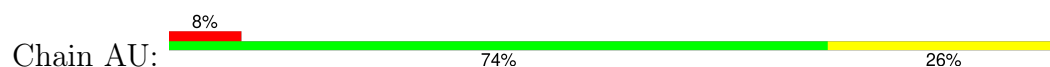
- Molecule 1: coat protein

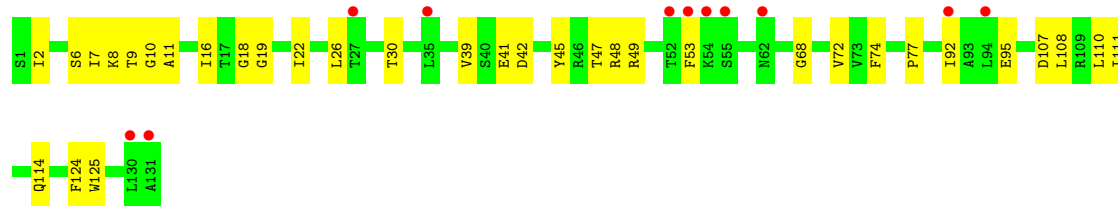


- Molecule 1: coat protein

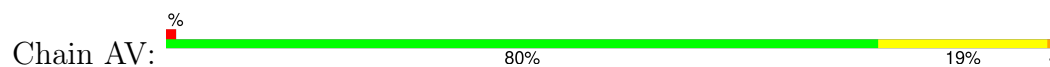


- Molecule 1: coat protein

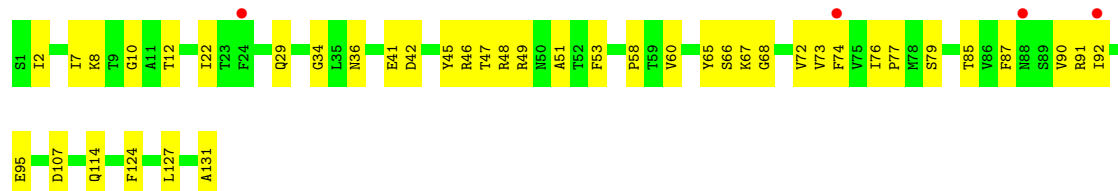
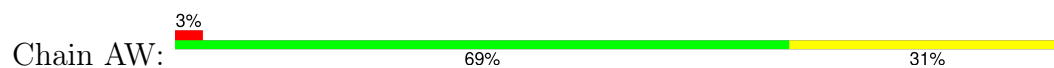




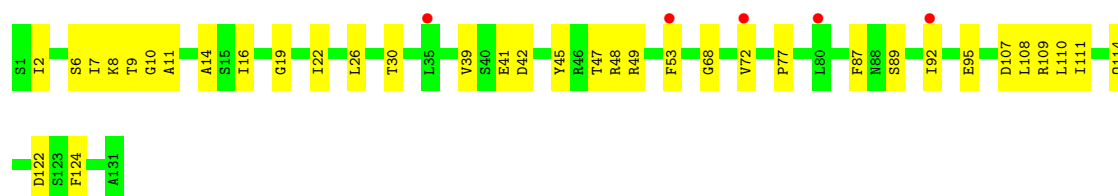
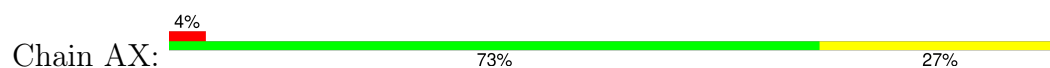
• Molecule 1: coat protein



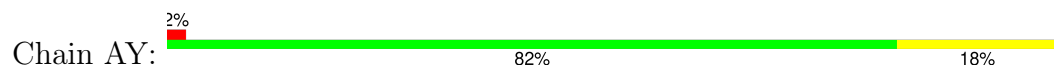
• Molecule 1: coat protein



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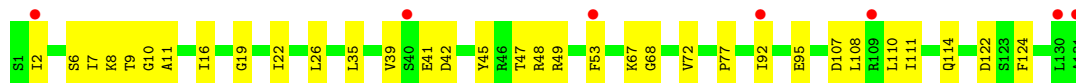
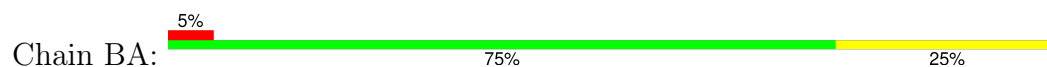
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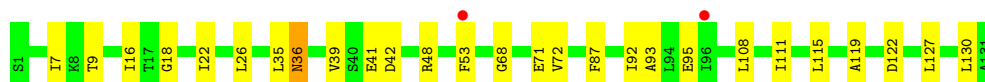
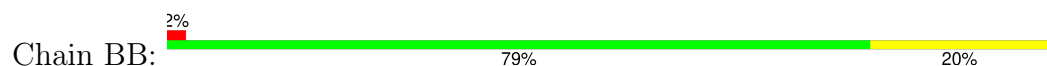




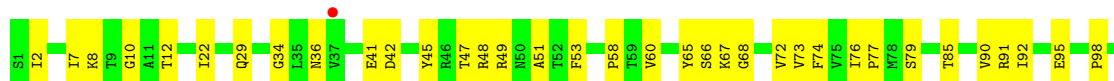
- Molecule 1: coat protein



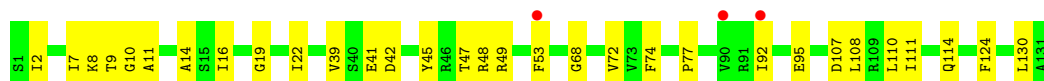
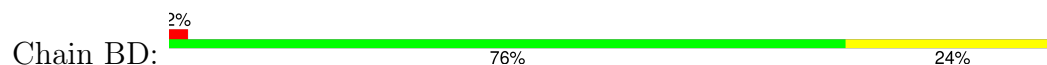
- Molecule 1: coat protein



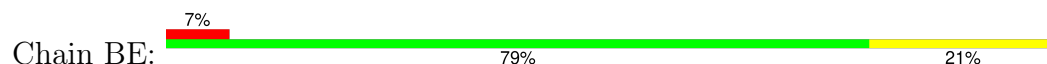
- Molecule 1: coat protein



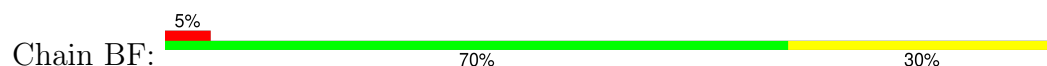
- Molecule 1: coat protein

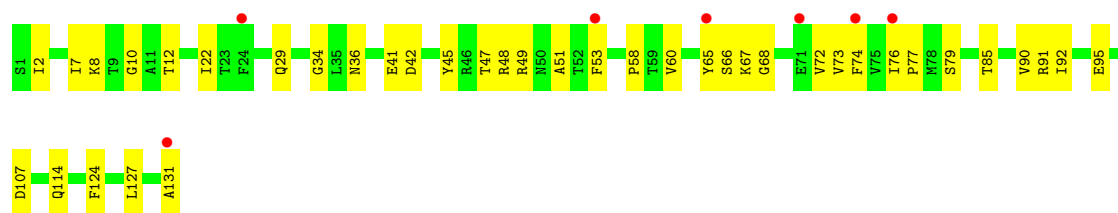


- Molecule 1: coat protein

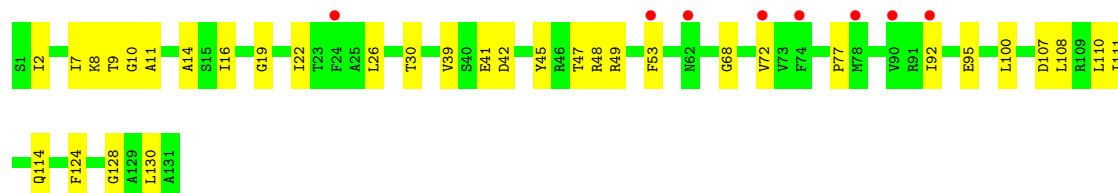
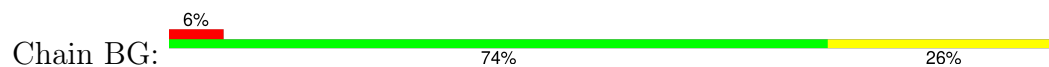


- Molecule 1: coat protein

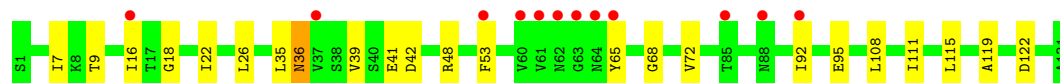
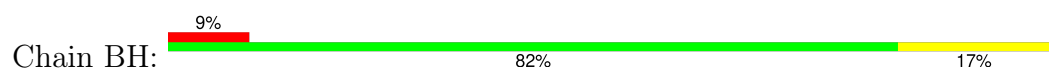




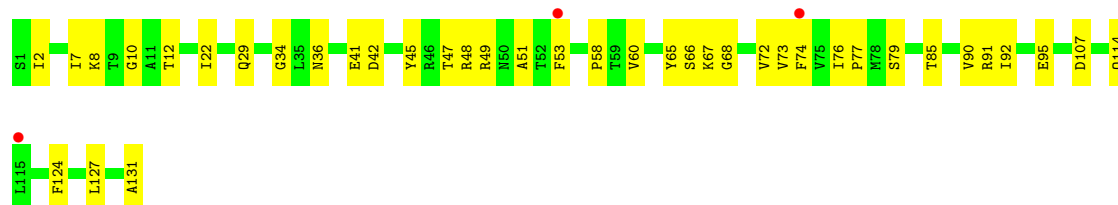
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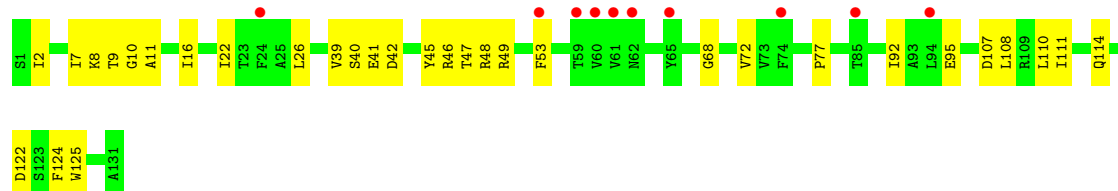
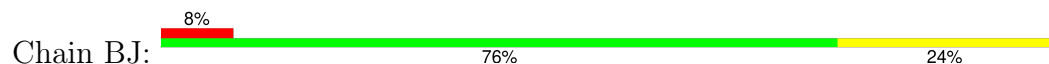
- Molecule 1: coat protein



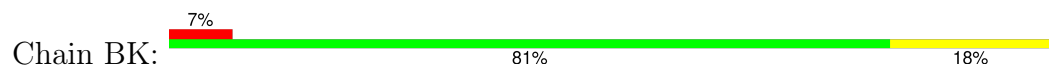
- Molecule 1: coat protein

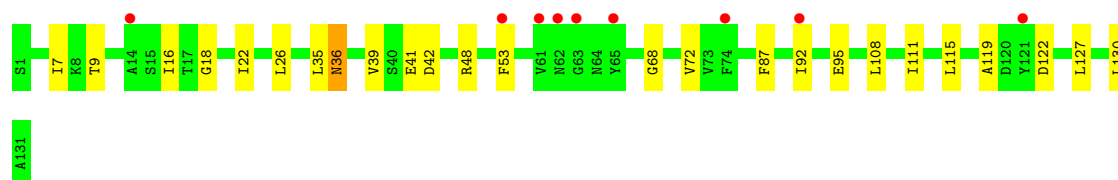


- Molecule 1: coat protein

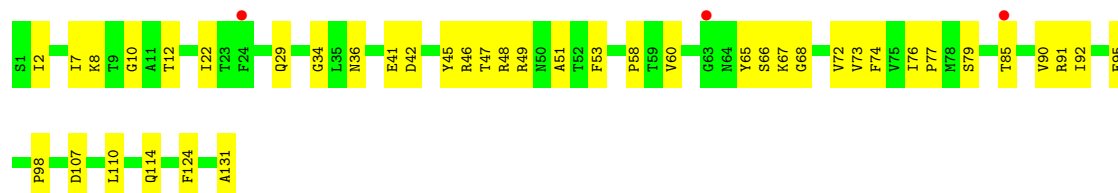


- Molecule 1: coat protein

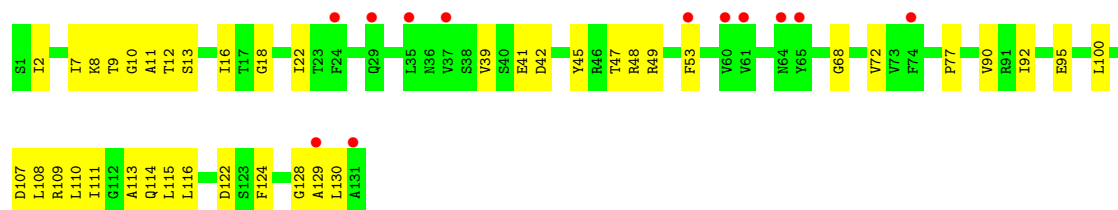




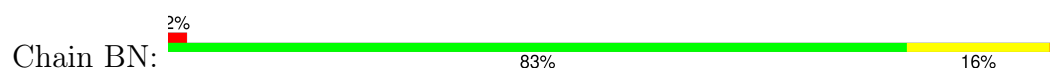
- Molecule 1: coat protein



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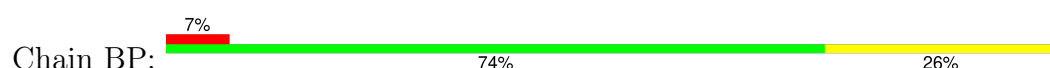
- Molecule 1: coat protein

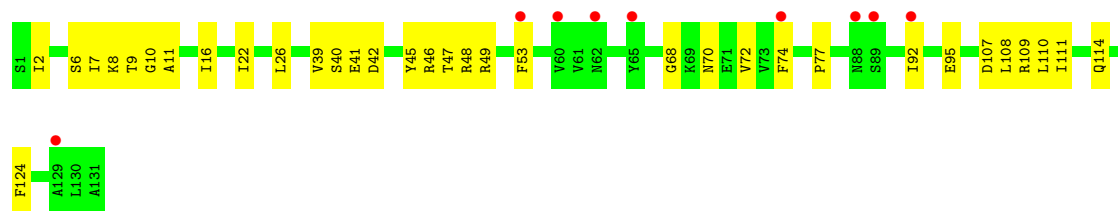


- Molecule 1: coat protein

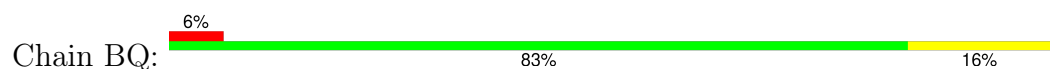


- Molecule 1: coat protein

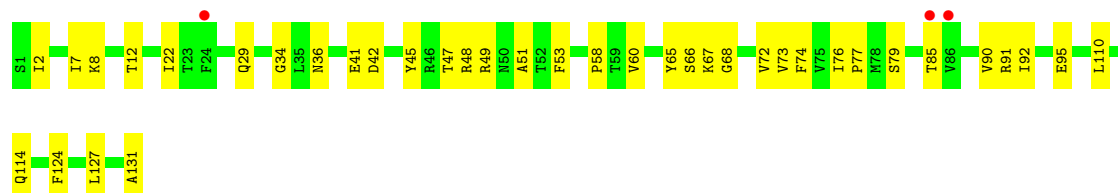
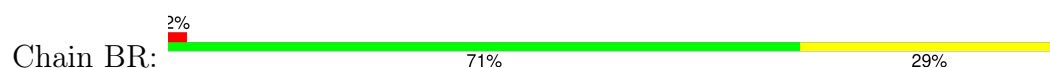




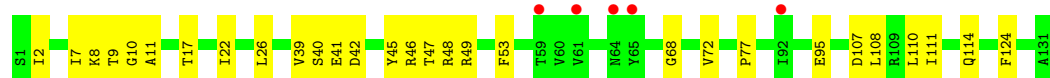
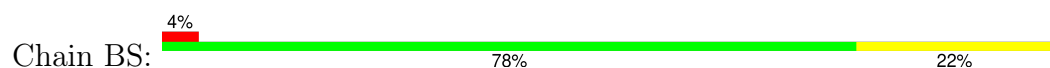
- Molecule 1: coat protein



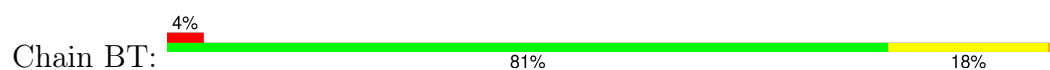
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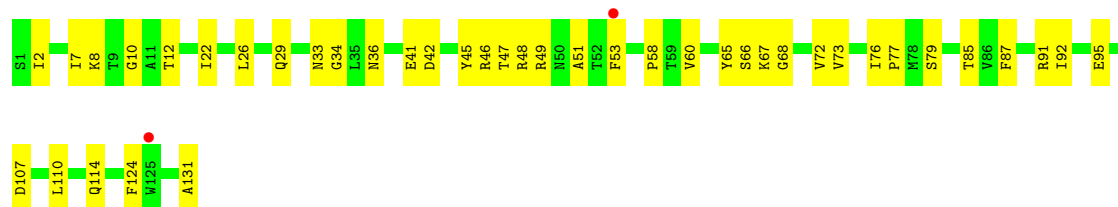
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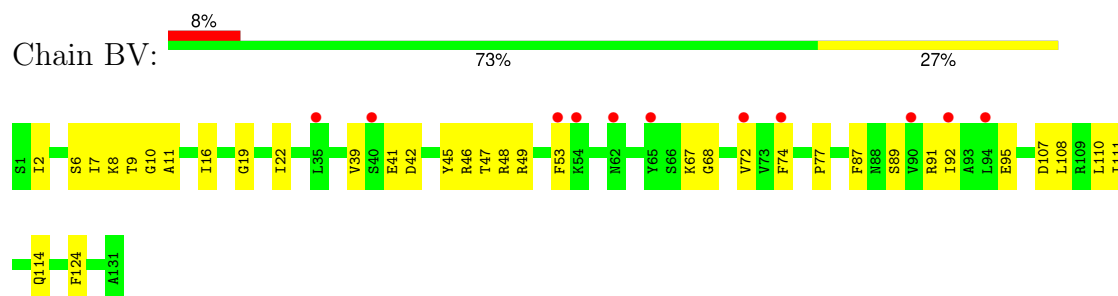
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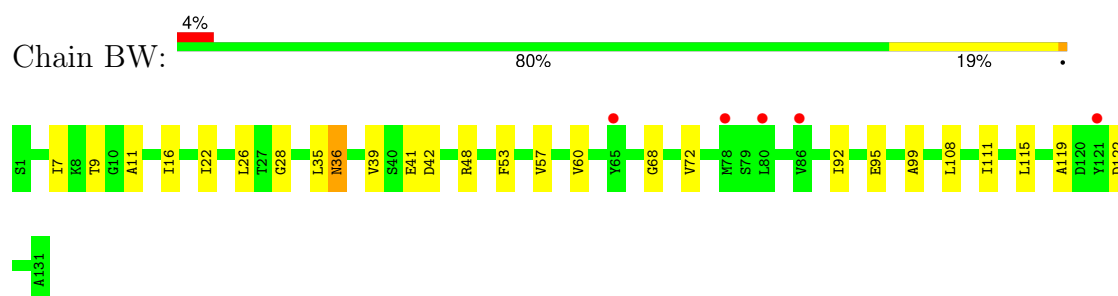
- Molecule 1: coat protein



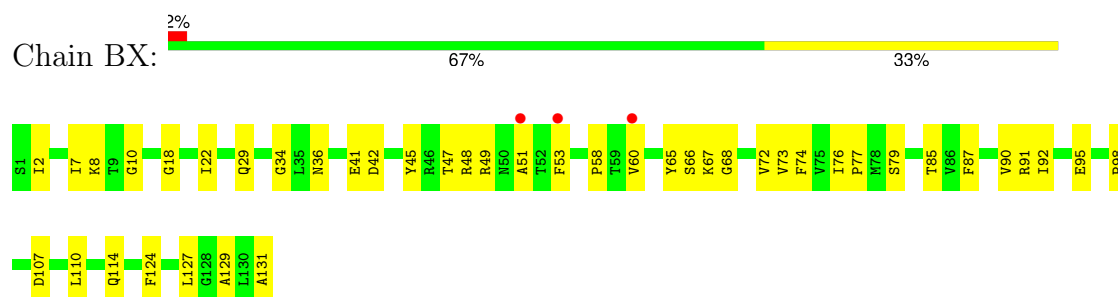
## ● Molecule 1: coat protein



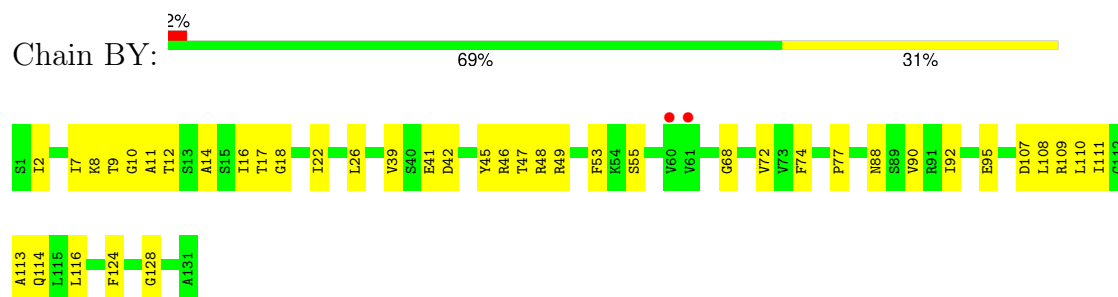
## ● Molecule 1: coat protein



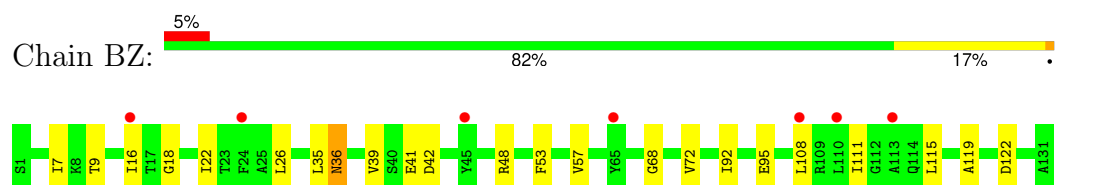
## ● Molecule 1: coat protein



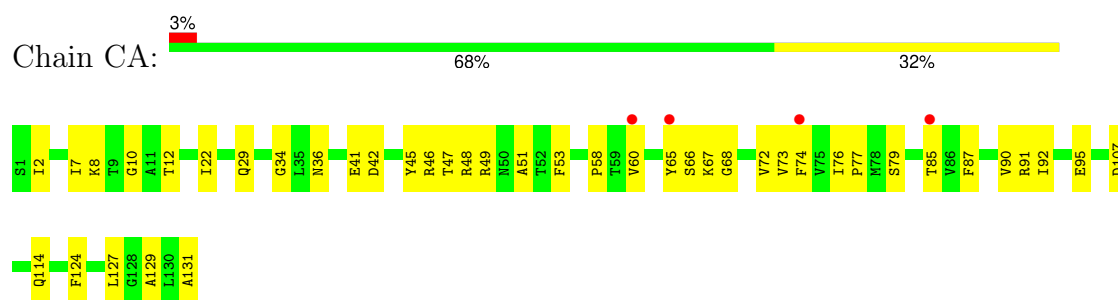
## ● Molecule 1: coat protein



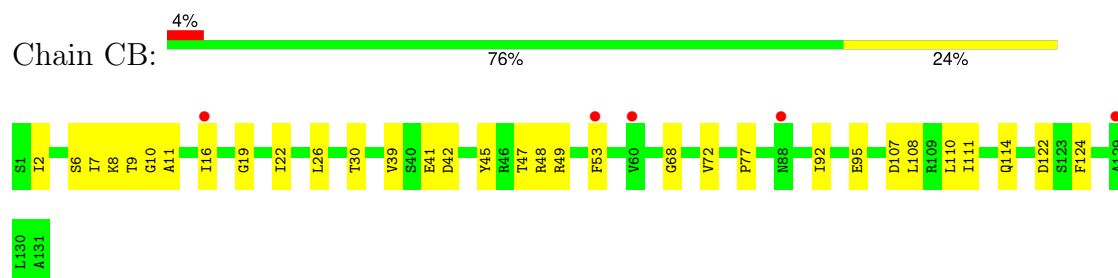
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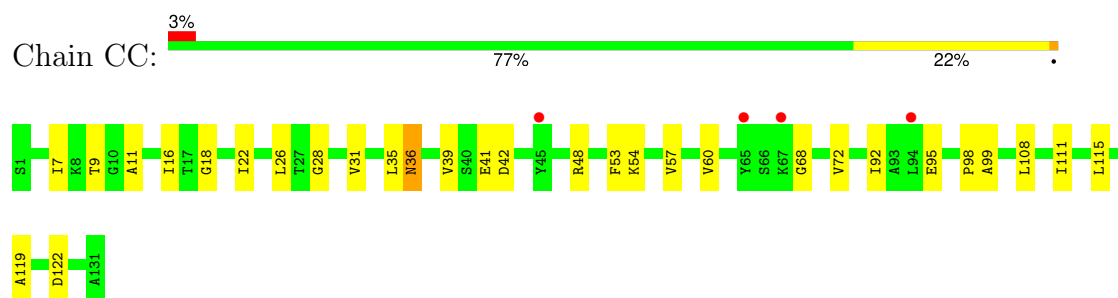
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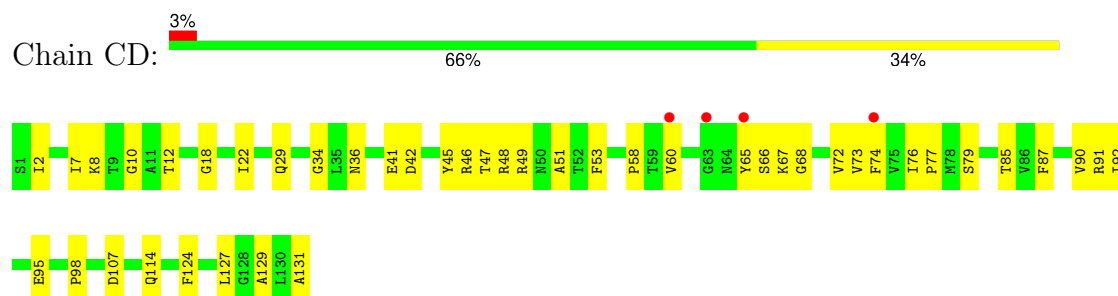
- Molecule 1: coat protein



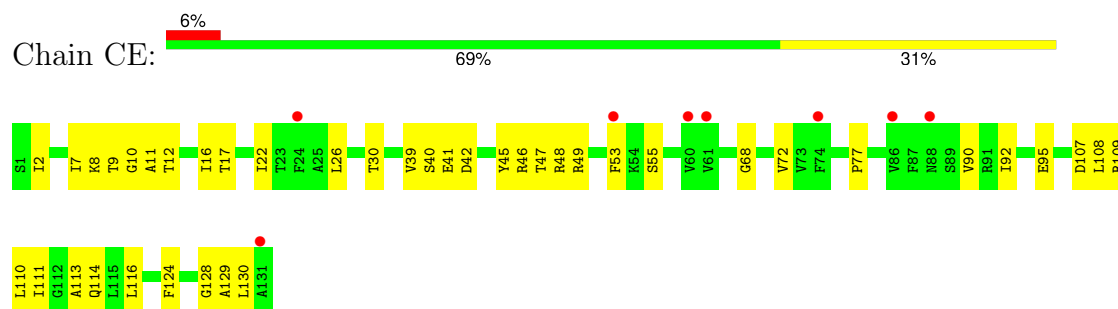
- Molecule 1: coat protein



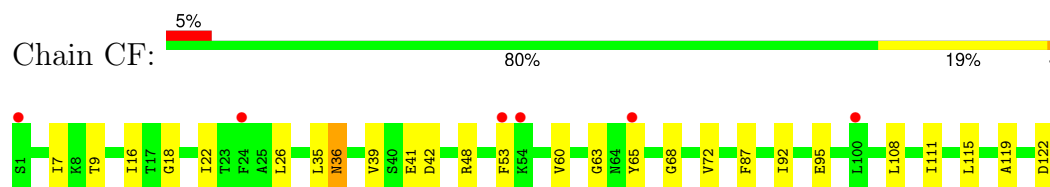
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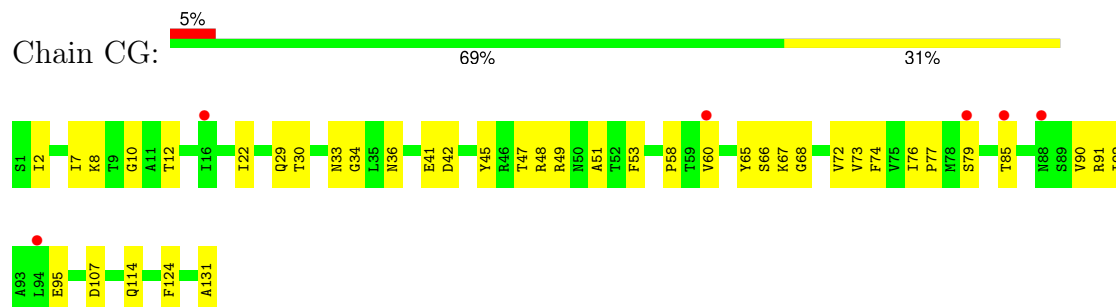
- Molecule 1: coat protein



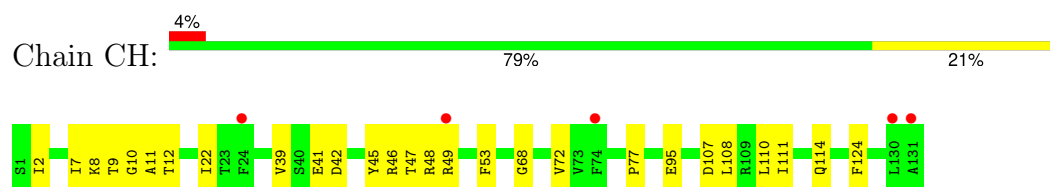
- Molecule 1: coat protein



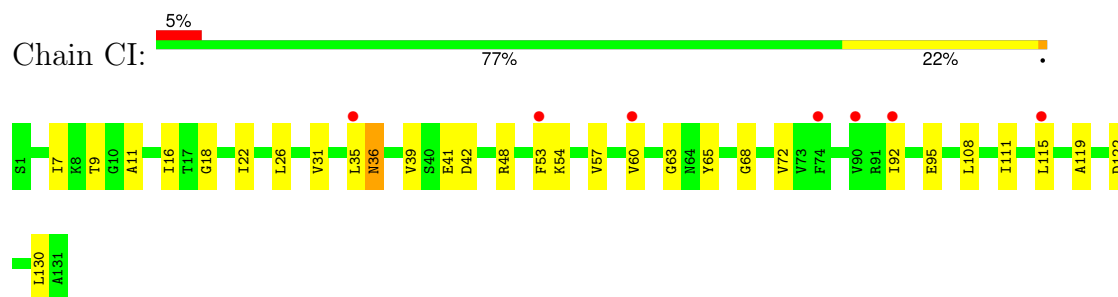
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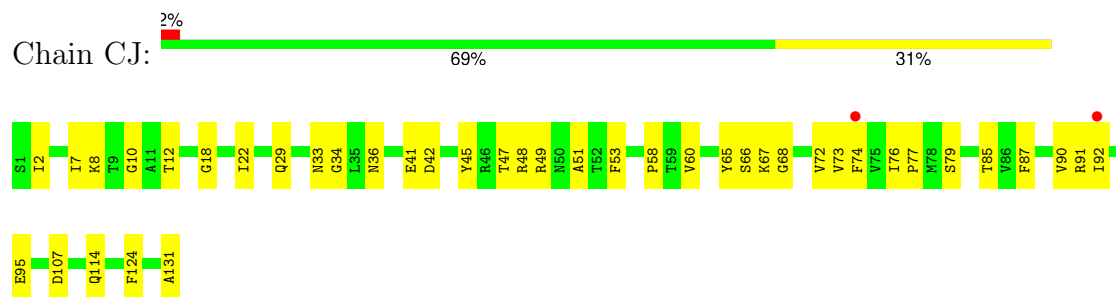
- Molecule 1: coat protein



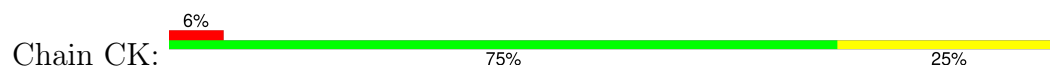
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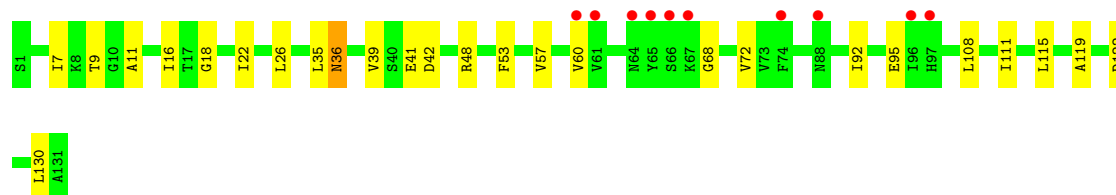
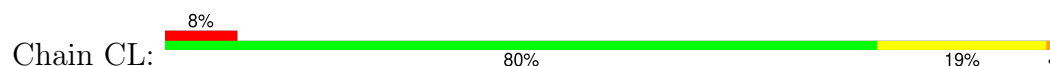


- Molecule 1: coat protein

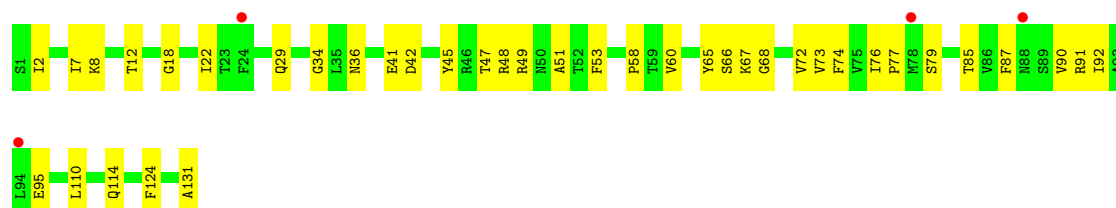
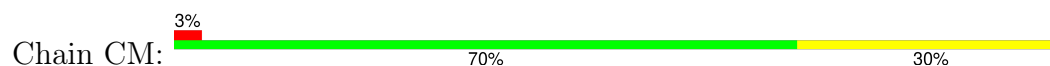




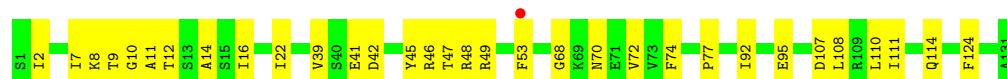
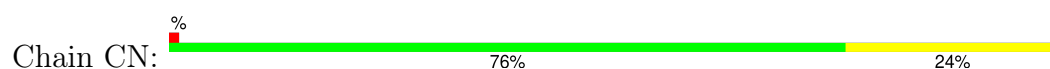
- Molecule 1: coat protein



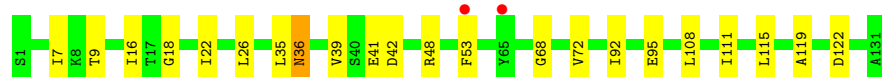
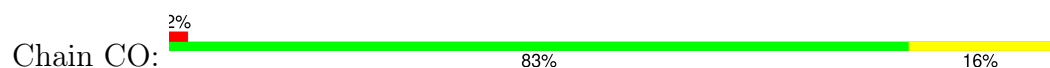
- Molecule 1: coat protein



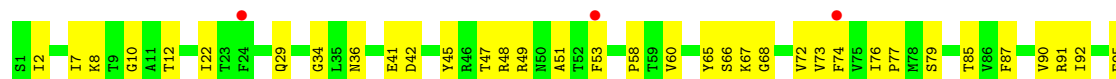
- Molecule 1: coat protein



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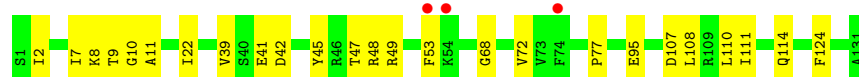
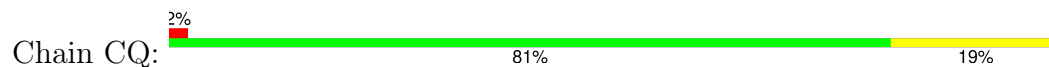
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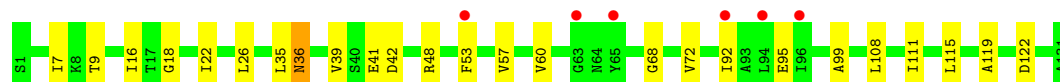
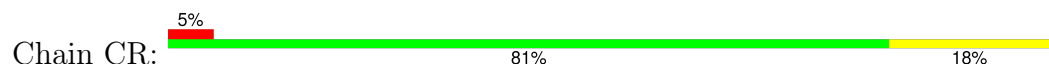




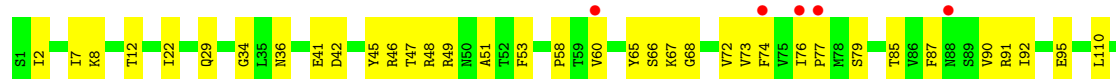
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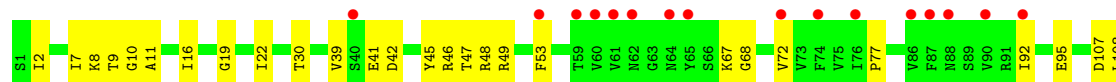
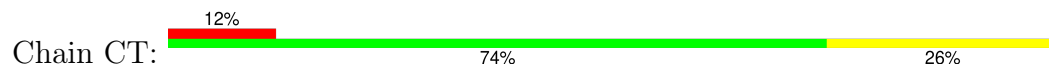
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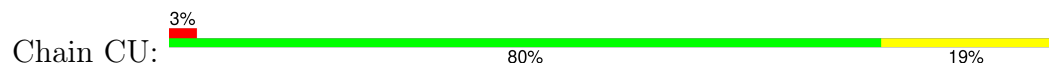
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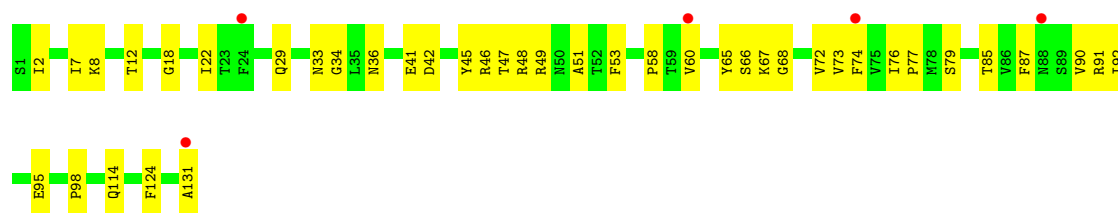


- Molecule 1: coat protein

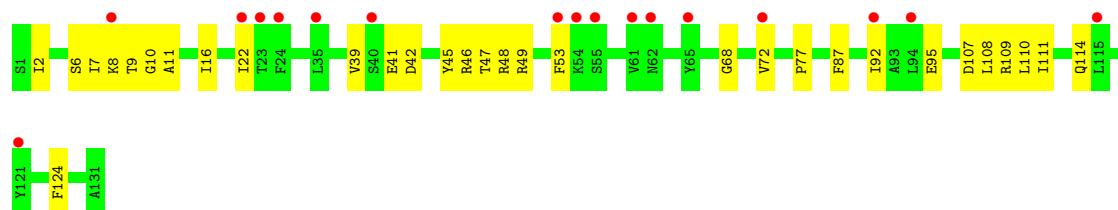
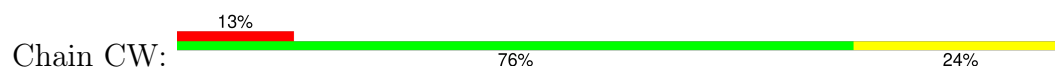


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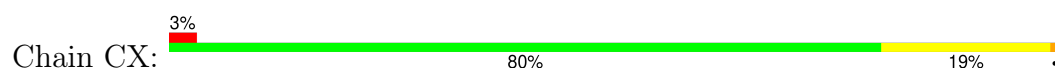




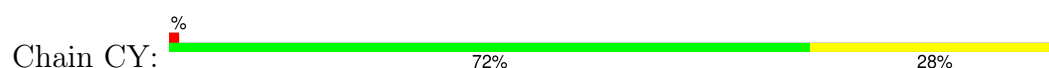
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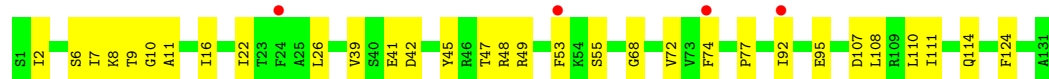
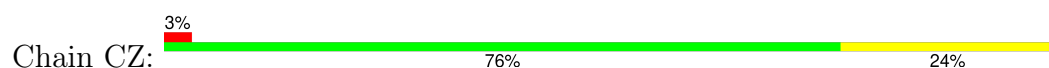
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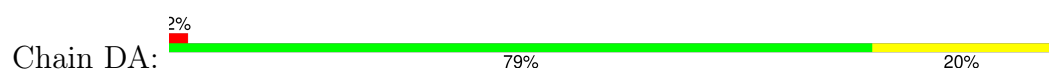
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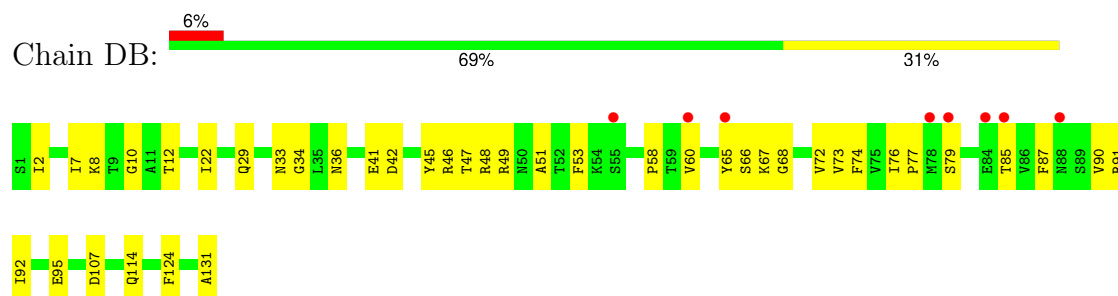
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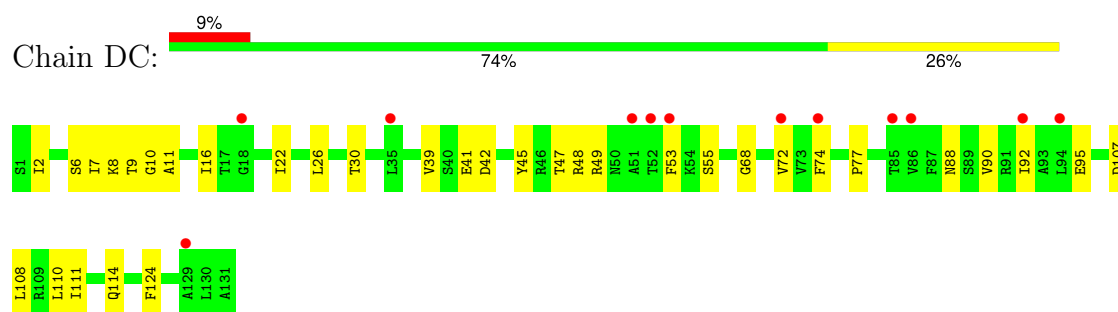
- Molecule 1: coat protein



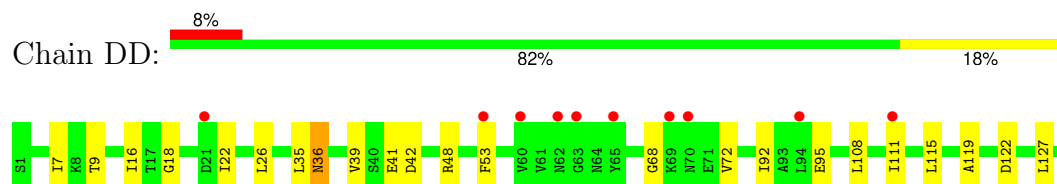
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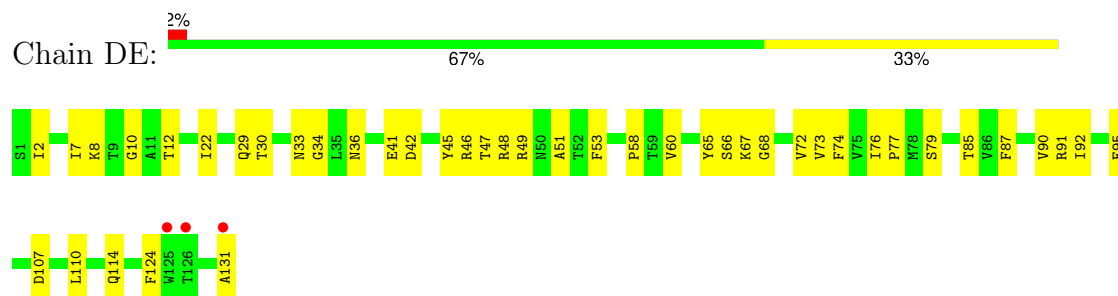
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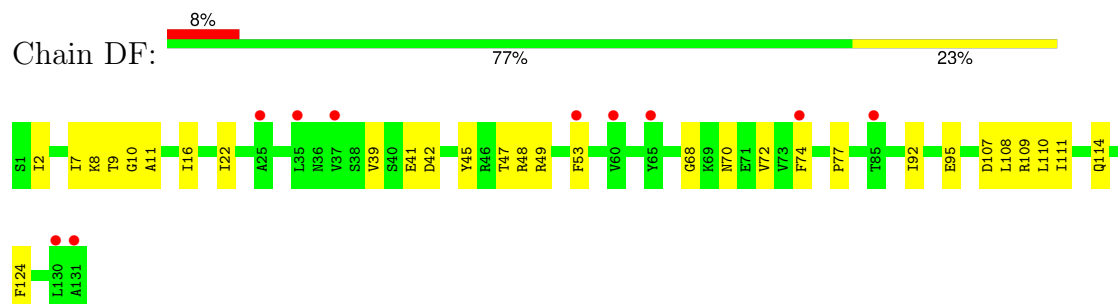
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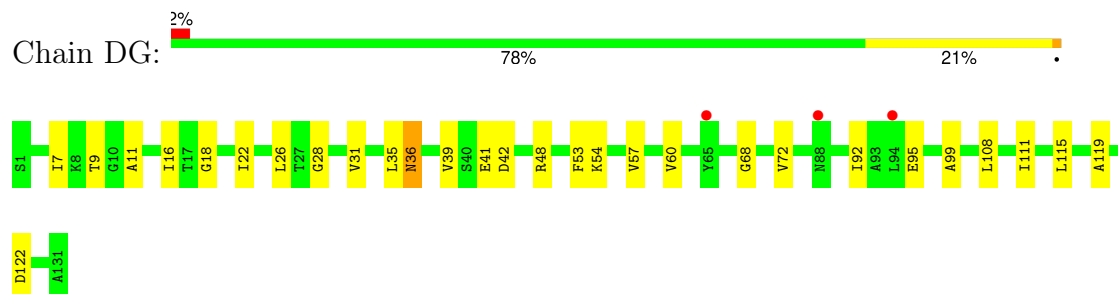
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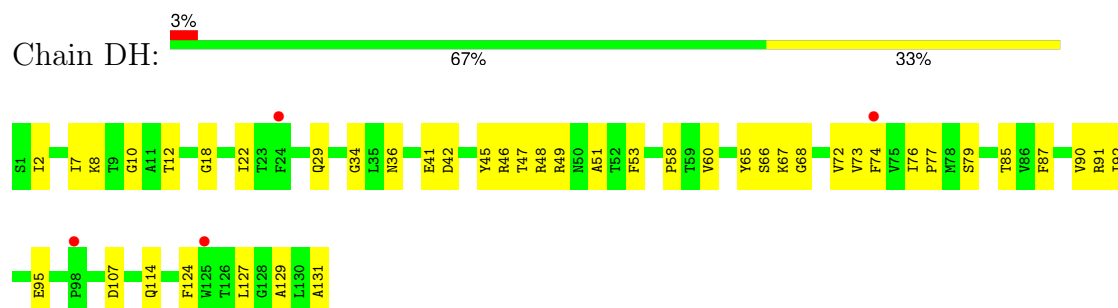
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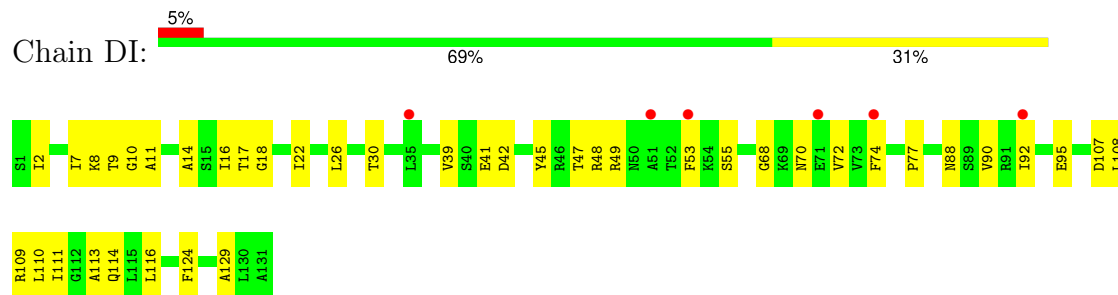
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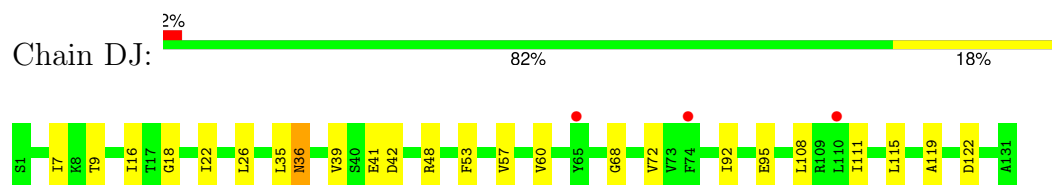
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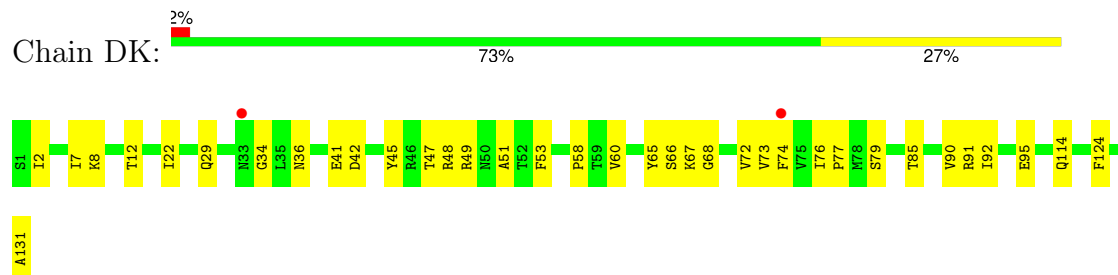
- Molecule 1: coat protein



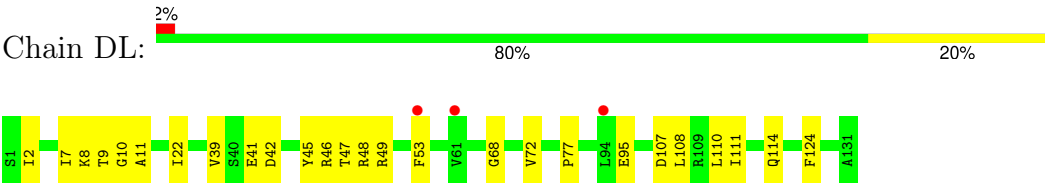
- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	415.01Å 335.00Å 291.78Å 90.00° 134.66° 90.00°	Depositor
Resolution (Å)	49.14 – 3.48 49.14 – 3.48	Depositor EDS
% Data completeness (in resolution range)	96.5 (49.14-3.48) 98.2 (49.14-3.48)	Depositor EDS
$R_{merge}$	0.45	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.97 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, $R_{free}$	0.269 , 0.271 0.273 , 0.275	Depositor DCC
$R_{free}$ test set	10004 reflections (2.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	121.7	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 72.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.079 for h+2*k,-h-l 0.094 for h,-k,-h-l 0.095 for -h-2*k,-k,l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	87480	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	AA	0.32	0/985	0.57	0/1338
1	AB	0.31	0/985	0.57	0/1338
1	AC	0.31	0/985	0.56	0/1338
1	AD	0.32	0/985	0.57	0/1338
1	AE	0.31	0/985	0.57	0/1338
1	AF	0.31	0/985	0.57	0/1338
1	AG	0.32	0/985	0.57	0/1338
1	AH	0.31	0/985	0.57	0/1338
1	AI	0.31	0/985	0.56	0/1338
1	AJ	0.32	0/985	0.57	0/1338
1	AK	0.31	0/985	0.57	0/1338
1	AL	0.31	0/985	0.56	0/1338
1	AM	0.32	0/985	0.57	0/1338
1	AN	0.31	0/985	0.57	0/1338
1	AO	0.31	0/985	0.56	0/1338
1	AP	0.32	0/985	0.57	0/1338
1	AQ	0.31	0/985	0.57	0/1338
1	AR	0.31	0/985	0.56	0/1338
1	AS	0.32	0/985	0.57	0/1338
1	AT	0.31	0/985	0.57	0/1338
1	AU	0.31	0/985	0.56	0/1338
1	AV	0.32	0/985	0.57	0/1338
1	AW	0.31	0/985	0.57	0/1338
1	AX	0.31	0/985	0.56	0/1338
1	AY	0.32	0/985	0.57	0/1338
1	AZ	0.31	0/985	0.57	0/1338
1	BA	0.31	0/985	0.57	0/1338
1	BB	0.32	0/985	0.57	0/1338
1	BC	0.31	0/985	0.57	0/1338
1	BD	0.31	0/985	0.57	0/1338
1	BE	0.32	0/985	0.57	0/1338
1	BF	0.31	0/985	0.57	0/1338
1	BG	0.31	0/985	0.56	0/1338
1	BH	0.32	0/985	0.57	0/1338

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	BI	0.31	0/985	0.57	0/1338
1	BJ	0.31	0/985	0.56	0/1338
1	BK	0.32	0/985	0.57	0/1338
1	BL	0.31	0/985	0.57	0/1338
1	BM	0.31	0/985	0.57	0/1338
1	BN	0.32	0/985	0.57	0/1338
1	BO	0.31	0/985	0.57	0/1338
1	BP	0.31	0/985	0.57	0/1338
1	BQ	0.32	0/985	0.57	0/1338
1	BR	0.31	0/985	0.57	0/1338
1	BS	0.31	0/985	0.57	0/1338
1	BT	0.32	0/985	0.57	0/1338
1	BU	0.31	0/985	0.57	0/1338
1	BV	0.31	0/985	0.56	0/1338
1	BW	0.32	0/985	0.58	0/1338
1	BX	0.31	0/985	0.57	0/1338
1	BY	0.31	0/985	0.57	0/1338
1	BZ	0.32	0/985	0.57	0/1338
1	CA	0.31	0/985	0.57	0/1338
1	CB	0.31	0/985	0.57	0/1338
1	CC	0.32	0/985	0.57	0/1338
1	CD	0.31	0/985	0.57	0/1338
1	CE	0.31	0/985	0.56	0/1338
1	CF	0.32	0/985	0.57	0/1338
1	CG	0.31	0/985	0.57	0/1338
1	CH	0.31	0/985	0.57	0/1338
1	CI	0.32	0/985	0.57	0/1338
1	CJ	0.31	0/985	0.57	0/1338
1	CK	0.31	0/985	0.56	0/1338
1	CL	0.32	0/985	0.57	0/1338
1	CM	0.31	0/985	0.57	0/1338
1	CN	0.31	0/985	0.57	0/1338
1	CO	0.32	0/985	0.57	0/1338
1	CP	0.31	0/985	0.57	0/1338
1	CQ	0.31	0/985	0.57	0/1338
1	CR	0.32	0/985	0.57	0/1338
1	CS	0.31	0/985	0.57	0/1338
1	CT	0.31	0/985	0.57	0/1338
1	CU	0.32	0/985	0.57	0/1338
1	CV	0.31	0/985	0.57	0/1338
1	CW	0.31	0/985	0.57	0/1338
1	CX	0.32	0/985	0.57	0/1338
1	CY	0.31	0/985	0.57	0/1338



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	CZ	0.31	0/985	0.57	0/1338
1	DA	0.32	0/985	0.57	0/1338
1	DB	0.31	0/985	0.57	0/1338
1	DC	0.31	0/985	0.56	0/1338
1	DD	0.32	0/985	0.57	0/1338
1	DE	0.31	0/985	0.57	0/1338
1	DF	0.31	0/985	0.57	0/1338
1	DG	0.32	0/985	0.57	0/1338
1	DH	0.31	0/985	0.57	0/1338
1	DI	0.31	0/985	0.57	0/1338
1	DJ	0.32	0/985	0.57	0/1338
1	DK	0.31	0/985	0.57	0/1338
1	DL	0.31	0/985	0.57	0/1338
All	All	0.31	0/88650	0.57	0/120420

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	972	0	977	26	0
1	AB	972	0	977	39	0
1	AC	972	0	977	39	0
1	AD	972	0	977	25	0
1	AE	972	0	977	41	0
1	AF	972	0	977	41	0
1	AG	972	0	977	27	0
1	AH	972	0	977	38	0
1	AI	972	0	977	52	0
1	AJ	972	0	977	26	0
1	AK	972	0	977	40	0
1	AL	972	0	977	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AM	972	0	977	26	0
1	AN	972	0	977	33	0
1	AO	972	0	977	51	0
1	AP	972	0	977	20	1
1	AQ	972	0	977	29	0
1	AR	972	0	977	35	1
1	AS	972	0	977	28	0
1	AT	972	0	977	39	0
1	AU	972	0	977	37	0
1	AV	972	0	977	25	0
1	AW	972	0	977	38	0
1	AX	972	0	977	35	0
1	AY	972	0	977	21	0
1	AZ	972	0	977	29	0
1	BA	972	0	977	31	0
1	BB	972	0	977	24	0
1	BC	972	0	977	39	0
1	BD	972	0	977	33	0
1	BE	972	0	977	29	0
1	BF	972	0	977	41	0
1	BG	972	0	977	39	0
1	BH	972	0	977	21	0
1	BI	972	0	977	31	0
1	BJ	972	0	977	42	0
1	BK	972	0	977	24	0
1	BL	972	0	977	42	0
1	BM	972	0	977	55	0
1	BN	972	0	977	20	0
1	BO	972	0	977	36	0
1	BP	972	0	977	45	0
1	BQ	972	0	977	21	0
1	BR	972	0	977	33	0
1	BS	972	0	977	29	1
1	BT	972	0	977	24	0
1	BU	972	0	977	36	0
1	BV	972	0	977	40	0
1	BW	972	0	977	26	0
1	BX	972	0	977	43	0
1	BY	972	0	977	53	0
1	BZ	972	0	977	21	0
1	CA	972	0	977	44	0
1	CB	972	0	977	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CC	972	0	977	29	0
1	CD	972	0	977	46	0
1	CE	972	0	977	51	0
1	CF	972	0	977	27	0
1	CG	972	0	977	30	2
1	CH	972	0	977	26	1
1	CI	972	0	977	28	0
1	CJ	972	0	977	34	0
1	CK	972	0	977	44	0
1	CL	972	0	977	25	0
1	CM	972	0	977	34	0
1	CN	972	0	977	42	0
1	CO	972	0	977	20	0
1	CP	972	0	977	36	0
1	CQ	972	0	977	19	0
1	CR	972	0	977	24	0
1	CS	972	0	977	36	0
1	CT	972	0	977	35	0
1	CU	972	0	977	24	0
1	CV	972	0	977	38	0
1	CW	972	0	977	35	0
1	CX	972	0	977	24	0
1	CY	972	0	977	35	0
1	CZ	972	0	977	34	0
1	DA	972	0	977	25	0
1	DB	972	0	977	35	0
1	DC	972	0	977	38	0
1	DD	972	0	977	24	0
1	DE	972	0	977	38	0
1	DF	972	0	977	32	0
1	DG	972	0	977	29	0
1	DH	972	0	977	40	0
1	DI	972	0	977	55	0
1	DJ	972	0	977	23	0
1	DK	972	0	977	28	0
1	DL	972	0	977	21	0
All	All	87480	0	87930	2312	3

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 13.

All (2312) 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:BA:16:ILE:HD13	1:CW:114:GLN:HE21	1.10	1.14
1:AX:16:ILE:HD13	1:CT:114:GLN:HE21	1.12	1.12
1:BA:114:GLN:HE21	1:CW:16:ILE:HD13	1.11	1.10
1:AX:114:GLN:HE21	1:CT:16:ILE:HD13	1.18	1.08
1:AL:16:ILE:HD13	1:CB:114:GLN:HE21	1.19	1.07
1:AL:114:GLN:HE21	1:CB:16:ILE:HD13	1.17	1.03
1:BF:65:TYR:CD2	1:BS:46:ARG:HG2	1.98	0.97
1:AR:114:GLN:HE21	1:CK:16:ILE:HD13	1.28	0.96
1:AF:92:ILE:HG12	1:BV:92:ILE:HG12	1.53	0.91
1:AI:110:LEU:HD23	1:BY:16:ILE:HD11	1.50	0.91
1:BA:16:ILE:HD13	1:CW:114:GLN:NE2	1.86	0.90
1:BM:16:ILE:HD13	1:DI:114:GLN:HE21	1.34	0.90
1:AR:16:ILE:HD13	1:CK:114:GLN:HE21	1.37	0.89
1:AF:16:ILE:HD13	1:BV:114:GLN:HE21	1.37	0.89
1:AO:16:ILE:HD11	1:CE:110:LEU:HD23	1.54	0.89
1:AO:16:ILE:HD13	1:CE:114:GLN:HE21	1.36	0.88
1:BA:114:GLN:NE2	1:CW:16:ILE:HD13	1.87	0.88
1:BM:110:LEU:HD23	1:DI:16:ILE:HD11	1.55	0.88
1:BJ:16:ILE:HD13	1:DF:114:GLN:HE21	1.38	0.87
1:AF:26:LEU:HB3	1:DD:130:LEU:O	1.74	0.87
1:AX:114:GLN:NE2	1:CT:16:ILE:HD13	1.89	0.86
1:AX:16:ILE:HD13	1:CT:114:GLN:NE2	1.91	0.86
1:BG:16:ILE:HD13	1:DC:114:GLN:HE21	1.41	0.86
1:BM:108:LEU:HD22	1:DI:90:VAL:HG12	1.55	0.86
1:AO:114:GLN:HE21	1:CE:16:ILE:HD13	1.39	0.85
1:BM:16:ILE:HD11	1:DI:110:LEU:HD23	1.58	0.85
1:AC:16:ILE:HD13	1:BP:114:GLN:HE21	1.40	0.85
1:AF:114:GLN:HE21	1:BV:16:ILE:HD13	1.40	0.85
1:AO:110:LEU:HD23	1:CE:16:ILE:HD11	1.57	0.85
1:CD:65:TYR:HE2	1:CK:46:ARG:HA	1.40	0.84
1:BJ:114:GLN:HE21	1:DF:16:ILE:HD13	1.42	0.84
1:AL:16:ILE:HD13	1:CB:114:GLN:NE2	1.93	0.84
1:BF:65:TYR:HD2	1:BS:46:ARG:HG2	1.41	0.83
1:AE:87:PHE:CE2	1:BE:60:VAL:HG11	2.12	0.83
1:BX:65:TYR:HE2	1:CN:46:ARG:HA	1.43	0.83
1:AE:87:PHE:HE2	1:BE:60:VAL:HG11	1.43	0.82
1:AA:16:ILE:HD13	1:AB:114:GLN:HE21	1.45	0.82
1:CU:16:ILE:HD13	1:CV:114:GLN:HE21	1.45	0.82
1:AJ:16:ILE:HD13	1:AK:114:GLN:HE21	1.45	0.82
1:AU:114:GLN:HE21	1:CN:16:ILE:HD13	1.44	0.82
1:DD:16:ILE:HD13	1:DE:114:GLN:HE21	1.45	0.82
1:BZ:16:ILE:HD13	1:CA:114:GLN:HE21	1.45	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BJ:46:ARG:HG2	1:BL:65:TYR:CD2	2.14	0.82
1:BW:16:ILE:HD13	1:BX:114:GLN:HE21	1.45	0.82
1:DA:16:ILE:HD13	1:DB:114:GLN:HE21	1.45	0.82
1:AI:16:ILE:HD11	1:BY:110:LEU:HD23	1.62	0.82
1:BE:16:ILE:HD13	1:BF:114:GLN:HE21	1.44	0.82
1:BN:16:ILE:HD13	1:BO:114:GLN:HE21	1.45	0.82
1:BQ:16:ILE:HD13	1:BR:114:GLN:HE21	1.45	0.82
1:DJ:16:ILE:HD13	1:DK:114:GLN:HE21	1.45	0.82
1:AV:16:ILE:HD13	1:AW:114:GLN:HE21	1.45	0.82
1:BH:16:ILE:HD13	1:BI:114:GLN:HE21	1.45	0.82
1:BJ:46:ARG:HG2	1:BL:65:TYR:HD2	1.45	0.82
1:AL:114:GLN:NE2	1:CB:16:ILE:HD13	1.95	0.82
1:CI:16:ILE:HD13	1:CJ:114:GLN:HE21	1.45	0.82
1:AY:16:ILE:HD13	1:AZ:114:GLN:HE21	1.45	0.81
1:CX:16:ILE:HD13	1:CY:114:GLN:HE21	1.45	0.81
1:AD:16:ILE:HD13	1:AE:114:GLN:HE21	1.44	0.81
1:CC:16:ILE:HD13	1:CD:114:GLN:HE21	1.45	0.81
1:CF:16:ILE:HD13	1:CG:114:GLN:HE21	1.45	0.81
1:CR:16:ILE:HD13	1:CS:114:GLN:HE21	1.45	0.81
1:BD:16:ILE:HD13	1:CZ:114:GLN:HE21	1.43	0.81
1:DG:16:ILE:HD13	1:DH:114:GLN:HE21	1.45	0.81
1:AA:57:VAL:HG21	1:DH:29:GLN:HG3	1.62	0.80
1:AS:16:ILE:HD13	1:AT:114:GLN:HE21	1.45	0.80
1:AG:16:ILE:HD13	1:AH:114:GLN:HE21	1.45	0.80
1:CL:16:ILE:HD13	1:CM:114:GLN:HE21	1.45	0.80
1:CO:16:ILE:HD13	1:CP:114:GLN:HE21	1.45	0.80
1:AP:16:ILE:HD13	1:AQ:114:GLN:HE21	1.45	0.80
1:BT:16:ILE:HD13	1:BU:114:GLN:HE21	1.45	0.80
1:AI:16:ILE:HD13	1:BY:114:GLN:HE21	1.46	0.80
1:BB:16:ILE:HD13	1:BC:114:GLN:HE21	1.45	0.80
1:AM:16:ILE:HD13	1:AN:114:GLN:HE21	1.45	0.80
1:BK:16:ILE:HD13	1:BL:114:GLN:HE21	1.45	0.79
1:BM:130:LEU:HD21	1:DI:55:SER:HB3	1.65	0.78
1:BG:7:ILE:O	1:DC:22:ILE:HG22	1.84	0.77
1:AA:130:LEU:O	1:AU:26:LEU:HB3	1.85	0.77
1:CD:87:PHE:HE2	1:CI:60:VAL:HG11	1.48	0.76
1:AU:16:ILE:HD13	1:CN:114:GLN:HE21	1.49	0.76
1:BC:65:TYR:CD2	1:BP:46:ARG:HG2	2.21	0.75
1:CA:65:TYR:CD2	1:CH:46:ARG:HG2	2.22	0.75
1:BD:114:GLN:HE21	1:CZ:16:ILE:HD13	1.51	0.75
1:DG:16:ILE:HD13	1:DH:114:GLN:NE2	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CU:16:ILE:HD13	1:CV:114:GLN:NE2	2.02	0.75
1:AS:16:ILE:HD13	1:AT:114:GLN:NE2	2.02	0.74
1:AY:16:ILE:HD13	1:AZ:114:GLN:NE2	2.02	0.74
1:CI:16:ILE:HD13	1:CJ:114:GLN:NE2	2.02	0.74
1:BF:65:TYR:CE2	1:BS:46:ARG:HG2	2.22	0.74
1:BZ:16:ILE:HD13	1:CA:114:GLN:NE2	2.02	0.74
1:CD:87:PHE:CE2	1:CI:60:VAL:HG11	2.22	0.74
1:CO:16:ILE:HD13	1:CP:114:GLN:NE2	2.02	0.74
1:BQ:16:ILE:HD13	1:BR:114:GLN:NE2	2.02	0.74
1:CX:16:ILE:HD13	1:CY:114:GLN:NE2	2.02	0.74
1:AD:16:ILE:HD13	1:AE:114:GLN:NE2	2.02	0.74
1:AJ:16:ILE:HD13	1:AK:114:GLN:NE2	2.02	0.74
1:BH:16:ILE:HD13	1:BI:114:GLN:NE2	2.02	0.74
1:CA:46:ARG:HG3	1:CF:65:TYR:CE2	2.21	0.74
1:CA:87:PHE:CE2	1:CF:60:VAL:HG11	2.21	0.74
1:BM:12:THR:OG1	1:DI:17:THR:O	2.06	0.74
1:DA:16:ILE:HD13	1:DB:114:GLN:NE2	2.02	0.74
1:AT:87:PHE:HE2	1:AV:60:VAL:HG11	1.53	0.74
1:BE:16:ILE:HD13	1:BF:114:GLN:NE2	2.02	0.74
1:BM:100:LEU:HD13	1:DI:88:ASN:ND2	2.02	0.74
1:BW:16:ILE:HD13	1:BX:114:GLN:NE2	2.02	0.74
1:DJ:16:ILE:HD13	1:DK:114:GLN:NE2	2.02	0.74
1:AA:16:ILE:HD13	1:AB:114:GLN:NE2	2.02	0.74
1:AM:16:ILE:HD13	1:AN:114:GLN:NE2	2.02	0.74
1:BB:16:ILE:HD13	1:BC:114:GLN:NE2	2.02	0.74
1:CC:16:ILE:HD13	1:CD:114:GLN:NE2	2.02	0.73
1:CR:16:ILE:HD13	1:CS:114:GLN:NE2	2.02	0.73
1:DD:16:ILE:HD13	1:DE:114:GLN:NE2	2.02	0.73
1:AP:16:ILE:HD13	1:AQ:114:GLN:NE2	2.02	0.73
1:BK:16:ILE:HD13	1:BL:114:GLN:NE2	2.02	0.73
1:BT:16:ILE:HD13	1:BU:114:GLN:NE2	2.02	0.73
1:CW:46:ARG:HG2	1:CY:65:TYR:CD2	2.23	0.73
1:AG:16:ILE:HD13	1:AH:114:GLN:NE2	2.02	0.73
1:AU:92:ILE:HG12	1:CN:92:ILE:HG12	1.70	0.73
1:CF:16:ILE:HD13	1:CG:114:GLN:NE2	2.02	0.73
1:AV:16:ILE:HD13	1:AW:114:GLN:NE2	2.02	0.72
1:BN:16:ILE:HD13	1:BO:114:GLN:NE2	2.02	0.72
1:BX:65:TYR:CD2	1:CN:46:ARG:HG2	2.24	0.72
1:CL:16:ILE:HD13	1:CM:114:GLN:NE2	2.02	0.72
1:BM:109:ARG:NH2	1:DI:116:LEU:O	2.22	0.72
1:CD:65:TYR:CE2	1:CK:46:ARG:HA	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AC:7:ILE:O	1:BP:22:ILE:HG22	1.89	0.72
1:AE:85:THR:N	1:BE:63:GLY:O	2.22	0.72
1:AF:30:THR:OG1	1:DE:33:ASN:OD1	2.08	0.71
1:AT:87:PHE:CE2	1:AV:60:VAL:HG11	2.25	0.71
1:CJ:8:LYS:HB2	1:CJ:114:GLN:HE22	1.56	0.71
1:AE:8:LYS:HB2	1:AE:114:GLN:HE22	1.56	0.71
1:AU:16:ILE:HD11	1:CN:110:LEU:HD23	1.73	0.71
1:DE:8:LYS:HB2	1:DE:114:GLN:HE22	1.56	0.71
1:AA:60:VAL:HG11	1:DH:87:PHE:HE2	1.55	0.71
1:CM:8:LYS:HB2	1:CM:114:GLN:HE22	1.56	0.71
1:CG:8:LYS:HB2	1:CG:114:GLN:HE22	1.56	0.71
1:AK:8:LYS:HB2	1:AK:114:GLN:HE22	1.56	0.71
1:AZ:8:LYS:HB2	1:AZ:114:GLN:HE22	1.56	0.71
1:BC:8:LYS:HB2	1:BC:114:GLN:HE22	1.56	0.71
1:BF:8:LYS:HB2	1:BF:114:GLN:HE22	1.56	0.71
1:BM:116:LEU:O	1:DI:109:ARG:NE	2.24	0.71
1:AN:8:LYS:HB2	1:AN:114:GLN:HE22	1.56	0.71
1:BM:109:ARG:HG2	1:DI:116:LEU:HD22	1.73	0.71
1:BR:8:LYS:HB2	1:BR:114:GLN:HE22	1.56	0.71
1:AC:92:ILE:HG12	1:BP:92:ILE:HG12	1.73	0.70
1:BG:111:ILE:HD13	1:DC:74:PHE:CZ	2.26	0.70
1:AB:8:LYS:HB2	1:AB:114:GLN:HE22	1.56	0.70
1:AQ:8:LYS:HB2	1:AQ:114:GLN:HE22	1.56	0.70
1:BX:8:LYS:HB2	1:BX:114:GLN:HE22	1.56	0.70
1:CR:60:VAL:HG11	1:DB:87:PHE:HE2	1.56	0.70
1:AH:8:LYS:HB2	1:AH:114:GLN:HE22	1.56	0.70
1:BM:129:ALA:HB2	1:DG:26:LEU:O	1.91	0.70
1:CV:8:LYS:HB2	1:CV:114:GLN:HE22	1.56	0.70
1:DH:8:LYS:HB2	1:DH:114:GLN:HE22	1.56	0.70
1:AW:8:LYS:HB2	1:AW:114:GLN:HE22	1.56	0.70
1:CA:8:LYS:HB2	1:CA:114:GLN:HE22	1.56	0.70
1:AI:130:LEU:HD21	1:BY:55:SER:HB3	1.73	0.70
1:BI:8:LYS:HB2	1:BI:114:GLN:HE22	1.56	0.70
1:BO:8:LYS:HB2	1:BO:114:GLN:HE22	1.56	0.70
1:CD:8:LYS:HB2	1:CD:114:GLN:HE22	1.56	0.70
1:CY:8:LYS:HB2	1:CY:114:GLN:HE22	1.56	0.70
1:BF:65:TYR:HE2	1:BS:46:ARG:HA	1.56	0.70
1:BL:8:LYS:HB2	1:BL:114:GLN:HE22	1.56	0.70
1:BU:8:LYS:HB2	1:BU:114:GLN:HE22	1.56	0.70
1:AC:114:GLN:HE21	1:BP:16:ILE:HD13	1.57	0.70
1:CA:85:THR:N	1:CF:63:GLY:O	2.19	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CD:65:TYR:CD2	1:CK:46:ARG:HG2	2.26	0.69
1:BX:65:TYR:CE2	1:CN:46:ARG:HA	2.26	0.69
1:DB:8:LYS:HB2	1:DB:114:GLN:HE22	1.56	0.69
1:DK:8:LYS:HB2	1:DK:114:GLN:HE22	1.56	0.69
1:CP:8:LYS:HB2	1:CP:114:GLN:HE22	1.56	0.69
1:CS:8:LYS:HB2	1:CS:114:GLN:HE22	1.56	0.69
1:AQ:2:ILE:HD11	1:AQ:124:PHE:HB2	1.75	0.69
1:AT:2:ILE:HD11	1:AT:124:PHE:HB2	1.75	0.69
1:CP:2:ILE:HD11	1:CP:124:PHE:HB2	1.75	0.69
1:AT:8:LYS:HB2	1:AT:114:GLN:HE22	1.56	0.69
1:AX:6:SER:HA	1:CT:22:ILE:O	1.93	0.69
1:BD:39:VAL:HG12	1:BD:41:GLU:H	1.58	0.69
1:BG:92:ILE:HG12	1:DC:92:ILE:HG12	1.74	0.69
1:CT:39:VAL:HG12	1:CT:41:GLU:H	1.58	0.69
1:AX:39:VAL:HG12	1:AX:41:GLU:H	1.58	0.68
1:AK:2:ILE:HD11	1:AK:124:PHE:HB2	1.75	0.68
1:CD:65:TYR:HD2	1:CK:46:ARG:HG2	1.56	0.68
1:CJ:2:ILE:HD11	1:CJ:124:PHE:HB2	1.75	0.68
1:DL:39:VAL:HG12	1:DL:41:GLU:H	1.59	0.68
1:AF:87:PHE:O	1:BV:67:LYS:NZ	2.20	0.68
1:BS:39:VAL:HG12	1:BS:41:GLU:H	1.58	0.68
1:DI:39:VAL:HG12	1:DI:41:GLU:H	1.59	0.68
1:AB:2:ILE:HD11	1:AB:124:PHE:HB2	1.75	0.68
1:AE:2:ILE:HD11	1:AE:124:PHE:HB2	1.75	0.68
1:AE:42:ASP:HB2	1:AE:48:ARG:HG2	1.76	0.68
1:AK:42:ASP:HB2	1:AK:48:ARG:HG2	1.76	0.68
1:BG:39:VAL:HG12	1:BG:41:GLU:H	1.58	0.68
1:BR:42:ASP:HB2	1:BR:48:ARG:HG2	1.76	0.68
1:BX:42:ASP:HB2	1:BX:48:ARG:HG2	1.76	0.68
1:CN:39:VAL:HG12	1:CN:41:GLU:H	1.59	0.68
1:DB:2:ILE:HD11	1:DB:124:PHE:HB2	1.75	0.68
1:DF:39:VAL:HG12	1:DF:41:GLU:H	1.58	0.68
1:BY:39:VAL:HG12	1:BY:41:GLU:H	1.58	0.68
1:CB:39:VAL:HG12	1:CB:41:GLU:H	1.58	0.68
1:AH:29:GLN:HG3	1:CC:57:VAL:HG21	1.75	0.68
1:AI:114:GLN:HE21	1:BY:16:ILE:HD13	1.57	0.68
1:AQ:42:ASP:HB2	1:AQ:48:ARG:HG2	1.76	0.68
1:AT:42:ASP:HB2	1:AT:48:ARG:HG2	1.76	0.68
1:BO:2:ILE:HD11	1:BO:124:PHE:HB2	1.76	0.68
1:BX:65:TYR:HD2	1:CN:46:ARG:HG2	1.57	0.68
1:CH:39:VAL:HG12	1:CH:41:GLU:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CJ:42:ASP:HB2	1:CJ:48:ARG:HG2	1.76	0.68
1:DA:42:ASP:HB2	1:DA:48:ARG:HG3	1.76	0.68
1:AI:39:VAL:HG12	1:AI:41:GLU:H	1.58	0.68
1:CY:2:ILE:HD11	1:CY:124:PHE:HB2	1.75	0.68
1:AF:39:VAL:HG12	1:AF:41:GLU:H	1.59	0.68
1:AW:42:ASP:HB2	1:AW:48:ARG:HG2	1.76	0.68
1:BM:39:VAL:HG12	1:BM:41:GLU:H	1.58	0.68
1:BU:42:ASP:HB2	1:BU:48:ARG:HG2	1.76	0.68
1:BX:2:ILE:HD11	1:BX:124:PHE:HB2	1.75	0.68
1:DG:42:ASP:HB2	1:DG:48:ARG:HG3	1.76	0.68
1:AM:42:ASP:HB2	1:AM:48:ARG:HG3	1.76	0.68
1:BK:42:ASP:HB2	1:BK:48:ARG:HG3	1.76	0.68
1:BP:39:VAL:HG12	1:BP:41:GLU:H	1.59	0.68
1:CO:42:ASP:HB2	1:CO:48:ARG:HG3	1.76	0.68
1:CQ:39:VAL:HG12	1:CQ:41:GLU:H	1.58	0.68
1:DK:42:ASP:HB2	1:DK:48:ARG:HG2	1.76	0.68
1:AD:42:ASP:HB2	1:AD:48:ARG:HG3	1.76	0.68
1:AP:92:ILE:HG12	1:AQ:92:ILE:HG12	1.76	0.68
1:CA:65:TYR:HD2	1:CH:46:ARG:HG2	1.58	0.68
1:CO:92:ILE:HG12	1:CP:92:ILE:HG12	1.76	0.68
1:CW:39:VAL:HG12	1:CW:41:GLU:H	1.59	0.68
1:DB:42:ASP:HB2	1:DB:48:ARG:HG2	1.76	0.68
1:DJ:42:ASP:HB2	1:DJ:48:ARG:HG3	1.76	0.68
1:AO:39:VAL:HG12	1:AO:41:GLU:H	1.59	0.67
1:BJ:16:ILE:HD11	1:DF:110:LEU:HD23	1.74	0.67
1:BK:92:ILE:HG12	1:BL:92:ILE:HG12	1.76	0.67
1:AE:29:GLN:OE1	1:AE:36:ASN:ND2	2.28	0.67
1:AH:42:ASP:HB2	1:AH:48:ARG:HG2	1.76	0.67
1:AU:39:VAL:HG12	1:AU:41:GLU:H	1.58	0.67
1:AZ:2:ILE:HD11	1:AZ:124:PHE:HB2	1.75	0.67
1:BB:42:ASP:HB2	1:BB:48:ARG:HG3	1.76	0.67
1:BC:42:ASP:HB2	1:BC:48:ARG:HG2	1.76	0.67
1:BJ:39:VAL:HG12	1:BJ:41:GLU:H	1.58	0.67
1:BO:42:ASP:HB2	1:BO:48:ARG:HG2	1.76	0.67
1:CV:29:GLN:OE1	1:CV:36:ASN:ND2	2.28	0.67
1:AJ:92:ILE:HG12	1:AK:92:ILE:HG12	1.76	0.67
1:AN:29:GLN:OE1	1:AN:36:ASN:ND2	2.28	0.67
1:AS:42:ASP:HB2	1:AS:48:ARG:HG3	1.76	0.67
1:BC:65:TYR:HD2	1:BP:46:ARG:HG2	1.57	0.67
1:BF:42:ASP:HB2	1:BF:48:ARG:HG2	1.76	0.67
1:BL:2:ILE:HD11	1:BL:124:PHE:HB2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BL:42:ASP:HB2	1:BL:48:ARG:HG2	1.76	0.67
1:CP:29:GLN:OE1	1:CP:36:ASN:ND2	2.28	0.67
1:AB:29:GLN:OE1	1:AB:36:ASN:ND2	2.28	0.67
1:AB:42:ASP:HB2	1:AB:48:ARG:HG2	1.76	0.67
1:AV:92:ILE:HG12	1:AW:92:ILE:HG12	1.76	0.67
1:BI:29:GLN:OE1	1:BI:36:ASN:ND2	2.28	0.67
1:BM:128:GLY:O	1:DG:28:GLY:HA3	1.95	0.67
1:CD:42:ASP:HB2	1:CD:48:ARG:HG2	1.76	0.67
1:CI:92:ILE:HG12	1:CJ:92:ILE:HG12	1.76	0.67
1:CP:42:ASP:HB2	1:CP:48:ARG:HG2	1.76	0.67
1:CU:42:ASP:HB2	1:CU:48:ARG:HG3	1.76	0.67
1:DH:2:ILE:HD11	1:DH:124:PHE:HB2	1.75	0.67
1:AG:92:ILE:HG12	1:AH:92:ILE:HG12	1.76	0.67
1:AK:29:GLN:OE1	1:AK:36:ASN:ND2	2.28	0.67
1:BO:29:GLN:OE1	1:BO:36:ASN:ND2	2.28	0.67
1:CE:39:VAL:HG12	1:CE:41:GLU:H	1.58	0.67
1:CG:29:GLN:OE1	1:CG:36:ASN:ND2	2.28	0.67
1:CU:92:ILE:HG12	1:CV:92:ILE:HG12	1.76	0.67
1:AM:92:ILE:HG12	1:AN:92:ILE:HG12	1.76	0.67
1:AT:29:GLN:OE1	1:AT:36:ASN:ND2	2.28	0.67
1:BR:29:GLN:OE1	1:BR:36:ASN:ND2	2.28	0.67
1:BV:39:VAL:HG12	1:BV:41:GLU:H	1.58	0.67
1:BX:29:GLN:OE1	1:BX:36:ASN:ND2	2.28	0.67
1:BZ:92:ILE:HG12	1:CA:92:ILE:HG12	1.76	0.67
1:CC:42:ASP:HB2	1:CC:48:ARG:HG3	1.76	0.67
1:CK:39:VAL:HG12	1:CK:41:GLU:H	1.59	0.67
1:CV:2:ILE:HD11	1:CV:124:PHE:HB2	1.75	0.67
1:CY:29:GLN:OE1	1:CY:36:ASN:ND2	2.28	0.67
1:DD:92:ILE:HG12	1:DE:92:ILE:HG12	1.76	0.67
1:AA:92:ILE:HG12	1:AB:92:ILE:HG12	1.76	0.67
1:AX:92:ILE:HG12	1:CT:92:ILE:HG12	1.76	0.67
1:BF:29:GLN:OE1	1:BF:36:ASN:ND2	2.28	0.67
1:BH:42:ASP:HB2	1:BH:48:ARG:HG3	1.76	0.67
1:BL:29:GLN:OE1	1:BL:36:ASN:ND2	2.28	0.67
1:BN:92:ILE:HG12	1:BO:92:ILE:HG12	1.76	0.67
1:BU:2:ILE:HD11	1:BU:124:PHE:HB2	1.75	0.67
1:CS:29:GLN:OE1	1:CS:36:ASN:ND2	2.28	0.67
1:DK:2:ILE:HD11	1:DK:124:PHE:HB2	1.75	0.67
1:AG:42:ASP:HB2	1:AG:48:ARG:HG3	1.76	0.67
1:AQ:29:GLN:OE1	1:AQ:36:ASN:ND2	2.28	0.67
1:AR:39:VAL:HG12	1:AR:41:GLU:H	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AW:29:GLN:OE1	1:AW:36:ASN:ND2	2.28	0.67
1:BC:2:ILE:HD11	1:BC:124:PHE:HB2	1.75	0.67
1:BT:92:ILE:HG12	1:BU:92:ILE:HG12	1.76	0.67
1:BU:29:GLN:OE1	1:BU:36:ASN:ND2	2.28	0.67
1:CL:92:ILE:HG12	1:CM:92:ILE:HG12	1.76	0.67
1:CM:42:ASP:HB2	1:CM:48:ARG:HG2	1.76	0.67
1:CR:42:ASP:HB2	1:CR:48:ARG:HG3	1.76	0.67
1:CX:92:ILE:HG12	1:CY:92:ILE:HG12	1.76	0.67
1:DE:29:GLN:OE1	1:DE:36:ASN:ND2	2.28	0.67
1:AL:39:VAL:HG12	1:AL:41:GLU:H	1.58	0.67
1:AR:114:GLN:NE2	1:CK:16:ILE:HD13	2.07	0.67
1:AW:2:ILE:HD11	1:AW:124:PHE:HB2	1.75	0.67
1:AY:92:ILE:HG12	1:AZ:92:ILE:HG12	1.76	0.67
1:BW:42:ASP:HB2	1:BW:48:ARG:HG3	1.76	0.67
1:CA:87:PHE:HE2	1:CF:60:VAL:HG11	1.56	0.67
1:CD:29:GLN:OE1	1:CD:36:ASN:ND2	2.28	0.67
1:CJ:29:GLN:OE1	1:CJ:36:ASN:ND2	2.28	0.67
1:DD:42:ASP:HB2	1:DD:48:ARG:HG3	1.76	0.67
1:DE:2:ILE:HD11	1:DE:124:PHE:HB2	1.75	0.67
1:DH:42:ASP:HB2	1:DH:48:ARG:HG2	1.76	0.67
1:AN:2:ILE:HD11	1:AN:124:PHE:HB2	1.75	0.67
1:CS:2:ILE:HD11	1:CS:124:PHE:HB2	1.75	0.67
1:CX:42:ASP:HB2	1:CX:48:ARG:HG3	1.76	0.67
1:AH:2:ILE:HD11	1:AH:124:PHE:HB2	1.75	0.66
1:AP:42:ASP:HB2	1:AP:48:ARG:HG3	1.76	0.66
1:AZ:29:GLN:OE1	1:AZ:36:ASN:ND2	2.28	0.66
1:BI:2:ILE:HD11	1:BI:124:PHE:HB2	1.75	0.66
1:BR:2:ILE:HD11	1:BR:124:PHE:HB2	1.75	0.66
1:BX:45:TYR:HD1	1:BX:48:ARG:HH21	1.44	0.66
1:CG:2:ILE:HD11	1:CG:124:PHE:HB2	1.75	0.66
1:CI:42:ASP:HB2	1:CI:48:ARG:HG3	1.76	0.66
1:CL:42:ASP:HB2	1:CL:48:ARG:HG3	1.76	0.66
1:CM:2:ILE:HD11	1:CM:124:PHE:HB2	1.75	0.66
1:DA:92:ILE:HG12	1:DB:92:ILE:HG12	1.76	0.66
1:DB:29:GLN:OE1	1:DB:36:ASN:ND2	2.28	0.66
1:DG:92:ILE:HG12	1:DH:92:ILE:HG12	1.76	0.66
1:DH:29:GLN:OE1	1:DH:36:ASN:ND2	2.28	0.66
1:DK:29:GLN:OE1	1:DK:36:ASN:ND2	2.28	0.66
1:AA:42:ASP:HB2	1:AA:48:ARG:HG3	1.76	0.66
1:AN:42:ASP:HB2	1:AN:48:ARG:HG2	1.76	0.66
1:AZ:42:ASP:HB2	1:AZ:48:ARG:HG2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BE:42:ASP:HB2	1:BE:48:ARG:HG3	1.76	0.66
1:BF:2:ILE:HD11	1:BF:124:PHE:HB2	1.75	0.66
1:BL:45:TYR:HD1	1:BL:48:ARG:HH21	1.44	0.66
1:CA:45:TYR:HD1	1:CA:48:ARG:HH21	1.43	0.66
1:DJ:92:ILE:HG12	1:DK:92:ILE:HG12	1.76	0.66
1:AH:29:GLN:OE1	1:AH:36:ASN:ND2	2.28	0.66
1:AJ:42:ASP:HB2	1:AJ:48:ARG:HG3	1.76	0.66
1:BC:29:GLN:OE1	1:BC:36:ASN:ND2	2.28	0.66
1:BH:92:ILE:HG12	1:BI:92:ILE:HG12	1.76	0.66
1:BQ:42:ASP:HB2	1:BQ:48:ARG:HG3	1.76	0.66
1:BW:92:ILE:HG12	1:BX:92:ILE:HG12	1.76	0.66
1:CA:42:ASP:HB2	1:CA:48:ARG:HG2	1.76	0.66
1:CC:92:ILE:HG12	1:CD:92:ILE:HG12	1.76	0.66
1:CF:42:ASP:HB2	1:CF:48:ARG:HG3	1.76	0.66
1:CV:42:ASP:HB2	1:CV:48:ARG:HG2	1.76	0.66
1:AC:39:VAL:HG12	1:AC:41:GLU:H	1.59	0.66
1:AV:42:ASP:HB2	1:AV:48:ARG:HG3	1.76	0.66
1:BZ:42:ASP:HB2	1:BZ:48:ARG:HG3	1.76	0.66
1:CD:2:ILE:HD11	1:CD:124:PHE:HB2	1.75	0.66
1:CD:45:TYR:HD1	1:CD:48:ARG:HH21	1.43	0.66
1:CP:45:TYR:HD1	1:CP:48:ARG:HH21	1.44	0.66
1:DB:45:TYR:HD1	1:DB:48:ARG:HH21	1.44	0.66
1:DE:42:ASP:HB2	1:DE:48:ARG:HG2	1.76	0.66
1:AT:45:TYR:HD1	1:AT:48:ARG:HH21	1.43	0.66
1:CA:2:ILE:HD11	1:CA:124:PHE:HB2	1.75	0.66
1:CS:42:ASP:HB2	1:CS:48:ARG:HG2	1.76	0.66
1:AS:92:ILE:HG12	1:AT:92:ILE:HG12	1.76	0.66
1:AZ:45:TYR:HD1	1:AZ:48:ARG:HH21	1.43	0.66
1:BA:39:VAL:HG12	1:BA:41:GLU:H	1.58	0.66
1:BE:92:ILE:HG12	1:BF:92:ILE:HG12	1.76	0.66
1:CY:42:ASP:HB2	1:CY:48:ARG:HG2	1.76	0.66
1:BM:16:ILE:HG21	1:DI:114:GLN:NE2	2.10	0.66
1:CG:42:ASP:HB2	1:CG:48:ARG:HG2	1.76	0.66
1:AY:42:ASP:HB2	1:AY:48:ARG:HG3	1.76	0.66
1:BB:92:ILE:HG12	1:BC:92:ILE:HG12	1.76	0.66
1:BC:45:TYR:HD1	1:BC:48:ARG:HH21	1.44	0.66
1:BN:42:ASP:HB2	1:BN:48:ARG:HG3	1.76	0.66
1:BT:42:ASP:HB2	1:BT:48:ARG:HG3	1.76	0.66
1:CM:29:GLN:OE1	1:CM:36:ASN:ND2	2.28	0.66
1:DK:45:TYR:HD1	1:DK:48:ARG:HH21	1.43	0.66
1:AH:87:PHE:HE2	1:CC:60:VAL:HG11	1.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BI:42:ASP:HB2	1:BI:48:ARG:HG2	1.76	0.66
1:CA:29:GLN:OE1	1:CA:36:ASN:ND2	2.28	0.66
1:CA:46:ARG:HG3	1:CF:65:TYR:CD2	2.31	0.66
1:DH:45:TYR:HD1	1:DH:48:ARG:HH21	1.44	0.66
1:AQ:45:TYR:HD1	1:AQ:48:ARG:HH21	1.43	0.66
1:BJ:110:LEU:HD23	1:DF:16:ILE:HD11	1.78	0.66
1:CY:45:TYR:HD1	1:CY:48:ARG:HH21	1.44	0.66
1:CZ:39:VAL:HG12	1:CZ:41:GLU:H	1.59	0.66
1:AB:33:ASN:OD1	1:AU:30:THR:OG1	2.13	0.65
1:AI:108:LEU:HD22	1:BY:90:VAL:HG12	1.77	0.65
1:AW:45:TYR:HD1	1:AW:48:ARG:HH21	1.44	0.65
1:BD:7:ILE:O	1:CZ:22:ILE:HG22	1.96	0.65
1:BQ:92:ILE:HG12	1:BR:92:ILE:HG12	1.76	0.65
1:CM:45:TYR:HD1	1:CM:48:ARG:HH21	1.44	0.65
1:CV:45:TYR:HD1	1:CV:48:ARG:HH21	1.43	0.65
1:DC:39:VAL:HG12	1:DC:41:GLU:H	1.59	0.65
1:AD:92:ILE:HG12	1:AE:92:ILE:HG12	1.76	0.65
1:CR:92:ILE:HG12	1:CS:92:ILE:HG12	1.76	0.65
1:DE:45:TYR:HD1	1:DE:48:ARG:HH21	1.43	0.65
1:AK:45:TYR:HD1	1:AK:48:ARG:HH21	1.44	0.65
1:BR:45:TYR:HD1	1:BR:48:ARG:HH21	1.43	0.65
1:CF:92:ILE:HG12	1:CG:92:ILE:HG12	1.76	0.65
1:CJ:45:TYR:HD1	1:CJ:48:ARG:HH21	1.44	0.65
1:BG:100:LEU:HD13	1:DC:88:ASN:ND2	2.12	0.65
1:BI:45:TYR:HD1	1:BI:48:ARG:HH21	1.43	0.65
1:BF:45:TYR:HD1	1:BF:48:ARG:HH21	1.44	0.64
1:BM:116:LEU:HD22	1:DI:109:ARG:HG2	1.79	0.64
1:CG:45:TYR:HD1	1:CG:48:ARG:HH21	1.44	0.64
1:AE:45:TYR:HD1	1:AE:48:ARG:HH21	1.44	0.64
1:AN:45:TYR:HD1	1:AN:48:ARG:HH21	1.43	0.64
1:CS:45:TYR:HD1	1:CS:48:ARG:HH21	1.44	0.64
1:BG:114:GLN:HE21	1:DC:16:ILE:HD13	1.63	0.64
1:BO:87:PHE:HE2	1:DJ:60:VAL:HG11	1.62	0.64
1:AL:92:ILE:HG12	1:CB:92:ILE:HG12	1.79	0.64
1:AC:46:ARG:HA	1:DH:65:TYR:HE2	1.61	0.64
1:AH:45:TYR:HD1	1:AH:48:ARG:HH21	1.43	0.64
1:AI:12:THR:OG1	1:BY:17:THR:O	2.11	0.64
1:AH:26:LEU:O	1:CD:129:ALA:HB2	1.97	0.64
1:AO:16:ILE:HG21	1:CE:114:GLN:NE2	2.13	0.64
1:BO:45:TYR:HD1	1:BO:48:ARG:HH21	1.44	0.64
1:BU:45:TYR:HD1	1:BU:48:ARG:HH21	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:92:ILE:HG12	1:CW:92:ILE:HG12	1.80	0.63
1:AE:46:ARG:HG3	1:BE:65:TYR:CE2	2.33	0.63
1:AB:45:TYR:HD1	1:AB:48:ARG:HH21	1.44	0.63
1:BE:127:LEU:HD13	1:BS:40:SER:HB2	1.79	0.63
1:BM:7:ILE:O	1:DI:22:ILE:HG22	1.98	0.63
1:CR:57:VAL:HG21	1:DB:29:GLN:HG3	1.80	0.63
1:AR:16:ILE:HD11	1:CK:110:LEU:HD23	1.81	0.62
1:AF:6:SER:HA	1:BV:22:ILE:O	1.98	0.62
1:BD:92:ILE:HG12	1:CZ:92:ILE:HG12	1.80	0.62
1:CR:60:VAL:HG11	1:DB:87:PHE:CE2	2.33	0.62
1:AA:60:VAL:HG11	1:DH:87:PHE:CE2	2.33	0.62
1:AH:87:PHE:CE2	1:CC:60:VAL:HG11	2.33	0.62
1:AB:30:THR:OG1	1:AS:33:ASN:OD1	2.16	0.62
1:AE:127:LEU:HD21	1:DE:48:ARG:HH12	1.63	0.62
1:CB:47:THR:HA	1:CB:77:PRO:HG2	1.82	0.62
1:DC:47:THR:HA	1:DC:77:PRO:HG2	1.82	0.62
1:AL:22:ILE:O	1:CB:6:SER:HA	1.99	0.62
1:BC:65:TYR:HE2	1:BP:46:ARG:HA	1.63	0.62
1:BS:47:THR:HA	1:BS:77:PRO:HG2	1.82	0.62
1:CE:47:THR:HA	1:CE:77:PRO:HG2	1.82	0.62
1:CQ:47:THR:HA	1:CQ:77:PRO:HG2	1.82	0.62
1:AW:65:TYR:CD2	1:BV:46:ARG:HG2	2.35	0.62
1:BJ:47:THR:HA	1:BJ:77:PRO:HG2	1.82	0.62
1:AF:8:LYS:HB2	1:AF:114:GLN:HE22	1.65	0.62
1:BJ:46:ARG:HA	1:BL:65:TYR:HE2	1.64	0.62
1:CK:47:THR:HA	1:CK:77:PRO:HG2	1.82	0.62
1:CW:47:THR:HA	1:CW:77:PRO:HG2	1.82	0.62
1:CZ:47:THR:HA	1:CZ:77:PRO:HG2	1.82	0.62
1:AI:8:LYS:HB2	1:AI:114:GLN:HE22	1.65	0.62
1:AL:8:LYS:HB2	1:AL:114:GLN:HE22	1.65	0.62
1:BJ:8:LYS:HB2	1:BJ:114:GLN:HE22	1.65	0.62
1:BJ:92:ILE:HG12	1:DF:92:ILE:HG12	1.82	0.62
1:BV:8:LYS:HB2	1:BV:114:GLN:HE22	1.65	0.62
1:DL:8:LYS:HB2	1:DL:114:GLN:HE22	1.65	0.62
1:BD:8:LYS:HB2	1:BD:114:GLN:HE22	1.65	0.61
1:BG:47:THR:HA	1:BG:77:PRO:HG2	1.82	0.61
1:AO:8:LYS:HB2	1:AO:114:GLN:HE22	1.65	0.61
1:BM:47:THR:HA	1:BM:77:PRO:HG2	1.82	0.61
1:BV:47:THR:HA	1:BV:77:PRO:HG2	1.82	0.61
1:CT:42:ASP:HB2	1:CT:48:ARG:HG2	1.83	0.61
1:DI:8:LYS:HB2	1:DI:114:GLN:HE22	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AI:47:THR:HA	1:AI:77:PRO:HG2	1.82	0.61
1:AO:46:ARG:HG2	1:CP:65:TYR:CD2	2.34	0.61
1:AU:8:LYS:HB2	1:AU:114:GLN:HE22	1.65	0.61
1:BA:8:LYS:HB2	1:BA:114:GLN:HE22	1.65	0.61
1:BD:22:ILE:HG22	1:CZ:7:ILE:O	2.01	0.61
1:BP:47:THR:HA	1:BP:77:PRO:HG2	1.82	0.61
1:BY:42:ASP:HB2	1:BY:48:ARG:HG2	1.83	0.61
1:CW:8:LYS:HB2	1:CW:114:GLN:HE22	1.65	0.61
1:AO:42:ASP:HB2	1:AO:48:ARG:HG2	1.83	0.61
1:BG:8:LYS:HB2	1:BG:114:GLN:HE22	1.65	0.61
1:BM:8:LYS:HB2	1:BM:114:GLN:HE22	1.65	0.61
1:BM:111:ILE:HD13	1:DI:74:PHE:CZ	2.34	0.61
1:BS:42:ASP:HB2	1:BS:48:ARG:HG2	1.83	0.61
1:CK:8:LYS:HB2	1:CK:114:GLN:HE22	1.65	0.61
1:CZ:8:LYS:HB2	1:CZ:114:GLN:HE22	1.65	0.61
1:CN:42:ASP:HB2	1:CN:48:ARG:HG2	1.83	0.61
1:AC:8:LYS:HB2	1:AC:114:GLN:HE22	1.65	0.61
1:AO:47:THR:HA	1:AO:77:PRO:HG2	1.82	0.61
1:AX:42:ASP:HB2	1:AX:48:ARG:HG2	1.83	0.61
1:DI:47:THR:HA	1:DI:77:PRO:HG2	1.82	0.61
1:AC:47:THR:HA	1:AC:77:PRO:HG2	1.82	0.61
1:AF:19:GLY:O	1:BV:8:LYS:HD2	2.00	0.61
1:AF:42:ASP:HB2	1:AF:48:ARG:HG2	1.83	0.61
1:BY:8:LYS:HB2	1:BY:114:GLN:HE22	1.65	0.61
1:CN:47:THR:HA	1:CN:77:PRO:HG2	1.82	0.61
1:CQ:8:LYS:HB2	1:CQ:114:GLN:HE22	1.65	0.61
1:AU:47:THR:HA	1:AU:77:PRO:HG2	1.82	0.61
1:AX:47:THR:HA	1:AX:77:PRO:HG2	1.82	0.61
1:BG:42:ASP:HB2	1:BG:48:ARG:HG2	1.83	0.61
1:BM:114:GLN:HE21	1:DI:16:ILE:HD13	1.65	0.61
1:CK:42:ASP:HB2	1:CK:48:ARG:HG2	1.83	0.61
1:AI:42:ASP:HB2	1:AI:48:ARG:HG2	1.83	0.61
1:AR:8:LYS:HB2	1:AR:114:GLN:HE22	1.65	0.61
1:AR:42:ASP:HB2	1:AR:48:ARG:HG2	1.83	0.61
1:AU:42:ASP:HB2	1:AU:48:ARG:HG2	1.83	0.61
1:BM:42:ASP:HB2	1:BM:48:ARG:HG2	1.83	0.61
1:BP:8:LYS:HB2	1:BP:114:GLN:HE22	1.65	0.61
1:BP:42:ASP:HB2	1:BP:48:ARG:HG2	1.83	0.61
1:CE:8:LYS:HB2	1:CE:114:GLN:HE22	1.65	0.61
1:DF:47:THR:HA	1:DF:77:PRO:HG2	1.82	0.61
1:AJ:65:TYR:CE2	1:CV:46:ARG:HG3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AL:47:THR:HA	1:AL:77:PRO:HG2	1.82	0.60
1:BF:65:TYR:CE2	1:BS:46:ARG:HA	2.36	0.60
1:BS:8:LYS:HB2	1:BS:114:GLN:HE22	1.65	0.60
1:BY:47:THR:HA	1:BY:77:PRO:HG2	1.82	0.60
1:CH:8:LYS:HB2	1:CH:114:GLN:HE22	1.65	0.60
1:CZ:42:ASP:HB2	1:CZ:48:ARG:HG2	1.83	0.60
1:AF:47:THR:HA	1:AF:77:PRO:HG2	1.82	0.60
1:AU:110:LEU:HD23	1:CN:16:ILE:HD11	1.83	0.60
1:CT:47:THR:HA	1:CT:77:PRO:HG2	1.82	0.60
1:DC:42:ASP:HB2	1:DC:48:ARG:HG2	1.83	0.60
1:BD:42:ASP:HB2	1:BD:48:ARG:HG2	1.83	0.60
1:BD:47:THR:HA	1:BD:77:PRO:HG2	1.82	0.60
1:CQ:42:ASP:HB2	1:CQ:48:ARG:HG2	1.83	0.60
1:AC:110:LEU:HD23	1:BP:16:ILE:HD11	1.83	0.60
1:AX:8:LYS:HB2	1:AX:114:GLN:HE22	1.65	0.60
1:BV:42:ASP:HB2	1:BV:48:ARG:HG2	1.83	0.60
1:AB:87:PHE:CE2	1:AS:60:VAL:HG11	2.37	0.60
1:AN:29:GLN:HG3	1:BZ:57:VAL:HG21	1.84	0.60
1:CN:8:LYS:HB2	1:CN:114:GLN:HE22	1.65	0.60
1:AC:42:ASP:HB2	1:AC:48:ARG:HG2	1.83	0.60
1:CT:8:LYS:HB2	1:CT:114:GLN:HE22	1.65	0.60
1:CW:46:ARG:HG2	1:CY:65:TYR:CE2	2.36	0.60
1:AC:16:ILE:HD11	1:BP:110:LEU:HD23	1.84	0.60
1:CB:42:ASP:HB2	1:CB:48:ARG:HG2	1.83	0.60
1:CH:47:THR:HA	1:CH:77:PRO:HG2	1.82	0.60
1:CB:8:LYS:HB2	1:CB:114:GLN:HE22	1.65	0.60
1:AR:47:THR:HA	1:AR:77:PRO:HG2	1.82	0.60
1:BJ:42:ASP:HB2	1:BJ:48:ARG:HG2	1.83	0.60
1:CH:42:ASP:HB2	1:CH:48:ARG:HG2	1.83	0.60
1:AF:22:ILE:O	1:BV:6:SER:HA	2.02	0.60
1:BD:110:LEU:HD23	1:CZ:16:ILE:HD11	1.83	0.60
1:DL:47:THR:HA	1:DL:77:PRO:HG2	1.82	0.60
1:CE:42:ASP:HB2	1:CE:48:ARG:HG2	1.83	0.59
1:CW:42:ASP:HB2	1:CW:48:ARG:HG2	1.83	0.59
1:AF:8:LYS:HD2	1:BV:19:GLY:O	2.02	0.59
1:AF:114:GLN:NE2	1:BV:16:ILE:HD13	2.15	0.59
1:AO:109:ARG:HG2	1:CE:116:LEU:HD22	1.84	0.59
1:BA:42:ASP:HB2	1:BA:48:ARG:HG2	1.83	0.59
1:DC:8:LYS:HB2	1:DC:114:GLN:HE22	1.65	0.59
1:DF:8:LYS:HB2	1:DF:114:GLN:HE22	1.65	0.59
1:DL:42:ASP:HB2	1:DL:48:ARG:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AC:111:ILE:HD13	1:BP:74:PHE:CZ	2.37	0.59
1:AM:130:LEU:O	1:CB:26:LEU:HB3	2.02	0.59
1:BA:47:THR:HA	1:BA:77:PRO:HG2	1.82	0.59
1:CW:10:GLY:N	1:CW:107:ASP:OD1	2.34	0.59
1:DF:42:ASP:HB2	1:DF:48:ARG:HG2	1.83	0.59
1:AB:46:ARG:HG3	1:AS:65:TYR:CE2	2.38	0.59
1:DI:42:ASP:HB2	1:DI:48:ARG:HG2	1.83	0.59
1:DF:10:GLY:N	1:DF:107:ASP:OD1	2.34	0.59
1:AH:46:ARG:NH2	1:CC:99:ALA:HA	2.18	0.59
1:AI:116:LEU:HD22	1:BY:109:ARG:HG2	1.85	0.59
1:BO:87:PHE:CE2	1:DJ:60:VAL:HG11	2.38	0.59
1:CD:65:TYR:HE2	1:CK:46:ARG:CA	2.14	0.59
1:AG:130:LEU:O	1:CE:26:LEU:HB3	2.03	0.59
1:AL:42:ASP:HB2	1:AL:48:ARG:HG2	1.83	0.59
1:BU:29:GLN:HG3	1:DG:57:VAL:HG21	1.85	0.59
1:AE:33:ASN:OD1	1:BG:30:THR:OG1	2.20	0.59
1:BI:127:LEU:HD21	1:BL:48:ARG:HH12	1.68	0.59
1:BM:115:LEU:HD13	1:DI:72:VAL:HG11	1.84	0.59
1:AH:33:ASN:OD1	1:CE:30:THR:OG1	2.20	0.59
1:AO:108:LEU:HD22	1:CE:90:VAL:HG12	1.85	0.58
1:BG:110:LEU:HD23	1:DC:16:ILE:HD11	1.85	0.58
1:BM:116:LEU:O	1:DI:109:ARG:NH2	2.35	0.58
1:AF:16:ILE:HD13	1:BV:114:GLN:NE2	2.13	0.58
1:BG:16:ILE:HD11	1:DC:110:LEU:HD23	1.85	0.58
1:CW:46:ARG:HA	1:CY:65:TYR:HE2	1.67	0.58
1:AO:109:ARG:NH2	1:CE:116:LEU:O	2.37	0.58
1:CZ:10:GLY:N	1:CZ:107:ASP:OD1	2.34	0.58
1:AK:65:TYR:CD2	1:BY:46:ARG:HG2	2.39	0.58
1:BK:39:VAL:O	1:BK:48:ARG:HD2	2.04	0.58
1:AG:39:VAL:O	1:AG:48:ARG:HD2	2.04	0.58
1:BZ:39:VAL:O	1:BZ:48:ARG:HD2	2.04	0.58
1:DL:10:GLY:N	1:DL:107:ASP:OD1	2.34	0.58
1:AI:116:LEU:O	1:BY:109:ARG:NH2	2.36	0.58
1:AM:39:VAL:O	1:AM:48:ARG:HD2	2.04	0.58
1:AO:46:ARG:HG2	1:CP:65:TYR:CE2	2.39	0.58
1:AT:46:ARG:NH2	1:AV:99:ALA:HA	2.19	0.58
1:CO:39:VAL:O	1:CO:48:ARG:HD2	2.04	0.58
1:CR:39:VAL:O	1:CR:48:ARG:HD2	2.04	0.58
1:AA:39:VAL:O	1:AA:48:ARG:HD2	2.04	0.58
1:AY:39:VAL:O	1:AY:48:ARG:HD2	2.04	0.58
1:BE:39:VAL:O	1:BE:48:ARG:HD2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AJ:39:VAL:O	1:AJ:48:ARG:HD2	2.04	0.57
1:AO:113:ALA:HB1	1:CE:113:ALA:HB1	1.85	0.57
1:BT:39:VAL:O	1:BT:48:ARG:HD2	2.04	0.57
1:AS:39:VAL:O	1:AS:48:ARG:HD2	2.04	0.57
1:CK:10:GLY:N	1:CK:107:ASP:OD1	2.34	0.57
1:CX:39:VAL:O	1:CX:48:ARG:HD2	2.04	0.57
1:DA:39:VAL:O	1:DA:48:ARG:HD2	2.04	0.57
1:AC:10:GLY:N	1:AC:107:ASP:OD1	2.34	0.57
1:DJ:39:VAL:O	1:DJ:48:ARG:HD2	2.04	0.57
1:BH:39:VAL:O	1:BH:48:ARG:HD2	2.04	0.57
1:BJ:7:ILE:O	1:DF:22:ILE:HG22	2.04	0.57
1:BQ:39:VAL:O	1:BQ:48:ARG:HD2	2.04	0.57
1:CI:39:VAL:O	1:CI:48:ARG:HD2	2.04	0.57
1:CT:10:GLY:N	1:CT:107:ASP:OD1	2.34	0.57
1:DC:10:GLY:N	1:DC:107:ASP:OD1	2.34	0.57
1:AB:47:THR:HA	1:AB:77:PRO:HG2	1.87	0.57
1:AJ:60:VAL:HG11	1:CV:87:PHE:CE2	2.39	0.57
1:AQ:47:THR:HA	1:AQ:77:PRO:HG2	1.87	0.57
1:AX:10:GLY:N	1:AX:107:ASP:OD1	2.34	0.57
1:DG:39:VAL:O	1:DG:48:ARG:HD2	2.04	0.57
1:AP:39:VAL:O	1:AP:48:ARG:HD2	2.04	0.57
1:BA:10:GLY:N	1:BA:107:ASP:OD1	2.34	0.57
1:BB:39:VAL:O	1:BB:48:ARG:HD2	2.04	0.57
1:BU:47:THR:HA	1:BU:77:PRO:HG2	1.87	0.57
1:CA:60:VAL:HG13	1:CA:65:TYR:HE1	1.70	0.57
1:CC:39:VAL:O	1:CC:48:ARG:HD2	2.04	0.57
1:DD:39:VAL:O	1:DD:48:ARG:HD2	2.04	0.57
1:DE:47:THR:HA	1:DE:77:PRO:HG2	1.87	0.57
1:AO:116:LEU:HD22	1:CE:109:ARG:HG2	1.87	0.57
1:AZ:47:THR:HA	1:AZ:77:PRO:HG2	1.87	0.57
1:AZ:60:VAL:HG13	1:AZ:65:TYR:HE1	1.70	0.57
1:BG:10:GLY:N	1:BG:107:ASP:OD1	2.34	0.57
1:AO:116:LEU:O	1:CE:109:ARG:NE	2.36	0.57
1:AQ:60:VAL:HG13	1:AQ:65:TYR:HE1	1.70	0.57
1:AU:10:GLY:N	1:AU:107:ASP:OD1	2.34	0.57
1:BC:60:VAL:HG13	1:BC:65:TYR:HE1	1.70	0.57
1:BL:47:THR:HA	1:BL:77:PRO:HG2	1.87	0.57
1:BM:90:VAL:HG12	1:DI:108:LEU:HD22	1.86	0.57
1:BW:39:VAL:O	1:BW:48:ARG:HD2	2.04	0.57
1:CF:39:VAL:O	1:CF:48:ARG:HD2	2.04	0.57
1:CY:47:THR:HA	1:CY:77:PRO:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:47:THR:HA	1:DB:77:PRO:HG2	1.87	0.57
1:AR:6:SER:HA	1:CK:22:ILE:O	2.04	0.57
1:AT:47:THR:HA	1:AT:77:PRO:HG2	1.87	0.57
1:BP:10:GLY:N	1:BP:107:ASP:OD1	2.34	0.57
1:BU:60:VAL:HG13	1:BU:65:TYR:HE1	1.70	0.57
1:CG:60:VAL:HG13	1:CG:65:TYR:HE1	1.70	0.57
1:DE:60:VAL:HG13	1:DE:65:TYR:HE1	1.70	0.57
1:AI:129:ALA:HB2	1:BW:26:LEU:O	2.05	0.56
1:AK:60:VAL:HG13	1:AK:65:TYR:HE1	1.70	0.56
1:BM:10:GLY:N	1:BM:107:ASP:OD1	2.34	0.56
1:BR:47:THR:HA	1:BR:77:PRO:HG2	1.87	0.56
1:BR:60:VAL:HG13	1:BR:65:TYR:HE1	1.70	0.56
1:BX:47:THR:HA	1:BX:77:PRO:HG2	1.87	0.56
1:CD:47:THR:HA	1:CD:77:PRO:HG2	1.87	0.56
1:CP:47:THR:HA	1:CP:77:PRO:HG2	1.87	0.56
1:AI:109:ARG:NH2	1:BY:116:LEU:O	2.37	0.56
1:AT:60:VAL:HG13	1:AT:65:TYR:HE1	1.70	0.56
1:BN:39:VAL:O	1:BN:48:ARG:HD2	2.04	0.56
1:BX:60:VAL:HG13	1:BX:65:TYR:HE1	1.70	0.56
1:CD:60:VAL:HG13	1:CD:65:TYR:HE1	1.70	0.56
1:CN:10:GLY:N	1:CN:107:ASP:OD1	2.34	0.56
1:DK:60:VAL:HG13	1:DK:65:TYR:HE1	1.70	0.56
1:AD:39:VAL:O	1:AD:48:ARG:HD2	2.04	0.56
1:AN:47:THR:HA	1:AN:77:PRO:HG2	1.87	0.56
1:BF:47:THR:HA	1:BF:77:PRO:HG2	1.87	0.56
1:CP:60:VAL:HG13	1:CP:65:TYR:HE1	1.70	0.56
1:CU:39:VAL:O	1:CU:48:ARG:HD2	2.04	0.56
1:CV:60:VAL:HG13	1:CV:65:TYR:HE1	1.70	0.56
1:DH:47:THR:HA	1:DH:77:PRO:HG2	1.87	0.56
1:AB:60:VAL:HG13	1:AB:65:TYR:HE1	1.70	0.56
1:AU:7:ILE:O	1:CN:22:ILE:HG22	2.05	0.56
1:BU:87:PHE:HE2	1:DG:60:VAL:HG11	1.69	0.56
1:DB:60:VAL:HG13	1:DB:65:TYR:HE1	1.70	0.56
1:AI:10:GLY:N	1:AI:107:ASP:OD1	2.34	0.56
1:AK:87:PHE:HE2	1:BW:60:VAL:HG11	1.71	0.56
1:AO:109:ARG:NE	1:CE:116:LEU:O	2.39	0.56
1:CH:10:GLY:N	1:CH:107:ASP:OD1	2.34	0.56
1:CJ:47:THR:HA	1:CJ:77:PRO:HG2	1.87	0.56
1:AI:22:ILE:HG22	1:BY:7:ILE:O	2.05	0.56
1:BD:22:ILE:O	1:CZ:6:SER:HA	2.05	0.56
1:BO:47:THR:HA	1:BO:77:PRO:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CL:39:VAL:O	1:CL:48:ARG:HD2	2.04	0.56
1:CL:119:ALA:HA	1:CL:122:ASP:HB2	1.88	0.56
1:AE:60:VAL:HG13	1:AE:65:TYR:HE1	1.70	0.56
1:AR:92:ILE:HG12	1:CK:92:ILE:HG12	1.86	0.56
1:AU:6:SER:HA	1:CN:22:ILE:O	2.06	0.56
1:AV:39:VAL:O	1:AV:48:ARG:HD2	2.04	0.56
1:BC:47:THR:HA	1:BC:77:PRO:HG2	1.87	0.56
1:CA:65:TYR:HE2	1:CH:46:ARG:HA	1.71	0.56
1:CI:119:ALA:HA	1:CI:122:ASP:HB2	1.88	0.56
1:CJ:60:VAL:HG13	1:CJ:65:TYR:HE1	1.70	0.56
1:CX:119:ALA:HA	1:CX:122:ASP:HB2	1.88	0.56
1:CY:60:VAL:HG13	1:CY:65:TYR:HE1	1.70	0.56
1:DH:60:VAL:HG13	1:DH:65:TYR:HE1	1.70	0.56
1:AA:119:ALA:HA	1:AA:122:ASP:HB2	1.88	0.56
1:AM:119:ALA:HA	1:AM:122:ASP:HB2	1.88	0.56
1:AW:60:VAL:HG13	1:AW:65:TYR:HE1	1.70	0.56
1:BH:119:ALA:HA	1:BH:122:ASP:HB2	1.88	0.56
1:BI:60:VAL:HG13	1:BI:65:TYR:HE1	1.70	0.56
1:BU:22:ILE:HA	1:BU:41:GLU:OE1	2.06	0.56
1:BZ:119:ALA:HA	1:BZ:122:ASP:HB2	1.88	0.56
1:CJ:34:GLY:HA3	1:CJ:53:PHE:O	2.06	0.56
1:CW:46:ARG:HG2	1:CY:65:TYR:HD2	1.67	0.56
1:AW:22:ILE:HA	1:AW:41:GLU:OE1	2.06	0.56
1:BB:119:ALA:HA	1:BB:122:ASP:HB2	1.88	0.56
1:BF:60:VAL:HG13	1:BF:65:TYR:HE1	1.70	0.56
1:BR:22:ILE:HA	1:BR:41:GLU:OE1	2.06	0.56
1:CO:119:ALA:HA	1:CO:122:ASP:HB2	1.88	0.56
1:CP:22:ILE:HA	1:CP:41:GLU:OE1	2.06	0.56
1:CU:119:ALA:HA	1:CU:122:ASP:HB2	1.88	0.56
1:CV:22:ILE:HA	1:CV:41:GLU:OE1	2.06	0.56
1:DB:22:ILE:HA	1:DB:41:GLU:OE1	2.06	0.56
1:DG:119:ALA:HA	1:DG:122:ASP:HB2	1.88	0.56
1:AK:47:THR:HA	1:AK:77:PRO:HG2	1.87	0.56
1:AW:34:GLY:HA3	1:AW:53:PHE:O	2.06	0.56
1:BI:22:ILE:HA	1:BI:41:GLU:OE1	2.06	0.56
1:BL:22:ILE:HA	1:BL:41:GLU:OE1	2.06	0.56
1:BM:108:LEU:HD22	1:DI:90:VAL:CG1	2.33	0.56
1:BY:10:GLY:N	1:BY:107:ASP:OD1	2.34	0.56
1:CR:119:ALA:HA	1:CR:122:ASP:HB2	1.88	0.56
1:CV:47:THR:HA	1:CV:77:PRO:HG2	1.87	0.56
1:AD:119:ALA:HA	1:AD:122:ASP:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AK:34:GLY:HA3	1:AK:53:PHE:O	2.06	0.55
1:AN:22:ILE:HA	1:AN:41:GLU:OE1	2.06	0.55
1:AW:47:THR:HA	1:AW:77:PRO:HG2	1.87	0.55
1:BC:22:ILE:HA	1:BC:41:GLU:OE1	2.06	0.55
1:CA:47:THR:HA	1:CA:77:PRO:HG2	1.87	0.55
1:CD:22:ILE:HA	1:CD:41:GLU:OE1	2.06	0.55
1:CD:98:PRO:HB2	1:CK:46:ARG:HG3	1.87	0.55
1:AE:47:THR:HA	1:AE:77:PRO:HG2	1.87	0.55
1:AH:60:VAL:HG13	1:AH:65:TYR:HE1	1.70	0.55
1:AN:34:GLY:HA3	1:AN:53:PHE:O	2.06	0.55
1:AS:119:ALA:HA	1:AS:122:ASP:HB2	1.88	0.55
1:BF:65:TYR:HE2	1:BS:46:ARG:CA	2.19	0.55
1:BK:119:ALA:HA	1:BK:122:ASP:HB2	1.88	0.55
1:BO:22:ILE:HA	1:BO:41:GLU:OE1	2.06	0.55
1:CF:119:ALA:HA	1:CF:122:ASP:HB2	1.88	0.55
1:CG:22:ILE:HA	1:CG:41:GLU:OE1	2.06	0.55
1:CP:34:GLY:HA3	1:CP:53:PHE:O	2.06	0.55
1:CS:22:ILE:HA	1:CS:41:GLU:OE1	2.06	0.55
1:CV:34:GLY:HA3	1:CV:53:PHE:O	2.06	0.55
1:DH:34:GLY:HA3	1:DH:53:PHE:O	2.06	0.55
1:AF:10:GLY:N	1:AF:107:ASP:OD1	2.34	0.55
1:AI:109:ARG:HG2	1:BY:116:LEU:HD22	1.88	0.55
1:AP:119:ALA:HA	1:AP:122:ASP:HB2	1.88	0.55
1:BC:34:GLY:HA3	1:BC:53:PHE:O	2.06	0.55
1:BO:60:VAL:HG13	1:BO:65:TYR:HE1	1.70	0.55
1:CA:22:ILE:HA	1:CA:41:GLU:OE1	2.06	0.55
1:CC:119:ALA:HA	1:CC:122:ASP:HB2	1.88	0.55
1:CG:34:GLY:HA3	1:CG:53:PHE:O	2.06	0.55
1:CM:47:THR:HA	1:CM:77:PRO:HG2	1.87	0.55
1:CM:60:VAL:HG13	1:CM:65:TYR:HE1	1.70	0.55
1:DJ:119:ALA:HA	1:DJ:122:ASP:HB2	1.88	0.55
1:AR:10:GLY:N	1:AR:107:ASP:OD1	2.34	0.55
1:BI:47:THR:HA	1:BI:77:PRO:HG2	1.87	0.55
1:BN:119:ALA:HA	1:BN:122:ASP:HB2	1.88	0.55
1:BX:22:ILE:HA	1:BX:41:GLU:OE1	2.06	0.55
1:CS:34:GLY:HA3	1:CS:53:PHE:O	2.06	0.55
1:CS:47:THR:HA	1:CS:77:PRO:HG2	1.87	0.55
1:CY:22:ILE:HA	1:CY:41:GLU:OE1	2.06	0.55
1:DE:34:GLY:HA3	1:DE:53:PHE:O	2.06	0.55
1:DH:22:ILE:HA	1:DH:41:GLU:OE1	2.06	0.55
1:DK:34:GLY:HA3	1:DK:53:PHE:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:22:ILE:HA	1:AB:41:GLU:OE1	2.06	0.55
1:AE:34:GLY:HA3	1:AE:53:PHE:O	2.06	0.55
1:AH:34:GLY:HA3	1:AH:53:PHE:O	2.06	0.55
1:AZ:34:GLY:HA3	1:AZ:53:PHE:O	2.06	0.55
1:BQ:119:ALA:HA	1:BQ:122:ASP:HB2	1.88	0.55
1:BT:119:ALA:HA	1:BT:122:ASP:HB2	1.88	0.55
1:CM:22:ILE:HA	1:CM:41:GLU:OE1	2.06	0.55
1:CS:60:VAL:HG13	1:CS:65:TYR:HE1	1.70	0.55
1:DK:22:ILE:HA	1:DK:41:GLU:OE1	2.06	0.55
1:DK:47:THR:HA	1:DK:77:PRO:HG2	1.87	0.55
1:AH:22:ILE:HA	1:AH:41:GLU:OE1	2.06	0.55
1:AT:34:GLY:HA3	1:AT:53:PHE:O	2.06	0.55
1:BE:119:ALA:HA	1:BE:122:ASP:HB2	1.88	0.55
1:CA:34:GLY:HA3	1:CA:53:PHE:O	2.06	0.55
1:AV:119:ALA:HA	1:AV:122:ASP:HB2	1.88	0.55
1:BO:34:GLY:HA3	1:BO:53:PHE:O	2.06	0.55
1:BR:34:GLY:HA3	1:BR:53:PHE:O	2.06	0.55
1:CG:47:THR:HA	1:CG:77:PRO:HG2	1.87	0.55
1:DB:34:GLY:HA3	1:DB:53:PHE:O	2.06	0.55
1:AF:48:ARG:HH12	1:DD:127:LEU:HB3	1.72	0.55
1:AH:47:THR:HA	1:AH:77:PRO:HG2	1.87	0.55
1:AT:22:ILE:HA	1:AT:41:GLU:OE1	2.06	0.55
1:BX:34:GLY:HA3	1:BX:53:PHE:O	2.06	0.55
1:CE:10:GLY:N	1:CE:107:ASP:OD1	2.34	0.55
1:AZ:22:ILE:HA	1:AZ:41:GLU:OE1	2.06	0.55
1:BF:22:ILE:HA	1:BF:41:GLU:OE1	2.06	0.55
1:BL:60:VAL:HG13	1:BL:65:TYR:HE1	1.70	0.55
1:CD:34:GLY:HA3	1:CD:53:PHE:O	2.06	0.55
1:AI:12:THR:H	1:BY:18:GLY:HA2	1.71	0.55
1:AK:22:ILE:HA	1:AK:41:GLU:OE1	2.06	0.55
1:BI:34:GLY:HA3	1:BI:53:PHE:O	2.06	0.55
1:BS:10:GLY:N	1:BS:107:ASP:OD1	2.34	0.55
1:AI:90:VAL:HG12	1:BY:108:LEU:HD22	1.87	0.54
1:BF:34:GLY:HA3	1:BF:53:PHE:O	2.06	0.54
1:BU:34:GLY:HA3	1:BU:53:PHE:O	2.06	0.54
1:CQ:10:GLY:N	1:CQ:107:ASP:OD1	2.34	0.54
1:DD:119:ALA:HA	1:DD:122:ASP:HB2	1.88	0.54
1:AL:10:GLY:N	1:AL:107:ASP:OD1	2.34	0.54
1:AN:60:VAL:HG13	1:AN:65:TYR:HE1	1.70	0.54
1:BU:87:PHE:CE2	1:DG:60:VAL:HG11	2.43	0.54
1:DA:119:ALA:HA	1:DA:122:ASP:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AS:22:ILE:HD11	1:AS:39:VAL:HG11	1.90	0.54
1:AY:119:ALA:HA	1:AY:122:ASP:HB2	1.88	0.54
1:BJ:46:ARG:HG3	1:BL:98:PRO:HB2	1.88	0.54
1:BL:34:GLY:HA3	1:BL:53:PHE:O	2.06	0.54
1:CD:29:GLN:HG3	1:CI:57:VAL:HG21	1.90	0.54
1:CU:22:ILE:HD11	1:CU:39:VAL:HG11	1.90	0.54
1:CY:34:GLY:HA3	1:CY:53:PHE:O	2.06	0.54
1:DI:10:GLY:N	1:DI:107:ASP:OD1	2.34	0.54
1:DJ:22:ILE:HD11	1:DJ:39:VAL:HG11	1.90	0.54
1:AE:22:ILE:HA	1:AE:41:GLU:OE1	2.06	0.54
1:AQ:34:GLY:HA3	1:AQ:53:PHE:O	2.06	0.54
1:AR:109:ARG:NH1	1:CK:122:ASP:OD1	2.35	0.54
1:BB:22:ILE:HD11	1:BB:39:VAL:HG11	1.90	0.54
1:BH:22:ILE:HD11	1:BH:39:VAL:HG11	1.90	0.54
1:BT:22:ILE:HD11	1:BT:39:VAL:HG11	1.90	0.54
1:BW:119:ALA:HA	1:BW:122:ASP:HB2	1.88	0.54
1:DE:22:ILE:HA	1:DE:41:GLU:OE1	2.06	0.54
1:AB:34:GLY:HA3	1:AB:53:PHE:O	2.06	0.54
1:AE:46:ARG:HG3	1:BE:65:TYR:CD2	2.42	0.54
1:AG:119:ALA:HA	1:AG:122:ASP:HB2	1.88	0.54
1:AI:116:LEU:O	1:BY:109:ARG:NE	2.38	0.54
1:AJ:119:ALA:HA	1:AJ:122:ASP:HB2	1.88	0.54
1:AM:22:ILE:HD11	1:AM:39:VAL:HG11	1.90	0.54
1:AQ:22:ILE:HA	1:AQ:41:GLU:OE1	2.06	0.54
1:BD:16:ILE:HD11	1:CZ:110:LEU:HD23	1.90	0.54
1:BJ:46:ARG:HA	1:BL:65:TYR:CE2	2.41	0.54
1:CJ:22:ILE:HA	1:CJ:41:GLU:OE1	2.06	0.54
1:CM:34:GLY:HA3	1:CM:53:PHE:O	2.06	0.54
1:AM:60:VAL:HG11	1:CP:87:PHE:CE2	2.43	0.54
1:CD:58:PRO:HB2	1:CK:45:TYR:CE2	2.43	0.54
1:AA:22:ILE:HD11	1:AA:39:VAL:HG11	1.90	0.54
1:AD:22:ILE:HD11	1:AD:39:VAL:HG11	1.90	0.54
1:BI:127:LEU:HD23	1:BL:48:ARG:HH22	1.72	0.54
1:AP:22:ILE:HD11	1:AP:39:VAL:HG11	1.90	0.54
1:DD:22:ILE:HD11	1:DD:39:VAL:HG11	1.90	0.54
1:AD:33:ASN:OD1	1:DE:30:THR:OG1	2.20	0.53
1:AI:130:LEU:HD21	1:BY:55:SER:CB	2.37	0.53
1:BO:29:GLN:HG3	1:DJ:57:VAL:HG21	1.90	0.53
1:BD:111:ILE:HD13	1:CZ:74:PHE:CZ	2.42	0.53
1:CC:22:ILE:HD11	1:CC:39:VAL:HG11	1.90	0.53
1:AJ:60:VAL:HG11	1:CV:87:PHE:HE2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AO:10:GLY:N	1:AO:107:ASP:OD1	2.34	0.53
1:AY:22:ILE:HD11	1:AY:39:VAL:HG11	1.90	0.53
1:CR:22:ILE:HD11	1:CR:39:VAL:HG11	1.90	0.53
1:DG:22:ILE:HD11	1:DG:39:VAL:HG11	1.90	0.53
1:AJ:22:ILE:HD11	1:AJ:39:VAL:HG11	1.90	0.53
1:AO:116:LEU:O	1:CE:109:ARG:NH2	2.40	0.53
1:AG:22:ILE:HD11	1:AG:39:VAL:HG11	1.90	0.53
1:AO:90:VAL:HG12	1:CE:108:LEU:HD22	1.89	0.53
1:BN:39:VAL:HG23	1:BN:42:ASP:H	1.74	0.53
1:BW:22:ILE:HD11	1:BW:39:VAL:HG11	1.90	0.53
1:CI:22:ILE:HD11	1:CI:39:VAL:HG11	1.90	0.53
1:CJ:29:GLN:HG3	1:DA:57:VAL:HG21	1.91	0.53
1:DJ:39:VAL:HG23	1:DJ:42:ASP:H	1.74	0.53
1:AV:22:ILE:HD11	1:AV:39:VAL:HG11	1.90	0.53
1:BJ:10:GLY:N	1:BJ:107:ASP:OD1	2.34	0.53
1:BW:39:VAL:HG23	1:BW:42:ASP:H	1.74	0.53
1:BX:87:PHE:HE2	1:CL:60:VAL:HG11	1.74	0.53
1:CF:39:VAL:HG23	1:CF:42:ASP:H	1.74	0.53
1:CX:22:ILE:HD11	1:CX:39:VAL:HG11	1.90	0.53
1:AA:39:VAL:HG23	1:AA:42:ASP:H	1.74	0.53
1:AV:39:VAL:HG23	1:AV:42:ASP:H	1.74	0.53
1:AG:39:VAL:HG23	1:AG:42:ASP:H	1.74	0.53
1:BK:22:ILE:HD11	1:BK:39:VAL:HG11	1.90	0.53
1:BQ:22:ILE:HD11	1:BQ:39:VAL:HG11	1.90	0.53
1:CB:10:GLY:N	1:CB:107:ASP:OD1	2.34	0.53
1:CI:39:VAL:HG23	1:CI:42:ASP:H	1.74	0.53
1:CM:29:GLN:HG3	1:CX:57:VAL:HG21	1.90	0.53
1:DA:22:ILE:HD11	1:DA:39:VAL:HG11	1.90	0.53
1:AF:22:ILE:HD12	1:AF:49:ARG:HH21	1.74	0.53
1:AK:48:ARG:HH12	1:BX:127:LEU:HD21	1.73	0.53
1:BL:49:ARG:HG2	1:BL:76:ILE:HG12	1.91	0.53
1:CF:22:ILE:HD11	1:CF:39:VAL:HG11	1.90	0.53
1:DG:39:VAL:HG23	1:DG:42:ASP:H	1.74	0.53
1:DH:49:ARG:HG2	1:DH:76:ILE:HG12	1.91	0.53
1:AO:22:ILE:HD12	1:AO:49:ARG:HH21	1.74	0.53
1:BA:22:ILE:HD12	1:BA:49:ARG:HH21	1.74	0.53
1:BD:22:ILE:HD12	1:BD:49:ARG:HH21	1.74	0.53
1:BM:130:LEU:HD21	1:DI:55:SER:CB	2.35	0.53
1:CE:22:ILE:HD12	1:CE:49:ARG:HH21	1.74	0.53
1:AG:60:VAL:HG11	1:CS:87:PHE:CE2	2.44	0.52
1:AX:2:ILE:HD11	1:AX:124:PHE:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:67:LYS:NZ	1:CW:87:PHE:O	2.34	0.52
1:BG:2:ILE:HD11	1:BG:124:PHE:HB2	1.91	0.52
1:BH:39:VAL:HG23	1:BH:42:ASP:H	1.74	0.52
1:BN:22:ILE:HD11	1:BN:39:VAL:HG11	1.90	0.52
1:BO:49:ARG:HG2	1:BO:76:ILE:HG12	1.91	0.52
1:CO:39:VAL:HG23	1:CO:42:ASP:H	1.74	0.52
1:DI:22:ILE:HD12	1:DI:49:ARG:HH21	1.74	0.52
1:DL:22:ILE:HD12	1:DL:49:ARG:HH21	1.74	0.52
1:AD:39:VAL:HG23	1:AD:42:ASP:H	1.74	0.52
1:AL:2:ILE:HD11	1:AL:124:PHE:HB2	1.92	0.52
1:AT:49:ARG:HG2	1:AT:76:ILE:HG12	1.91	0.52
1:BJ:2:ILE:HD11	1:BJ:124:PHE:HB2	1.92	0.52
1:BT:39:VAL:HG23	1:BT:42:ASP:H	1.74	0.52
1:BX:49:ARG:HG2	1:BX:76:ILE:HG12	1.91	0.52
1:BY:22:ILE:HD12	1:BY:49:ARG:HH21	1.74	0.52
1:CT:2:ILE:HD11	1:CT:124:PHE:HB2	1.92	0.52
1:DE:49:ARG:HG2	1:DE:76:ILE:HG12	1.91	0.52
1:AE:49:ARG:HG2	1:AE:76:ILE:HG12	1.91	0.52
1:AI:7:ILE:O	1:BY:22:ILE:HG22	2.08	0.52
1:AN:49:ARG:HG2	1:AN:76:ILE:HG12	1.91	0.52
1:AR:22:ILE:HD12	1:AR:49:ARG:HH21	1.74	0.52
1:AZ:49:ARG:HG2	1:AZ:76:ILE:HG12	1.91	0.52
1:BD:10:GLY:N	1:BD:107:ASP:OD1	2.34	0.52
1:CD:85:THR:N	1:CI:63:GLY:O	2.35	0.52
1:CE:2:ILE:HD11	1:CE:124:PHE:HB2	1.92	0.52
1:CN:22:ILE:HD12	1:CN:49:ARG:HH21	1.74	0.52
1:CO:22:ILE:HD11	1:CO:39:VAL:HG11	1.90	0.52
1:CQ:22:ILE:HD12	1:CQ:49:ARG:HH21	1.74	0.52
1:CR:39:VAL:HG23	1:CR:42:ASP:H	1.74	0.52
1:CZ:45:TYR:HA	1:CZ:48:ARG:HE	1.75	0.52
1:DC:22:ILE:HD12	1:DC:49:ARG:HH21	1.74	0.52
1:AC:45:TYR:HA	1:AC:48:ARG:HE	1.75	0.52
1:AX:22:ILE:HD12	1:AX:49:ARG:HH21	1.74	0.52
1:BA:2:ILE:HD11	1:BA:124:PHE:HB2	1.92	0.52
1:BC:49:ARG:HG2	1:BC:76:ILE:HG12	1.91	0.52
1:BM:113:ALA:HB1	1:DI:113:ALA:HB1	1.90	0.52
1:BQ:39:VAL:HG23	1:BQ:42:ASP:H	1.74	0.52
1:CJ:49:ARG:HG2	1:CJ:76:ILE:HG12	1.92	0.52
1:CL:22:ILE:HD11	1:CL:39:VAL:HG11	1.90	0.52
1:AI:2:ILE:HD11	1:AI:124:PHE:HB2	1.92	0.52
1:AO:2:ILE:HD11	1:AO:124:PHE:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:45:TYR:HA	1:AR:48:ARG:HE	1.75	0.52
1:BD:45:TYR:HA	1:BD:48:ARG:HE	1.75	0.52
1:BE:39:VAL:HG23	1:BE:42:ASP:H	1.74	0.52
1:BG:108:LEU:HD22	1:DC:90:VAL:HG12	1.92	0.52
1:BJ:45:TYR:HA	1:BJ:48:ARG:HE	1.75	0.52
1:BP:45:TYR:HA	1:BP:48:ARG:HE	1.75	0.52
1:CH:45:TYR:HB2	1:CH:48:ARG:HH21	1.75	0.52
1:CQ:2:ILE:HD11	1:CQ:124:PHE:HB2	1.92	0.52
1:CS:49:ARG:HG2	1:CS:76:ILE:HG12	1.91	0.52
1:CW:2:ILE:HD11	1:CW:124:PHE:HB2	1.92	0.52
1:CW:22:ILE:HD12	1:CW:49:ARG:HH21	1.74	0.52
1:CX:39:VAL:HG23	1:CX:42:ASP:H	1.74	0.52
1:DF:2:ILE:HD11	1:DF:124:PHE:HB2	1.92	0.52
1:DF:45:TYR:HA	1:DF:48:ARG:HE	1.75	0.52
1:AL:22:ILE:HD12	1:AL:49:ARG:HH21	1.74	0.52
1:AL:45:TYR:HB2	1:AL:48:ARG:HH21	1.75	0.52
1:AU:45:TYR:HB2	1:AU:48:ARG:HH21	1.75	0.52
1:BE:22:ILE:HD11	1:BE:39:VAL:HG11	1.90	0.52
1:CG:49:ARG:HG2	1:CG:76:ILE:HG12	1.92	0.52
1:CH:2:ILE:HD11	1:CH:124:PHE:HB2	1.92	0.52
1:CH:22:ILE:HD12	1:CH:49:ARG:HH21	1.74	0.52
1:CK:45:TYR:HA	1:CK:48:ARG:HE	1.75	0.52
1:DF:22:ILE:HD12	1:DF:49:ARG:HH21	1.74	0.52
1:AF:45:TYR:HA	1:AF:48:ARG:HE	1.75	0.52
1:AJ:39:VAL:HG23	1:AJ:42:ASP:H	1.74	0.52
1:AK:87:PHE:CE2	1:BW:60:VAL:HG11	2.45	0.52
1:AS:39:VAL:HG23	1:AS:42:ASP:H	1.74	0.52
1:AX:45:TYR:HA	1:AX:48:ARG:HE	1.75	0.52
1:BB:39:VAL:HG23	1:BB:42:ASP:H	1.74	0.52
1:BM:22:ILE:HD12	1:BM:49:ARG:HH21	1.74	0.52
1:BS:22:ILE:HD12	1:BS:49:ARG:HH21	1.74	0.52
1:BV:45:TYR:HA	1:BV:48:ARG:HE	1.75	0.52
1:BX:65:TYR:HE2	1:CN:46:ARG:CA	2.17	0.52
1:CK:22:ILE:HD12	1:CK:49:ARG:HH21	1.74	0.52
1:CL:39:VAL:HG23	1:CL:42:ASP:H	1.74	0.52
1:AC:2:ILE:HD11	1:AC:124:PHE:HB2	1.92	0.52
1:AO:114:GLN:NE2	1:CE:16:ILE:HG21	2.24	0.52
1:BS:2:ILE:HD11	1:BS:124:PHE:HB2	1.92	0.52
1:BV:45:TYR:HB2	1:BV:48:ARG:HH21	1.75	0.52
1:BZ:22:ILE:HD11	1:BZ:39:VAL:HG11	1.90	0.52
1:CT:22:ILE:HD12	1:CT:49:ARG:HH21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DC:2:ILE:HD11	1:DC:124:PHE:HB2	1.92	0.52
1:DJ:68:GLY:O	1:DJ:95:GLU:HA	2.10	0.52
1:AB:49:ARG:HG2	1:AB:76:ILE:HG12	1.91	0.52
1:AI:45:TYR:HA	1:AI:48:ARG:HE	1.75	0.52
1:AM:39:VAL:HG23	1:AM:42:ASP:H	1.74	0.52
1:AQ:49:ARG:HG2	1:AQ:76:ILE:HG12	1.91	0.52
1:BA:22:ILE:HA	1:BA:41:GLU:OE1	2.10	0.52
1:BJ:22:ILE:HD12	1:BJ:49:ARG:HH21	1.74	0.52
1:BW:68:GLY:O	1:BW:95:GLU:HA	2.10	0.52
1:BX:29:GLN:HG3	1:CL:57:VAL:HG21	1.90	0.52
1:BZ:68:GLY:O	1:BZ:95:GLU:HA	2.10	0.52
1:CB:45:TYR:HA	1:CB:48:ARG:HE	1.75	0.52
1:CE:45:TYR:HA	1:CE:48:ARG:HE	1.75	0.52
1:DD:39:VAL:HG23	1:DD:42:ASP:H	1.74	0.52
1:DF:45:TYR:HB2	1:DF:48:ARG:HH21	1.75	0.52
1:AG:60:VAL:HG11	1:CS:87:PHE:HE2	1.75	0.52
1:AI:22:ILE:HA	1:AI:41:GLU:OE1	2.10	0.52
1:AJ:68:GLY:O	1:AJ:95:GLU:HA	2.10	0.52
1:BF:49:ARG:HG2	1:BF:76:ILE:HG12	1.91	0.52
1:BG:45:TYR:HB2	1:BG:48:ARG:HH21	1.75	0.52
1:BI:49:ARG:HG2	1:BI:76:ILE:HG12	1.91	0.52
1:BK:39:VAL:HG23	1:BK:42:ASP:H	1.74	0.52
1:BN:68:GLY:O	1:BN:95:GLU:HA	2.10	0.52
1:BP:22:ILE:HA	1:BP:41:GLU:OE1	2.10	0.52
1:BY:45:TYR:HB2	1:BY:48:ARG:HH21	1.75	0.52
1:CB:22:ILE:HD12	1:CB:49:ARG:HH21	1.74	0.52
1:CK:2:ILE:HD11	1:CK:124:PHE:HB2	1.92	0.52
1:CM:49:ARG:HG2	1:CM:76:ILE:HG12	1.91	0.52
1:DB:49:ARG:HG2	1:DB:76:ILE:HG12	1.92	0.52
1:AC:22:ILE:HA	1:AC:41:GLU:OE1	2.10	0.51
1:AO:45:TYR:HB2	1:AO:48:ARG:HH21	1.75	0.51
1:AP:39:VAL:HG23	1:AP:42:ASP:H	1.74	0.51
1:AP:68:GLY:O	1:AP:95:GLU:HA	2.10	0.51
1:AT:48:ARG:HH12	1:AW:127:LEU:HD21	1.74	0.51
1:AU:22:ILE:HD12	1:AU:49:ARG:HH21	1.74	0.51
1:AX:45:TYR:HB2	1:AX:48:ARG:HH21	1.75	0.51
1:BB:68:GLY:O	1:BB:95:GLU:HA	2.10	0.51
1:BM:45:TYR:HB2	1:BM:48:ARG:HH21	1.75	0.51
1:BP:2:ILE:HD11	1:BP:124:PHE:HB2	1.92	0.51
1:BV:22:ILE:HD12	1:BV:49:ARG:HH21	1.74	0.51
1:CB:22:ILE:HA	1:CB:41:GLU:OE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CB:45:TYR:HB2	1:CB:48:ARG:HH21	1.75	0.51
1:CC:39:VAL:HG23	1:CC:42:ASP:H	1.74	0.51
1:CE:22:ILE:HA	1:CE:41:GLU:OE1	2.10	0.51
1:CT:22:ILE:HA	1:CT:41:GLU:OE1	2.10	0.51
1:CU:68:GLY:O	1:CU:95:GLU:HA	2.10	0.51
1:CZ:22:ILE:HA	1:CZ:41:GLU:OE1	2.10	0.51
1:DD:68:GLY:O	1:DD:95:GLU:HA	2.10	0.51
1:AD:68:GLY:O	1:AD:95:GLU:HA	2.10	0.51
1:AF:45:TYR:HB2	1:AF:48:ARG:HH21	1.75	0.51
1:AI:22:ILE:HD12	1:AI:49:ARG:HH21	1.74	0.51
1:AL:45:TYR:HA	1:AL:48:ARG:HE	1.75	0.51
1:AR:22:ILE:HA	1:AR:41:GLU:OE1	2.10	0.51
1:AU:2:ILE:HD11	1:AU:124:PHE:HB2	1.91	0.51
1:AV:68:GLY:O	1:AV:95:GLU:HA	2.10	0.51
1:BA:45:TYR:HB2	1:BA:48:ARG:HH21	1.75	0.51
1:BD:45:TYR:HB2	1:BD:48:ARG:HH21	1.75	0.51
1:CD:49:ARG:HG2	1:CD:76:ILE:HG12	1.91	0.51
1:CE:45:TYR:HB2	1:CE:48:ARG:HH21	1.75	0.51
1:CN:45:TYR:HB2	1:CN:48:ARG:HH21	1.75	0.51
1:CR:68:GLY:O	1:CR:95:GLU:HA	2.10	0.51
1:CU:39:VAL:HG23	1:CU:42:ASP:H	1.74	0.51
1:CZ:22:ILE:HD12	1:CZ:49:ARG:HH21	1.74	0.51
1:DA:39:VAL:HG23	1:DA:42:ASP:H	1.74	0.51
1:AD:65:TYR:CE2	1:DE:46:ARG:HG3	2.45	0.51
1:AL:22:ILE:HA	1:AL:41:GLU:OE1	2.10	0.51
1:AS:68:GLY:O	1:AS:95:GLU:HA	2.10	0.51
1:AU:45:TYR:HA	1:AU:48:ARG:HE	1.75	0.51
1:AY:68:GLY:O	1:AY:95:GLU:HA	2.10	0.51
1:BA:45:TYR:HA	1:BA:48:ARG:HE	1.75	0.51
1:BD:16:ILE:HD13	1:CZ:114:GLN:NE2	2.22	0.51
1:BG:45:TYR:HA	1:BG:48:ARG:HE	1.75	0.51
1:BJ:45:TYR:HB2	1:BJ:48:ARG:HH21	1.75	0.51
1:BS:45:TYR:HA	1:BS:48:ARG:HE	1.75	0.51
1:BT:68:GLY:O	1:BT:95:GLU:HA	2.10	0.51
1:BY:22:ILE:HA	1:BY:41:GLU:OE1	2.10	0.51
1:BZ:39:VAL:HG23	1:BZ:42:ASP:H	1.74	0.51
1:CB:2:ILE:HD11	1:CB:124:PHE:HB2	1.92	0.51
1:CH:45:TYR:HA	1:CH:48:ARG:HE	1.75	0.51
1:CQ:22:ILE:HA	1:CQ:41:GLU:OE1	2.10	0.51
1:CQ:45:TYR:HA	1:CQ:48:ARG:HE	1.75	0.51
1:CT:45:TYR:HB2	1:CT:48:ARG:HH21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CV:49:ARG:HG2	1:CV:76:ILE:HG12	1.92	0.51
1:CY:49:ARG:HG2	1:CY:76:ILE:HG12	1.91	0.51
1:BD:22:ILE:HA	1:BD:41:GLU:OE1	2.10	0.51
1:BH:68:GLY:O	1:BH:95:GLU:HA	2.10	0.51
1:BM:2:ILE:HD11	1:BM:124:PHE:HB2	1.92	0.51
1:BM:22:ILE:HA	1:BM:41:GLU:OE1	2.10	0.51
1:BM:45:TYR:HA	1:BM:48:ARG:HE	1.75	0.51
1:BR:49:ARG:HG2	1:BR:76:ILE:HG12	1.91	0.51
1:BS:45:TYR:HB2	1:BS:48:ARG:HH21	1.75	0.51
1:BY:2:ILE:HD11	1:BY:124:PHE:HB2	1.92	0.51
1:DL:45:TYR:HB2	1:DL:48:ARG:HH21	1.75	0.51
1:AI:45:TYR:HB2	1:AI:48:ARG:HH21	1.75	0.51
1:AM:60:VAL:HG11	1:CP:87:PHE:HE2	1.74	0.51
1:AO:22:ILE:HA	1:AO:41:GLU:OE1	2.10	0.51
1:BF:65:TYR:HE2	1:BS:46:ARG:CB	2.23	0.51
1:CN:22:ILE:HA	1:CN:41:GLU:OE1	2.10	0.51
1:CN:45:TYR:HA	1:CN:48:ARG:HE	1.75	0.51
1:CP:49:ARG:HG2	1:CP:76:ILE:HG12	1.92	0.51
1:AA:7:ILE:HD12	1:AA:111:ILE:HG13	1.93	0.51
1:AC:22:ILE:HD12	1:AC:49:ARG:HH21	1.74	0.51
1:AF:2:ILE:HD11	1:AF:124:PHE:HB2	1.92	0.51
1:AO:130:LEU:HD21	1:CE:55:SER:HB3	1.92	0.51
1:AR:2:ILE:HD11	1:AR:124:PHE:HB2	1.92	0.51
1:BK:68:GLY:O	1:BK:95:GLU:HA	2.10	0.51
1:BV:22:ILE:HA	1:BV:41:GLU:OE1	2.10	0.51
1:CC:9:THR:HG22	1:CC:111:ILE:HD12	1.93	0.51
1:CN:2:ILE:HD11	1:CN:124:PHE:HB2	1.92	0.51
1:DF:22:ILE:HA	1:DF:41:GLU:OE1	2.10	0.51
1:DI:45:TYR:HA	1:DI:48:ARG:HE	1.75	0.51
1:AD:9:THR:HG22	1:AD:111:ILE:HD12	1.93	0.51
1:AO:45:TYR:HA	1:AO:48:ARG:HE	1.75	0.51
1:BH:7:ILE:HD12	1:BH:111:ILE:HG13	1.93	0.51
1:BN:7:ILE:HD12	1:BN:111:ILE:HG13	1.93	0.51
1:BQ:68:GLY:O	1:BQ:95:GLU:HA	2.10	0.51
1:BU:46:ARG:NH2	1:DG:99:ALA:HA	2.25	0.51
1:BU:49:ARG:HG2	1:BU:76:ILE:HG12	1.91	0.51
1:CF:9:THR:HG22	1:CF:111:ILE:HD12	1.93	0.51
1:CL:68:GLY:O	1:CL:95:GLU:HA	2.10	0.51
1:CO:68:GLY:O	1:CO:95:GLU:HA	2.10	0.51
1:CR:9:THR:HG22	1:CR:111:ILE:HD12	1.93	0.51
1:CU:9:THR:HG22	1:CU:111:ILE:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CX:7:ILE:HD12	1:CX:111:ILE:HG13	1.93	0.51
1:DC:45:TYR:HB2	1:DC:48:ARG:HH21	1.75	0.51
1:DG:7:ILE:HD12	1:DG:111:ILE:HG13	1.93	0.51
1:DL:2:ILE:HD11	1:DL:124:PHE:HB2	1.92	0.51
1:DL:22:ILE:HA	1:DL:41:GLU:OE1	2.10	0.51
1:DL:45:TYR:HA	1:DL:48:ARG:HE	1.75	0.51
1:AG:68:GLY:O	1:AG:95:GLU:HA	2.10	0.51
1:AH:49:ARG:HG2	1:AH:76:ILE:HG12	1.91	0.51
1:AW:49:ARG:HG2	1:AW:76:ILE:HG12	1.91	0.51
1:AY:7:ILE:HD12	1:AY:111:ILE:HG13	1.93	0.51
1:AY:39:VAL:HG23	1:AY:42:ASP:H	1.74	0.51
1:BC:65:TYR:CE2	1:BP:46:ARG:HA	2.45	0.51
1:BE:9:THR:HG22	1:BE:111:ILE:HD12	1.93	0.51
1:BG:22:ILE:HA	1:BG:41:GLU:OE1	2.10	0.51
1:BJ:22:ILE:HA	1:BJ:41:GLU:OE1	2.10	0.51
1:BV:2:ILE:HD11	1:BV:124:PHE:HB2	1.91	0.51
1:BV:10:GLY:N	1:BV:107:ASP:OD1	2.34	0.51
1:DA:68:GLY:O	1:DA:95:GLU:HA	2.10	0.51
1:DC:22:ILE:HA	1:DC:41:GLU:OE1	2.10	0.51
1:DG:68:GLY:O	1:DG:95:GLU:HA	2.10	0.51
1:DI:22:ILE:HA	1:DI:41:GLU:OE1	2.10	0.51
1:DK:49:ARG:HG2	1:DK:76:ILE:HG12	1.91	0.51
1:AA:68:GLY:O	1:AA:95:GLU:HA	2.10	0.51
1:AR:110:LEU:HD23	1:CK:16:ILE:HD11	1.92	0.51
1:BB:9:THR:HG22	1:BB:111:ILE:HD12	1.93	0.51
1:BE:68:GLY:O	1:BE:95:GLU:HA	2.10	0.51
1:CA:49:ARG:HG2	1:CA:76:ILE:HG12	1.91	0.51
1:CU:7:ILE:HD12	1:CU:111:ILE:HG13	1.93	0.51
1:CW:45:TYR:HA	1:CW:48:ARG:HE	1.75	0.51
1:CZ:2:ILE:HD11	1:CZ:124:PHE:HB2	1.92	0.51
1:AE:48:ARG:HH12	1:BF:127:LEU:HD21	1.76	0.51
1:AM:7:ILE:HD12	1:AM:111:ILE:HG13	1.93	0.51
1:AM:68:GLY:O	1:AM:95:GLU:HA	2.10	0.51
1:AS:7:ILE:HD12	1:AS:111:ILE:HG13	1.93	0.51
1:AV:9:THR:HG22	1:AV:111:ILE:HD12	1.93	0.51
1:AX:22:ILE:HA	1:AX:41:GLU:OE1	2.10	0.51
1:BJ:26:LEU:HB3	1:BK:130:LEU:O	2.11	0.51
1:BK:7:ILE:HD12	1:BK:111:ILE:HG13	1.93	0.51
1:CA:65:TYR:CE2	1:CH:46:ARG:HG2	2.46	0.51
1:CI:68:GLY:O	1:CI:95:GLU:HA	2.10	0.51
1:CM:87:PHE:HE2	1:CX:60:VAL:HG11	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CW:45:TYR:HB2	1:CW:48:ARG:HH21	1.75	0.51
1:AF:22:ILE:HA	1:AF:41:GLU:OE1	2.10	0.50
1:AK:49:ARG:HG2	1:AK:76:ILE:HG12	1.91	0.50
1:BA:22:ILE:O	1:CW:6:SER:HA	2.11	0.50
1:BN:9:THR:HG22	1:BN:111:ILE:HD12	1.93	0.50
1:BT:7:ILE:HD12	1:BT:111:ILE:HG13	1.93	0.50
1:BW:7:ILE:HD12	1:BW:111:ILE:HG13	1.93	0.50
1:BZ:7:ILE:HD12	1:BZ:111:ILE:HG13	1.93	0.50
1:BZ:9:THR:HG22	1:BZ:111:ILE:HD12	1.93	0.50
1:CC:7:ILE:HD12	1:CC:111:ILE:HG13	1.93	0.50
1:CH:22:ILE:HA	1:CH:41:GLU:OE1	2.10	0.50
1:CQ:45:TYR:HB2	1:CQ:48:ARG:HH21	1.75	0.50
1:CT:45:TYR:HA	1:CT:48:ARG:HE	1.75	0.50
1:CZ:45:TYR:HB2	1:CZ:48:ARG:HH21	1.75	0.50
1:DD:7:ILE:HD12	1:DD:111:ILE:HG13	1.93	0.50
1:DG:9:THR:HG22	1:DG:111:ILE:HD12	1.93	0.50
1:AG:7:ILE:HD12	1:AG:111:ILE:HG13	1.93	0.50
1:AK:46:ARG:NH2	1:BW:99:ALA:HA	2.26	0.50
1:AY:9:THR:HG22	1:AY:111:ILE:HD12	1.93	0.50
1:BH:9:THR:HG22	1:BH:111:ILE:HD12	1.93	0.50
1:BP:22:ILE:HD12	1:BP:49:ARG:HH21	1.74	0.50
1:BS:22:ILE:HA	1:BS:41:GLU:OE1	2.10	0.50
1:CO:9:THR:HG22	1:CO:111:ILE:HD12	1.93	0.50
1:DJ:7:ILE:HD12	1:DJ:111:ILE:HG13	1.93	0.50
1:AA:9:THR:HG22	1:AA:111:ILE:HD12	1.93	0.50
1:AC:45:TYR:HB2	1:AC:48:ARG:HH21	1.75	0.50
1:AH:48:ARG:HH12	1:CD:127:LEU:HD21	1.76	0.50
1:AI:128:GLY:O	1:BW:28:GLY:HA3	2.11	0.50
1:AM:22:ILE:HA	1:AM:41:GLU:OE1	2.12	0.50
1:AR:45:TYR:HB2	1:AR:48:ARG:HH21	1.75	0.50
1:AU:22:ILE:HA	1:AU:41:GLU:OE1	2.10	0.50
1:AX:16:ILE:HG21	1:CT:114:GLN:NE2	2.26	0.50
1:BE:7:ILE:HD12	1:BE:111:ILE:HG13	1.93	0.50
1:BQ:7:ILE:HD12	1:BQ:111:ILE:HG13	1.93	0.50
1:BW:9:THR:HG22	1:BW:111:ILE:HD12	1.93	0.50
1:BY:45:TYR:HA	1:BY:48:ARG:HE	1.75	0.50
1:CF:68:GLY:O	1:CF:95:GLU:HA	2.10	0.50
1:CL:7:ILE:HD12	1:CL:111:ILE:HG13	1.93	0.50
1:CX:68:GLY:O	1:CX:95:GLU:HA	2.10	0.50
1:DA:7:ILE:HD12	1:DA:111:ILE:HG13	1.93	0.50
1:DA:9:THR:HG22	1:DA:111:ILE:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:46:ARG:HG3	1:AS:65:TYR:CD2	2.46	0.50
1:AY:22:ILE:HA	1:AY:41:GLU:OE1	2.12	0.50
1:BB:7:ILE:HD12	1:BB:111:ILE:HG13	1.93	0.50
1:BD:2:ILE:HD11	1:BD:124:PHE:HB2	1.92	0.50
1:BG:22:ILE:HD12	1:BG:49:ARG:HH21	1.74	0.50
1:CC:68:GLY:O	1:CC:95:GLU:HA	2.10	0.50
1:CK:22:ILE:HA	1:CK:41:GLU:OE1	2.10	0.50
1:CL:22:ILE:HA	1:CL:41:GLU:OE1	2.12	0.50
1:CR:22:ILE:HA	1:CR:41:GLU:OE1	2.12	0.50
1:AC:125:TRP:O	1:BP:70:ASN:ND2	2.44	0.50
1:BH:22:ILE:HA	1:BH:41:GLU:OE1	2.12	0.50
1:BK:9:THR:HG22	1:BK:111:ILE:HD12	1.93	0.50
1:BP:45:TYR:HB2	1:BP:48:ARG:HH21	1.75	0.50
1:CK:45:TYR:HB2	1:CK:48:ARG:HH21	1.75	0.50
1:CX:22:ILE:HA	1:CX:41:GLU:OE1	2.12	0.50
1:AB:48:ARG:HH12	1:AT:127:LEU:HD21	1.76	0.50
1:AD:7:ILE:HD12	1:AD:111:ILE:HG13	1.93	0.50
1:AE:87:PHE:CZ	1:BE:60:VAL:HG11	2.46	0.50
1:AJ:22:ILE:HA	1:AJ:41:GLU:OE1	2.12	0.50
1:AN:33:ASN:OD1	1:CB:30:THR:OG1	2.30	0.50
1:BJ:40:SER:HB2	1:BK:127:LEU:HD13	1.93	0.50
1:BN:22:ILE:HA	1:BN:41:GLU:OE1	2.12	0.50
1:CL:9:THR:HG22	1:CL:111:ILE:HD12	1.93	0.50
1:CW:22:ILE:HA	1:CW:41:GLU:OE1	2.10	0.50
1:DD:22:ILE:HA	1:DD:41:GLU:OE1	2.12	0.50
1:DI:2:ILE:HD11	1:DI:124:PHE:HB2	1.92	0.50
1:AV:22:ILE:HA	1:AV:41:GLU:OE1	2.12	0.50
1:BE:22:ILE:HA	1:BE:41:GLU:OE1	2.12	0.50
1:BT:9:THR:HG22	1:BT:111:ILE:HD12	1.93	0.50
1:CF:22:ILE:HA	1:CF:41:GLU:OE1	2.12	0.50
1:DC:45:TYR:HA	1:DC:48:ARG:HE	1.75	0.50
1:DI:45:TYR:HB2	1:DI:48:ARG:HH21	1.75	0.50
1:BF:48:ARG:HH12	1:BR:127:LEU:HD21	1.77	0.50
1:BX:98:PRO:HB2	1:CN:46:ARG:HG3	1.94	0.50
1:CC:22:ILE:HA	1:CC:41:GLU:OE1	2.12	0.50
1:CF:7:ILE:HD12	1:CF:111:ILE:HG13	1.93	0.50
1:CU:22:ILE:HA	1:CU:41:GLU:OE1	2.12	0.50
1:AG:9:THR:HG22	1:AG:111:ILE:HD12	1.93	0.50
1:AM:9:THR:HG22	1:AM:111:ILE:HD12	1.93	0.50
1:BH:65:TYR:CE2	1:BL:46:ARG:HG3	2.47	0.50
1:BK:22:ILE:HA	1:BK:41:GLU:OE1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BW:22:ILE:HA	1:BW:41:GLU:OE1	2.12	0.50
1:CI:22:ILE:HA	1:CI:41:GLU:OE1	2.12	0.50
1:DG:22:ILE:HA	1:DG:41:GLU:OE1	2.12	0.50
1:DJ:22:ILE:HA	1:DJ:41:GLU:OE1	2.12	0.50
1:AI:46:ARG:HG2	1:CS:65:TYR:CD2	2.47	0.49
1:AW:65:TYR:HD2	1:BV:46:ARG:HG2	1.74	0.49
1:CI:7:ILE:HD12	1:CI:111:ILE:HG13	1.93	0.49
1:AP:9:THR:HG22	1:AP:111:ILE:HD12	1.93	0.49
1:CR:7:ILE:HD12	1:CR:111:ILE:HG13	1.93	0.49
1:DJ:9:THR:HG22	1:DJ:111:ILE:HD12	1.93	0.49
1:AO:55:SER:HB3	1:CE:130:LEU:HD21	1.94	0.49
1:AP:7:ILE:HD12	1:AP:111:ILE:HG13	1.93	0.49
1:AS:22:ILE:HA	1:AS:41:GLU:OE1	2.12	0.49
1:AV:7:ILE:HD12	1:AV:111:ILE:HG13	1.93	0.49
1:BQ:9:THR:HG22	1:BQ:111:ILE:HD12	1.93	0.49
1:AD:60:VAL:HG11	1:DE:87:PHE:CE2	2.48	0.49
1:AJ:9:THR:HG22	1:AJ:111:ILE:HD12	1.93	0.49
1:AO:108:LEU:HA	1:AO:111:ILE:HG22	1.95	0.49
1:BG:19:GLY:O	1:DC:8:LYS:HD2	2.13	0.49
1:BQ:22:ILE:HA	1:BQ:41:GLU:OE1	2.12	0.49
1:CI:9:THR:HG22	1:CI:111:ILE:HD12	1.93	0.49
1:CO:7:ILE:HD12	1:CO:111:ILE:HG13	1.93	0.49
1:CX:9:THR:HG22	1:CX:111:ILE:HD12	1.93	0.49
1:AD:22:ILE:HA	1:AD:41:GLU:OE1	2.12	0.49
1:AO:17:THR:O	1:CE:12:THR:OG1	2.23	0.49
1:AO:18:GLY:CA	1:CE:11:ALA:HA	2.42	0.49
1:BP:108:LEU:HA	1:BP:111:ILE:HG22	1.95	0.49
1:DA:22:ILE:HA	1:DA:41:GLU:OE1	2.12	0.49
1:AA:22:ILE:HA	1:AA:41:GLU:OE1	2.12	0.49
1:AR:108:LEU:HA	1:AR:111:ILE:HG22	1.95	0.49
1:BG:14:ALA:HB2	1:DC:16:ILE:HD12	1.95	0.49
1:BT:22:ILE:HA	1:BT:41:GLU:OE1	2.12	0.49
1:BY:9:THR:HG22	1:BY:111:ILE:HD12	1.95	0.49
1:BZ:22:ILE:HA	1:BZ:41:GLU:OE1	2.12	0.49
1:CO:22:ILE:HA	1:CO:41:GLU:OE1	2.12	0.49
1:DD:9:THR:HG22	1:DD:111:ILE:HD12	1.93	0.49
1:AB:87:PHE:HE2	1:AS:60:VAL:HG11	1.78	0.49
1:AC:108:LEU:HA	1:AC:111:ILE:HG22	1.95	0.49
1:AG:22:ILE:HA	1:AG:41:GLU:OE1	2.12	0.49
1:AJ:7:ILE:HD12	1:AJ:111:ILE:HG13	1.93	0.49
1:BG:108:LEU:HA	1:BG:111:ILE:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BM:108:LEU:HA	1:BM:111:ILE:HG22	1.95	0.49
1:BS:9:THR:HG22	1:BS:111:ILE:HD12	1.95	0.49
1:BS:108:LEU:HA	1:BS:111:ILE:HG22	1.95	0.49
1:CK:108:LEU:HA	1:CK:111:ILE:HG22	1.95	0.49
1:CQ:108:LEU:HA	1:CQ:111:ILE:HG22	1.95	0.49
1:AW:65:TYR:HE2	1:BV:46:ARG:HA	1.77	0.49
1:CN:108:LEU:HA	1:CN:111:ILE:HG22	1.95	0.49
1:CR:99:ALA:HA	1:DB:46:ARG:NH2	2.28	0.49
1:CZ:108:LEU:HA	1:CZ:111:ILE:HG22	1.95	0.49
1:DF:108:LEU:HA	1:DF:111:ILE:HG22	1.95	0.49
1:BJ:125:TRP:O	1:DF:70:ASN:ND2	2.46	0.49
1:BM:9:THR:HG22	1:BM:111:ILE:HD12	1.95	0.49
1:CI:130:LEU:O	1:DC:26:LEU:HB3	2.13	0.49
1:CK:9:THR:HG22	1:CK:111:ILE:HD12	1.95	0.49
1:AL:108:LEU:HA	1:AL:111:ILE:HG22	1.95	0.49
1:CU:57:VAL:HG21	1:CY:29:GLN:HG3	1.94	0.49
1:AC:22:ILE:O	1:BP:6:SER:HA	2.12	0.48
1:BD:108:LEU:HA	1:BD:111:ILE:HG22	1.95	0.48
1:CA:87:PHE:CZ	1:CF:60:VAL:HG11	2.47	0.48
1:CQ:9:THR:HG22	1:CQ:111:ILE:HD12	1.95	0.48
1:CT:9:THR:HG22	1:CT:111:ILE:HD12	1.95	0.48
1:DC:9:THR:HG22	1:DC:111:ILE:HD12	1.95	0.48
1:AD:130:LEU:O	1:BG:26:LEU:HB3	2.13	0.48
1:AW:87:PHE:CE2	1:BT:60:VAL:HG11	2.48	0.48
1:BB:22:ILE:HA	1:BB:41:GLU:OE1	2.12	0.48
1:BG:22:ILE:O	1:DC:6:SER:HA	2.13	0.48
1:BM:68:GLY:O	1:BM:95:GLU:HA	2.14	0.48
1:BX:79:SER:HA	1:BX:85:THR:HG22	1.96	0.48
1:DL:68:GLY:O	1:DL:95:GLU:HA	2.14	0.48
1:AL:9:THR:HG22	1:AL:111:ILE:HD12	1.95	0.48
1:AO:68:GLY:O	1:AO:95:GLU:HA	2.14	0.48
1:AR:9:THR:HG22	1:AR:111:ILE:HD12	1.95	0.48
1:AS:9:THR:HG22	1:AS:111:ILE:HD12	1.93	0.48
1:AU:9:THR:HG22	1:AU:111:ILE:HD12	1.95	0.48
1:AW:79:SER:HA	1:AW:85:THR:HG22	1.96	0.48
1:BA:108:LEU:HA	1:BA:111:ILE:HG22	1.95	0.48
1:CD:46:ARG:HG3	1:CI:65:TYR:CE2	2.48	0.48
1:CD:79:SER:HA	1:CD:85:THR:HG22	1.96	0.48
1:CH:68:GLY:O	1:CH:95:GLU:HA	2.14	0.48
1:DI:9:THR:HG22	1:DI:111:ILE:HD12	1.95	0.48
1:DI:108:LEU:HA	1:DI:111:ILE:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AE:79:SER:HA	1:AE:85:THR:HG22	1.96	0.48
1:AF:9:THR:HG22	1:AF:111:ILE:HD12	1.95	0.48
1:AO:18:GLY:HA2	1:CE:11:ALA:HA	1.96	0.48
1:AX:9:THR:HG22	1:AX:111:ILE:HD12	1.95	0.48
1:BG:68:GLY:O	1:BG:95:GLU:HA	2.14	0.48
1:BJ:68:GLY:O	1:BJ:95:GLU:HA	2.14	0.48
1:CA:65:TYR:CE2	1:CH:46:ARG:HA	2.48	0.48
1:CG:79:SER:HA	1:CG:85:THR:HG22	1.96	0.48
1:CN:68:GLY:O	1:CN:95:GLU:HA	2.14	0.48
1:CT:68:GLY:O	1:CT:95:GLU:HA	2.14	0.48
1:CZ:68:GLY:O	1:CZ:95:GLU:HA	2.14	0.48
1:DC:68:GLY:O	1:DC:95:GLU:HA	2.14	0.48
1:DH:79:SER:HA	1:DH:85:THR:HG22	1.96	0.48
1:AB:79:SER:HA	1:AB:85:THR:HG22	1.96	0.48
1:AI:111:ILE:HD13	1:BY:74:PHE:CZ	2.48	0.48
1:AK:79:SER:HA	1:AK:85:THR:HG22	1.96	0.48
1:AU:22:ILE:HG22	1:CN:7:ILE:O	2.14	0.48
1:BJ:46:ARG:HG2	1:BL:65:TYR:CE2	2.48	0.48
1:BT:130:LEU:O	1:DI:26:LEU:HB3	2.14	0.48
1:CA:79:SER:HA	1:CA:85:THR:HG22	1.96	0.48
1:DK:79:SER:HA	1:DK:85:THR:HG22	1.96	0.48
1:AA:7:ILE:O	1:AB:22:ILE:HG22	2.14	0.48
1:AI:108:LEU:HA	1:AI:111:ILE:HG22	1.95	0.48
1:AT:79:SER:HA	1:AT:85:THR:HG22	1.96	0.48
1:BA:9:THR:HG22	1:BA:111:ILE:HD12	1.95	0.48
1:BB:7:ILE:O	1:BC:22:ILE:HG22	2.14	0.48
1:BE:7:ILE:O	1:BF:22:ILE:HG22	2.14	0.48
1:BK:7:ILE:O	1:BL:22:ILE:HG22	2.14	0.48
1:BO:79:SER:HA	1:BO:85:THR:HG22	1.96	0.48
1:BP:68:GLY:O	1:BP:95:GLU:HA	2.14	0.48
1:BS:68:GLY:O	1:BS:95:GLU:HA	2.14	0.48
1:BV:68:GLY:O	1:BV:95:GLU:HA	2.14	0.48
1:BY:68:GLY:O	1:BY:95:GLU:HA	2.14	0.48
1:BZ:7:ILE:O	1:CA:22:ILE:HG22	2.14	0.48
1:CE:108:LEU:HA	1:CE:111:ILE:HG22	1.95	0.48
1:DF:9:THR:HG22	1:DF:111:ILE:HD12	1.95	0.48
1:AC:68:GLY:O	1:AC:95:GLU:HA	2.14	0.48
1:AD:7:ILE:O	1:AE:22:ILE:HG22	2.14	0.48
1:AL:68:GLY:O	1:AL:95:GLU:HA	2.14	0.48
1:BD:68:GLY:O	1:BD:95:GLU:HA	2.14	0.48
1:BJ:122:ASP:OD1	1:DF:109:ARG:NH1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BX:87:PHE:CE2	1:CL:60:VAL:HG11	2.49	0.48
1:CE:68:GLY:O	1:CE:95:GLU:HA	2.14	0.48
1:CH:9:THR:HG22	1:CH:111:ILE:HD12	1.95	0.48
1:CH:108:LEU:HA	1:CH:111:ILE:HG22	1.95	0.48
1:CM:87:PHE:CE2	1:CX:60:VAL:HG11	2.48	0.48
1:DD:7:ILE:O	1:DE:22:ILE:HG22	2.14	0.48
1:DF:68:GLY:O	1:DF:95:GLU:HA	2.14	0.48
1:AP:22:ILE:HA	1:AP:41:GLU:OE1	2.12	0.48
1:AT:29:GLN:HG3	1:AV:57:VAL:HG21	1.96	0.48
1:AX:108:LEU:HA	1:AX:111:ILE:HG22	1.95	0.48
1:BC:65:TYR:CE2	1:BP:46:ARG:HG2	2.48	0.48
1:BC:79:SER:HA	1:BC:85:THR:HG22	1.95	0.48
1:BR:79:SER:HA	1:BR:85:THR:HG22	1.96	0.48
1:CK:68:GLY:O	1:CK:95:GLU:HA	2.14	0.48
1:CN:9:THR:HG22	1:CN:111:ILE:HD12	1.95	0.48
1:CU:7:ILE:O	1:CV:22:ILE:HG22	2.14	0.48
1:DJ:7:ILE:O	1:DK:22:ILE:HG22	2.14	0.48
1:DL:9:THR:HG22	1:DL:111:ILE:HD12	1.95	0.48
1:AQ:79:SER:HA	1:AQ:85:THR:HG22	1.96	0.48
1:BD:9:THR:HG22	1:BD:111:ILE:HD12	1.95	0.48
1:CD:58:PRO:HG2	1:CK:45:TYR:CD2	2.49	0.48
1:CE:9:THR:HG22	1:CE:111:ILE:HD12	1.95	0.48
1:CJ:79:SER:HA	1:CJ:85:THR:HG22	1.96	0.48
1:DC:108:LEU:HA	1:DC:111:ILE:HG22	1.95	0.48
1:AI:68:GLY:O	1:AI:95:GLU:HA	2.14	0.48
1:AM:57:VAL:HG21	1:CP:29:GLN:HG3	1.95	0.48
1:AU:68:GLY:O	1:AU:95:GLU:HA	2.14	0.48
1:AX:8:LYS:HD2	1:CT:19:GLY:O	2.13	0.48
1:BV:108:LEU:HA	1:BV:111:ILE:HG22	1.95	0.48
1:CC:7:ILE:O	1:CD:22:ILE:HG22	2.14	0.48
1:CW:9:THR:HG22	1:CW:111:ILE:HD12	1.95	0.48
1:CX:7:ILE:O	1:CY:22:ILE:HG22	2.14	0.48
1:AK:29:GLN:HB3	1:AK:36:ASN:HD22	1.80	0.47
1:AP:7:ILE:O	1:AQ:22:ILE:HG22	2.14	0.47
1:AP:22:ILE:HG22	1:AQ:7:ILE:O	2.14	0.47
1:BA:68:GLY:O	1:BA:95:GLU:HA	2.14	0.47
1:BG:9:THR:HG22	1:BG:111:ILE:HD12	1.95	0.47
1:BK:22:ILE:HG22	1:BL:7:ILE:O	2.14	0.47
1:BR:29:GLN:HB3	1:BR:36:ASN:HD22	1.79	0.47
1:BW:7:ILE:O	1:BX:22:ILE:HG22	2.14	0.47
1:CW:108:LEU:HA	1:CW:111:ILE:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CY:29:GLN:HB3	1:CY:36:ASN:HD22	1.79	0.47
1:DG:7:ILE:O	1:DH:22:ILE:HG22	2.14	0.47
1:DI:68:GLY:O	1:DI:95:GLU:HA	2.14	0.47
1:AE:29:GLN:HB3	1:AE:36:ASN:HD22	1.80	0.47
1:AJ:7:ILE:O	1:AK:22:ILE:HG22	2.14	0.47
1:AN:29:GLN:HB3	1:AN:36:ASN:HD22	1.79	0.47
1:AU:108:LEU:HA	1:AU:111:ILE:HG22	1.95	0.47
1:AV:7:ILE:O	1:AW:22:ILE:HG22	2.14	0.47
1:BH:22:ILE:HG22	1:BI:7:ILE:O	2.14	0.47
1:BL:79:SER:HA	1:BL:85:THR:HG22	1.95	0.47
1:BU:79:SER:HA	1:BU:85:THR:HG22	1.96	0.47
1:CB:9:THR:HG22	1:CB:111:ILE:HD12	1.95	0.47
1:CF:22:ILE:HG22	1:CG:7:ILE:O	2.14	0.47
1:CM:29:GLN:HB3	1:CM:36:ASN:HD22	1.80	0.47
1:CM:79:SER:HA	1:CM:85:THR:HG22	1.96	0.47
1:CP:29:GLN:HB3	1:CP:36:ASN:HD22	1.80	0.47
1:CP:79:SER:HA	1:CP:85:THR:HG22	1.95	0.47
1:CT:108:LEU:HA	1:CT:111:ILE:HG22	1.95	0.47
1:CW:68:GLY:O	1:CW:95:GLU:HA	2.14	0.47
1:AA:22:ILE:HG22	1:AB:7:ILE:O	2.14	0.47
1:AD:22:ILE:HG22	1:AE:7:ILE:O	2.14	0.47
1:AE:46:ARG:NH2	1:BE:99:ALA:HA	2.28	0.47
1:AO:9:THR:HG22	1:AO:111:ILE:HD12	1.95	0.47
1:AS:130:LEU:O	1:AX:26:LEU:HB3	2.15	0.47
1:AT:33:ASN:OD1	1:AX:30:THR:OG1	2.32	0.47
1:BB:22:ILE:HG22	1:BC:7:ILE:O	2.14	0.47
1:BC:29:GLN:HB3	1:BC:36:ASN:HD22	1.80	0.47
1:BF:79:SER:HA	1:BF:85:THR:HG22	1.96	0.47
1:BL:29:GLN:HB3	1:BL:36:ASN:HD22	1.80	0.47
1:BQ:7:ILE:O	1:BR:22:ILE:HG22	2.14	0.47
1:BQ:22:ILE:HG22	1:BR:7:ILE:O	2.14	0.47
1:BY:108:LEU:HA	1:BY:111:ILE:HG22	1.95	0.47
1:CL:22:ILE:HG22	1:CM:7:ILE:O	2.14	0.47
1:CV:29:GLN:HB3	1:CV:36:ASN:HD22	1.80	0.47
1:AC:9:THR:HG22	1:AC:111:ILE:HD12	1.95	0.47
1:AI:92:ILE:HG12	1:BY:92:ILE:HG12	1.94	0.47
1:AT:29:GLN:HB3	1:AT:36:ASN:HD22	1.80	0.47
1:AY:7:ILE:O	1:AZ:22:ILE:HG22	2.14	0.47
1:BH:7:ILE:O	1:BI:22:ILE:HG22	2.14	0.47
1:BN:7:ILE:O	1:BO:22:ILE:HG22	2.14	0.47
1:BP:9:THR:HG22	1:BP:111:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CF:7:ILE:O	1:CG:22:ILE:HG22	2.14	0.47
1:CO:7:ILE:O	1:CP:22:ILE:HG22	2.14	0.47
1:CS:79:SER:HA	1:CS:85:THR:HG22	1.96	0.47
1:DA:22:ILE:HG22	1:DB:7:ILE:O	2.14	0.47
1:DJ:22:ILE:HG22	1:DK:7:ILE:O	2.14	0.47
1:AC:122:ASP:OD1	1:BP:109:ARG:NH1	2.44	0.47
1:AF:68:GLY:O	1:AF:95:GLU:HA	2.14	0.47
1:AF:108:LEU:HA	1:AF:111:ILE:HG22	1.95	0.47
1:AG:127:LEU:HD13	1:CE:40:SER:HB2	1.95	0.47
1:AH:29:GLN:HB3	1:AH:36:ASN:HD22	1.80	0.47
1:AH:79:SER:HA	1:AH:85:THR:HG22	1.95	0.47
1:AI:9:THR:HG22	1:AI:111:ILE:HD12	1.95	0.47
1:AM:7:ILE:O	1:AN:22:ILE:HG22	2.14	0.47
1:AW:87:PHE:HE2	1:BT:60:VAL:HG11	1.79	0.47
1:BC:48:ARG:HH12	1:BO:127:LEU:HD21	1.79	0.47
1:BE:22:ILE:HG22	1:BF:7:ILE:O	2.14	0.47
1:BJ:45:TYR:CE2	1:BL:58:PRO:HD2	2.50	0.47
1:CI:7:ILE:O	1:CJ:22:ILE:HG22	2.14	0.47
1:CP:53:PHE:CD1	1:CP:72:VAL:HG22	2.50	0.47
1:CZ:9:THR:HG22	1:CZ:111:ILE:HD12	1.95	0.47
1:DE:29:GLN:HB3	1:DE:36:ASN:HD22	1.80	0.47
1:AJ:130:LEU:O	1:BY:26:LEU:HB3	2.14	0.47
1:AO:128:GLY:O	1:CC:28:GLY:HA3	2.14	0.47
1:AZ:53:PHE:CD1	1:AZ:72:VAL:HG22	2.50	0.47
1:AZ:79:SER:HA	1:AZ:85:THR:HG22	1.96	0.47
1:BI:79:SER:HA	1:BI:85:THR:HG22	1.95	0.47
1:BU:29:GLN:HB3	1:BU:36:ASN:HD22	1.79	0.47
1:CB:108:LEU:HA	1:CB:111:ILE:HG22	1.95	0.47
1:CQ:68:GLY:O	1:CQ:95:GLU:HA	2.14	0.47
1:CS:29:GLN:HB3	1:CS:36:ASN:HD22	1.80	0.47
1:CU:22:ILE:HG22	1:CV:7:ILE:O	2.14	0.47
1:AB:53:PHE:CD1	1:AB:72:VAL:HG22	2.50	0.47
1:AE:53:PHE:CD1	1:AE:72:VAL:HG22	2.50	0.47
1:AG:7:ILE:O	1:AH:22:ILE:HG22	2.14	0.47
1:AI:113:ALA:HB1	1:BY:113:ALA:HB1	1.97	0.47
1:AN:48:ARG:HH12	1:CA:127:LEU:HD21	1.80	0.47
1:AQ:53:PHE:CD1	1:AQ:72:VAL:HG22	2.50	0.47
1:AR:22:ILE:HG22	1:CK:7:ILE:O	2.13	0.47
1:AR:68:GLY:O	1:AR:95:GLU:HA	2.14	0.47
1:AS:7:ILE:O	1:AT:22:ILE:HG22	2.14	0.47
1:AW:46:ARG:HG3	1:BT:65:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AX:68:GLY:O	1:AX:95:GLU:HA	2.14	0.47
1:BB:127:LEU:HD13	1:BP:40:SER:HB2	1.97	0.47
1:BJ:108:LEU:HA	1:BJ:111:ILE:HG22	1.95	0.47
1:BO:53:PHE:CD1	1:BO:72:VAL:HG22	2.50	0.47
1:BT:7:ILE:O	1:BU:22:ILE:HG22	2.14	0.47
1:BX:29:GLN:HB3	1:BX:36:ASN:HD22	1.80	0.47
1:CA:29:GLN:HB3	1:CA:36:ASN:HD22	1.79	0.47
1:CB:68:GLY:O	1:CB:95:GLU:HA	2.14	0.47
1:CG:53:PHE:CD1	1:CG:72:VAL:HG22	2.50	0.47
1:CJ:87:PHE:HE2	1:DA:60:VAL:HG11	1.79	0.47
1:CL:7:ILE:O	1:CM:22:ILE:HG22	2.14	0.47
1:CR:7:ILE:O	1:CS:22:ILE:HG22	2.14	0.47
1:CS:53:PHE:CD1	1:CS:72:VAL:HG22	2.50	0.47
1:CV:79:SER:HA	1:CV:85:THR:HG22	1.95	0.47
1:CX:22:ILE:HG22	1:CY:7:ILE:O	2.14	0.47
1:CY:79:SER:HA	1:CY:85:THR:HG22	1.95	0.47
1:DB:29:GLN:HB3	1:DB:36:ASN:HD22	1.79	0.47
1:DE:79:SER:HA	1:DE:85:THR:HG22	1.96	0.47
1:AB:29:GLN:HB3	1:AB:36:ASN:HD22	1.80	0.47
1:AR:16:ILE:HD13	1:CK:114:GLN:NE2	2.17	0.47
1:AS:22:ILE:HG22	1:AT:7:ILE:O	2.14	0.47
1:BC:53:PHE:CD1	1:BC:72:VAL:HG22	2.50	0.47
1:BF:53:PHE:CD1	1:BF:72:VAL:HG22	2.50	0.47
1:BG:128:GLY:O	1:DA:28:GLY:HA3	2.15	0.47
1:BR:53:PHE:CD1	1:BR:72:VAL:HG22	2.50	0.47
1:CC:22:ILE:HG22	1:CD:7:ILE:O	2.14	0.47
1:CR:22:ILE:HG22	1:CS:7:ILE:O	2.14	0.47
1:CY:53:PHE:CD1	1:CY:72:VAL:HG22	2.50	0.47
1:DE:53:PHE:CD1	1:DE:72:VAL:HG22	2.50	0.47
1:DK:29:GLN:HB3	1:DK:36:ASN:HD22	1.80	0.47
1:DL:108:LEU:HA	1:DL:111:ILE:HG22	1.95	0.47
1:AH:53:PHE:CD1	1:AH:72:VAL:HG22	2.50	0.47
1:AI:110:LEU:O	1:AI:114:GLN:HG3	2.15	0.47
1:AJ:22:ILE:HG22	1:AK:7:ILE:O	2.14	0.47
1:BJ:9:THR:HG22	1:BJ:111:ILE:HD12	1.95	0.47
1:BZ:22:ILE:HG22	1:CA:7:ILE:O	2.14	0.47
1:CG:29:GLN:HB3	1:CG:36:ASN:HD22	1.80	0.47
1:DA:7:ILE:O	1:DB:22:ILE:HG22	2.14	0.47
1:DB:53:PHE:CD1	1:DB:72:VAL:HG22	2.50	0.47
1:DB:79:SER:HA	1:DB:85:THR:HG22	1.95	0.47
1:DK:53:PHE:CD1	1:DK:72:VAL:HG22	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AM:22:ILE:HG22	1:AN:7:ILE:O	2.14	0.47
1:AN:53:PHE:CD1	1:AN:72:VAL:HG22	2.50	0.47
1:BP:110:LEU:O	1:BP:114:GLN:HG3	2.15	0.47
1:BV:9:THR:HG22	1:BV:111:ILE:HD12	1.95	0.47
1:BX:73:VAL:HG22	1:BX:91:ARG:HE	1.80	0.47
1:CJ:53:PHE:CD1	1:CJ:72:VAL:HG22	2.50	0.47
1:CJ:87:PHE:CE2	1:DA:60:VAL:HG11	2.50	0.47
1:AC:110:LEU:O	1:AC:114:GLN:HG3	2.15	0.46
1:AE:73:VAL:HG22	1:AE:91:ARG:HE	1.81	0.46
1:AK:53:PHE:CD1	1:AK:72:VAL:HG22	2.50	0.46
1:AL:110:LEU:O	1:AL:114:GLN:HG3	2.16	0.46
1:AO:110:LEU:O	1:AO:114:GLN:HG3	2.15	0.46
1:AT:53:PHE:CD1	1:AT:72:VAL:HG22	2.50	0.46
1:AY:22:ILE:HG22	1:AZ:7:ILE:O	2.14	0.46
1:BA:110:LEU:O	1:BA:114:GLN:HG3	2.15	0.46
1:BF:29:GLN:HB3	1:BF:36:ASN:HD22	1.79	0.46
1:BF:73:VAL:HG22	1:BF:91:ARG:HE	1.81	0.46
1:BR:73:VAL:HG22	1:BR:91:ARG:HE	1.80	0.46
1:BU:48:ARG:HH12	1:DH:127:LEU:HD21	1.80	0.46
1:BW:22:ILE:HG22	1:BX:7:ILE:O	2.14	0.46
1:CA:73:VAL:HG22	1:CA:91:ARG:HE	1.81	0.46
1:CD:29:GLN:HB3	1:CD:36:ASN:HD22	1.80	0.46
1:CT:110:LEU:O	1:CT:114:GLN:HG3	2.15	0.46
1:CV:53:PHE:CD1	1:CV:72:VAL:HG22	2.50	0.46
1:DL:110:LEU:O	1:DL:114:GLN:HG3	2.15	0.46
1:AG:22:ILE:HG22	1:AH:7:ILE:O	2.14	0.46
1:AG:28:GLY:HA3	1:BY:128:GLY:O	2.16	0.46
1:AN:79:SER:HA	1:AN:85:THR:HG22	1.96	0.46
1:AU:7:ILE:HB	1:AU:114:GLN:OE1	2.16	0.46
1:BL:53:PHE:CD1	1:BL:72:VAL:HG22	2.50	0.46
1:BT:22:ILE:HG22	1:BU:7:ILE:O	2.14	0.46
1:BU:53:PHE:CD1	1:BU:72:VAL:HG22	2.50	0.46
1:BV:110:LEU:O	1:BV:114:GLN:HG3	2.15	0.46
1:BX:53:PHE:CD1	1:BX:72:VAL:HG22	2.50	0.46
1:CH:110:LEU:O	1:CH:114:GLN:HG3	2.16	0.46
1:CI:22:ILE:HG22	1:CJ:7:ILE:O	2.14	0.46
1:CP:73:VAL:HG22	1:CP:91:ARG:HE	1.80	0.46
1:CQ:110:LEU:O	1:CQ:114:GLN:HG3	2.15	0.46
1:CS:73:VAL:HG22	1:CS:91:ARG:HE	1.80	0.46
1:DD:22:ILE:HG22	1:DE:7:ILE:O	2.14	0.46
1:AK:65:TYR:HE2	1:BY:46:ARG:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AK:73:VAL:HG22	1:AK:91:ARG:HE	1.81	0.46
1:AR:7:ILE:O	1:CK:22:ILE:HG22	2.15	0.46
1:AW:65:TYR:CE2	1:BV:46:ARG:HG2	2.50	0.46
1:AZ:29:GLN:HB3	1:AZ:36:ASN:HD22	1.79	0.46
1:BD:110:LEU:O	1:BD:114:GLN:HG3	2.15	0.46
1:BI:73:VAL:HG22	1:BI:91:ARG:HE	1.81	0.46
1:BN:22:ILE:HG22	1:BO:7:ILE:O	2.14	0.46
1:CB:110:LEU:O	1:CB:114:GLN:HG3	2.16	0.46
1:CD:53:PHE:CD1	1:CD:72:VAL:HG22	2.50	0.46
1:CD:73:VAL:HG22	1:CD:91:ARG:HE	1.81	0.46
1:CJ:33:ASN:OD1	1:DC:30:THR:OG1	2.33	0.46
1:CT:7:ILE:HB	1:CT:114:GLN:OE1	2.16	0.46
1:DH:53:PHE:CD1	1:DH:72:VAL:HG22	2.50	0.46
1:DK:73:VAL:HG22	1:DK:91:ARG:HE	1.81	0.46
1:AE:127:LEU:CD2	1:DE:48:ARG:HH12	2.27	0.46
1:AV:22:ILE:HG22	1:AW:7:ILE:O	2.14	0.46
1:AX:7:ILE:HB	1:AX:114:GLN:OE1	2.16	0.46
1:BA:7:ILE:HB	1:BA:114:GLN:OE1	2.16	0.46
1:BU:73:VAL:HG22	1:BU:91:ARG:HE	1.80	0.46
1:CA:53:PHE:CD1	1:CA:72:VAL:HG22	2.50	0.46
1:CM:53:PHE:CD1	1:CM:72:VAL:HG22	2.50	0.46
1:CW:7:ILE:HB	1:CW:114:GLN:OE1	2.16	0.46
1:DF:110:LEU:O	1:DF:114:GLN:HG3	2.16	0.46
1:DH:29:GLN:HB3	1:DH:36:ASN:HD22	1.80	0.46
1:DL:7:ILE:HB	1:DL:114:GLN:OE1	2.16	0.46
1:AK:29:GLN:HG3	1:BW:57:VAL:HG21	1.98	0.46
1:AK:65:TYR:HD2	1:BY:46:ARG:HG2	1.79	0.46
1:BI:53:PHE:CD1	1:BI:72:VAL:HG22	2.50	0.46
1:BM:18:GLY:HA2	1:DI:11:ALA:HA	1.97	0.46
1:BO:29:GLN:HB3	1:BO:36:ASN:HD22	1.79	0.46
1:CQ:7:ILE:HB	1:CQ:114:GLN:OE1	2.16	0.46
1:DC:7:ILE:HB	1:DC:114:GLN:OE1	2.16	0.46
1:DE:73:VAL:HG22	1:DE:91:ARG:HE	1.81	0.46
1:DG:22:ILE:HG22	1:DH:7:ILE:O	2.14	0.46
1:AR:110:LEU:O	1:AR:114:GLN:HG3	2.15	0.46
1:AT:73:VAL:HG22	1:AT:91:ARG:HE	1.80	0.46
1:AU:110:LEU:O	1:AU:114:GLN:HG3	2.15	0.46
1:AU:125:TRP:O	1:CN:70:ASN:ND2	2.49	0.46
1:AW:53:PHE:CD1	1:AW:72:VAL:HG22	2.50	0.46
1:AX:110:LEU:O	1:AX:114:GLN:HG3	2.15	0.46
1:BJ:7:ILE:HB	1:BJ:114:GLN:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BM:7:ILE:HB	1:BM:114:GLN:OE1	2.16	0.46
1:CB:7:ILE:HB	1:CB:114:GLN:OE1	2.16	0.46
1:CM:73:VAL:HG22	1:CM:91:ARG:HE	1.80	0.46
1:CY:73:VAL:HG22	1:CY:91:ARG:HE	1.80	0.46
1:DC:110:LEU:O	1:DC:114:GLN:HG3	2.15	0.46
1:DF:7:ILE:HB	1:DF:114:GLN:OE1	2.16	0.46
1:AW:29:GLN:HB3	1:AW:36:ASN:HD22	1.79	0.46
1:BG:7:ILE:HB	1:BG:114:GLN:OE1	2.16	0.46
1:BJ:16:ILE:HG21	1:DF:114:GLN:NE2	2.31	0.46
1:BJ:46:ARG:CA	1:BL:65:TYR:HE2	2.27	0.46
1:BM:110:LEU:O	1:BM:114:GLN:HG3	2.15	0.46
1:BS:7:ILE:HB	1:BS:114:GLN:OE1	2.16	0.46
1:CK:7:ILE:HB	1:CK:114:GLN:OE1	2.16	0.46
1:CN:110:LEU:O	1:CN:114:GLN:HG3	2.16	0.46
1:CO:22:ILE:HG22	1:CP:7:ILE:O	2.14	0.46
1:CV:73:VAL:HG22	1:CV:91:ARG:HE	1.81	0.46
1:DH:73:VAL:HG22	1:DH:91:ARG:HE	1.81	0.46
1:AO:46:ARG:HA	1:CP:65:TYR:HE2	1.80	0.46
1:AZ:73:VAL:HG22	1:AZ:91:ARG:HE	1.81	0.46
1:BI:29:GLN:HB3	1:BI:36:ASN:HD22	1.79	0.46
1:BY:110:LEU:O	1:BY:114:GLN:HG3	2.15	0.46
1:CJ:73:VAL:HG22	1:CJ:91:ARG:HE	1.81	0.46
1:CZ:7:ILE:HB	1:CZ:114:GLN:OE1	2.16	0.46
1:AL:30:THR:OG1	1:CV:33:ASN:OD1	2.32	0.46
1:BG:110:LEU:O	1:BG:114:GLN:HG3	2.15	0.46
1:BJ:11:ALA:HB3	1:BJ:110:LEU:HD23	1.98	0.46
1:CE:110:LEU:O	1:CE:114:GLN:HG3	2.15	0.46
1:CH:7:ILE:HB	1:CH:114:GLN:OE1	2.16	0.46
1:DI:7:ILE:HB	1:DI:114:GLN:OE1	2.16	0.46
1:AF:67:LYS:NZ	1:BV:87:PHE:O	2.27	0.46
1:AG:65:TYR:CE2	1:CS:46:ARG:HG3	2.50	0.46
1:AX:89:SER:HB2	1:CT:95:GLU:HB2	1.97	0.46
1:BA:11:ALA:HB3	1:BA:110:LEU:HD23	1.98	0.46
1:BC:73:VAL:HG22	1:BC:91:ARG:HE	1.81	0.46
1:CB:11:ALA:HB3	1:CB:110:LEU:HD23	1.98	0.46
1:CE:7:ILE:HB	1:CE:114:GLN:OE1	2.16	0.46
1:CT:11:ALA:HB3	1:CT:110:LEU:HD23	1.98	0.46
1:AE:48:ARG:HH22	1:BF:127:LEU:HD23	1.81	0.45
1:AI:14:ALA:HA	1:BY:16:ILE:HA	1.96	0.45
1:AO:114:GLN:NE2	1:CE:16:ILE:HD13	2.20	0.45
1:AQ:29:GLN:HB3	1:AQ:36:ASN:HD22	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AW:73:VAL:HG22	1:AW:91:ARG:HE	1.81	0.45
1:BA:6:SER:HA	1:CW:22:ILE:O	2.16	0.45
1:BF:65:TYR:CE2	1:BS:46:ARG:CG	2.97	0.45
1:BP:7:ILE:HB	1:BP:114:GLN:OE1	2.16	0.45
1:BS:11:ALA:HB3	1:BS:110:LEU:HD23	1.98	0.45
1:BS:110:LEU:O	1:BS:114:GLN:HG3	2.15	0.45
1:CG:73:VAL:HG22	1:CG:91:ARG:HE	1.80	0.45
1:CN:11:ALA:HB3	1:CN:110:LEU:HD23	1.98	0.45
1:AC:7:ILE:HB	1:AC:114:GLN:OE1	2.16	0.45
1:AH:73:VAL:HG22	1:AH:91:ARG:HE	1.80	0.45
1:AL:46:ARG:HG2	1:CV:65:TYR:CD2	2.51	0.45
1:AO:7:ILE:HB	1:AO:114:GLN:OE1	2.16	0.45
1:BD:7:ILE:HB	1:BD:114:GLN:OE1	2.16	0.45
1:BI:42:ASP:O	1:BI:48:ARG:HD3	2.17	0.45
1:BJ:114:GLN:NE2	1:DF:16:ILE:HD13	2.22	0.45
1:BP:11:ALA:HB3	1:BP:110:LEU:HD23	1.98	0.45
1:CJ:42:ASP:O	1:CJ:48:ARG:HD3	2.17	0.45
1:DF:11:ALA:HB3	1:DF:110:LEU:HD23	1.98	0.45
1:AL:7:ILE:HB	1:AL:114:GLN:OE1	2.16	0.45
1:AN:73:VAL:HG22	1:AN:91:ARG:HE	1.80	0.45
1:AX:19:GLY:O	1:CT:8:LYS:HD2	2.16	0.45
1:AX:87:PHE:O	1:CT:67:LYS:NZ	2.29	0.45
1:BG:111:ILE:HD13	1:DC:74:PHE:CE2	2.51	0.45
1:BM:18:GLY:CA	1:DI:11:ALA:HA	2.47	0.45
1:BY:7:ILE:HB	1:BY:114:GLN:OE1	2.16	0.45
1:CJ:29:GLN:HB3	1:CJ:36:ASN:HD22	1.79	0.45
1:CM:42:ASP:O	1:CM:48:ARG:HD3	2.17	0.45
1:CV:42:ASP:O	1:CV:48:ARG:HD3	2.17	0.45
1:CY:42:ASP:O	1:CY:48:ARG:HD3	2.17	0.45
1:DI:110:LEU:O	1:DI:114:GLN:HG3	2.16	0.45
1:AE:42:ASP:O	1:AE:48:ARG:HD3	2.17	0.45
1:AI:11:ALA:HB3	1:AI:110:LEU:HD23	1.98	0.45
1:BC:42:ASP:O	1:BC:48:ARG:HD3	2.17	0.45
1:BG:11:ALA:HB3	1:BG:110:LEU:HD23	1.98	0.45
1:BI:60:VAL:HG22	1:BI:65:TYR:CE1	2.52	0.45
1:BR:42:ASP:O	1:BR:48:ARG:HD3	2.17	0.45
1:BX:60:VAL:HG22	1:BX:65:TYR:CE1	2.52	0.45
1:CA:42:ASP:O	1:CA:48:ARG:HD3	2.17	0.45
1:CM:60:VAL:HG22	1:CM:65:TYR:CE1	2.52	0.45
1:CN:7:ILE:HB	1:CN:114:GLN:OE1	2.16	0.45
1:CS:42:ASP:O	1:CS:48:ARG:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CZ:110:LEU:O	1:CZ:114:GLN:HG3	2.15	0.45
1:AF:110:LEU:O	1:AF:114:GLN:HG3	2.15	0.45
1:AH:60:VAL:HG22	1:AH:65:TYR:CE1	2.52	0.45
1:AH:65:TYR:HE2	1:CE:46:ARG:HA	1.82	0.45
1:AI:7:ILE:HB	1:AI:114:GLN:OE1	2.16	0.45
1:AR:7:ILE:HB	1:AR:114:GLN:OE1	2.16	0.45
1:AX:11:ALA:HB3	1:AX:110:LEU:HD23	1.98	0.45
1:AZ:60:VAL:HG22	1:AZ:65:TYR:CE1	2.52	0.45
1:BL:73:VAL:HG22	1:BL:91:ARG:HE	1.81	0.45
1:BO:73:VAL:HG22	1:BO:91:ARG:HE	1.80	0.45
1:CD:42:ASP:O	1:CD:48:ARG:HD3	2.17	0.45
1:CS:60:VAL:HG22	1:CS:65:TYR:CE1	2.52	0.45
1:CW:110:LEU:O	1:CW:114:GLN:HG3	2.15	0.45
1:DB:42:ASP:O	1:DB:48:ARG:HD3	2.17	0.45
1:DH:60:VAL:HG22	1:DH:65:TYR:CE1	2.52	0.45
1:AB:42:ASP:O	1:AB:48:ARG:HD3	2.17	0.45
1:AC:11:ALA:HB3	1:AC:110:LEU:HD23	1.98	0.45
1:AF:7:ILE:HB	1:AF:114:GLN:OE1	2.16	0.45
1:AF:89:SER:HB2	1:BV:95:GLU:HB2	1.98	0.45
1:AN:42:ASP:O	1:AN:48:ARG:HD3	2.17	0.45
1:BL:42:ASP:O	1:BL:48:ARG:HD3	2.17	0.45
1:BV:7:ILE:HB	1:BV:114:GLN:OE1	2.16	0.45
1:CD:60:VAL:HG22	1:CD:65:TYR:CE1	2.52	0.45
1:CK:110:LEU:O	1:CK:114:GLN:HG3	2.16	0.45
1:DK:42:ASP:O	1:DK:48:ARG:HD3	2.17	0.45
1:AK:42:ASP:O	1:AK:48:ARG:HD3	2.17	0.45
1:AL:19:GLY:O	1:CB:8:LYS:HD2	2.15	0.45
1:AO:12:THR:OG1	1:CE:17:THR:O	2.20	0.45
1:AQ:73:VAL:HG22	1:AQ:91:ARG:HE	1.80	0.45
1:AW:60:VAL:HG22	1:AW:65:TYR:CE1	2.52	0.45
1:BU:26:LEU:O	1:DH:129:ALA:HB2	2.17	0.45
1:CG:42:ASP:O	1:CG:48:ARG:HD3	2.17	0.45
1:CG:60:VAL:HG22	1:CG:65:TYR:CE1	2.52	0.45
1:CH:11:ALA:HB3	1:CH:110:LEU:HD23	1.98	0.45
1:CY:60:VAL:HG22	1:CY:65:TYR:CE1	2.52	0.45
1:DC:11:ALA:HB3	1:DC:110:LEU:HD23	1.98	0.45
1:AO:92:ILE:HG12	1:CE:92:ILE:HG12	1.98	0.45
1:AQ:42:ASP:O	1:AQ:48:ARG:HD3	2.17	0.45
1:AZ:42:ASP:O	1:AZ:48:ARG:HD3	2.17	0.45
1:BJ:110:LEU:O	1:BJ:114:GLN:HG3	2.15	0.45
1:BL:60:VAL:HG22	1:BL:65:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CV:60:VAL:HG22	1:CV:65:TYR:CE1	2.52	0.45
1:CW:46:ARG:HA	1:CY:65:TYR:CE2	2.50	0.45
1:DB:60:VAL:HG22	1:DB:65:TYR:CE1	2.52	0.45
1:DK:60:VAL:HG22	1:DK:65:TYR:CE1	2.52	0.45
1:AB:60:VAL:HG22	1:AB:65:TYR:CE1	2.52	0.45
1:AI:39:VAL:HG12	1:AI:42:ASP:H	1.82	0.45
1:AK:60:VAL:HG22	1:AK:65:TYR:CE1	2.52	0.45
1:AT:42:ASP:O	1:AT:48:ARG:HD3	2.17	0.45
1:BB:130:LEU:O	1:BP:26:LEU:HB3	2.16	0.45
1:BF:60:VAL:HG22	1:BF:65:TYR:CE1	2.52	0.45
1:BO:60:VAL:HG22	1:BO:65:TYR:CE1	2.52	0.45
1:CQ:39:VAL:HG12	1:CQ:42:ASP:H	1.82	0.45
1:DC:39:VAL:HG12	1:DC:42:ASP:H	1.82	0.45
1:AB:48:ARG:HH12	1:AT:127:LEU:CD2	2.29	0.45
1:AL:11:ALA:HB3	1:AL:110:LEU:HD23	1.98	0.45
1:AP:26:LEU:HD12	1:AP:36:ASN:O	2.17	0.45
1:BD:11:ALA:HB3	1:BD:110:LEU:HD23	1.98	0.45
1:BM:13:SER:O	1:DI:16:ILE:HG13	2.16	0.45
1:BX:42:ASP:O	1:BX:48:ARG:HD3	2.17	0.45
1:BY:11:ALA:HB3	1:BY:110:LEU:HD23	1.98	0.45
1:CZ:39:VAL:HG12	1:CZ:42:ASP:H	1.82	0.45
1:DB:73:VAL:HG22	1:DB:91:ARG:HE	1.81	0.45
1:DH:42:ASP:O	1:DH:48:ARG:HD3	2.17	0.45
1:DL:39:VAL:HG12	1:DL:42:ASP:H	1.82	0.45
1:AF:11:ALA:HB3	1:AF:110:LEU:HD23	1.98	0.44
1:AJ:26:LEU:HD12	1:AJ:36:ASN:O	2.17	0.44
1:AN:60:VAL:HG22	1:AN:65:TYR:CE1	2.52	0.44
1:AT:60:VAL:HG22	1:AT:65:TYR:CE1	2.52	0.44
1:BC:60:VAL:HG22	1:BC:65:TYR:CE1	2.52	0.44
1:BQ:108:LEU:HA	1:BQ:111:ILE:HG22	2.00	0.44
1:CA:60:VAL:HG22	1:CA:65:TYR:CE1	2.52	0.44
1:CO:26:LEU:HD12	1:CO:36:ASN:O	2.18	0.44
1:AC:39:VAL:HG12	1:AC:42:ASP:H	1.82	0.44
1:AG:26:LEU:HD12	1:AG:36:ASN:O	2.17	0.44
1:AH:42:ASP:O	1:AH:48:ARG:HD3	2.17	0.44
1:AR:11:ALA:HB3	1:AR:110:LEU:HD23	1.98	0.44
1:AU:11:ALA:HB3	1:AU:110:LEU:HD23	1.99	0.44
1:BM:16:ILE:HA	1:DI:14:ALA:HA	1.99	0.44
1:BM:116:LEU:O	1:DI:109:ARG:CZ	2.65	0.44
1:BO:42:ASP:O	1:BO:48:ARG:HD3	2.17	0.44
1:BS:39:VAL:HG12	1:BS:42:ASP:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BU:42:ASP:O	1:BU:48:ARG:HD3	2.17	0.44
1:BY:39:VAL:HG12	1:BY:42:ASP:H	1.82	0.44
1:BZ:108:LEU:HA	1:BZ:111:ILE:HG22	2.00	0.44
1:CD:58:PRO:HD2	1:CK:45:TYR:CZ	2.52	0.44
1:CH:39:VAL:HG12	1:CH:42:ASP:H	1.82	0.44
1:CJ:60:VAL:HG22	1:CJ:65:TYR:CE1	2.52	0.44
1:CX:26:LEU:HD12	1:CX:36:ASN:O	2.18	0.44
1:DA:108:LEU:HA	1:DA:111:ILE:HG22	1.99	0.44
1:DE:42:ASP:O	1:DE:48:ARG:HD3	2.17	0.44
1:DI:11:ALA:HB3	1:DI:110:LEU:HD23	1.98	0.44
1:DJ:108:LEU:HA	1:DJ:111:ILE:HG22	2.00	0.44
1:AA:108:LEU:HA	1:AA:111:ILE:HG22	2.00	0.44
1:AB:73:VAL:HG22	1:AB:91:ARG:HE	1.80	0.44
1:AO:39:VAL:HG12	1:AO:42:ASP:H	1.82	0.44
1:AQ:60:VAL:HG22	1:AQ:65:TYR:CE1	2.52	0.44
1:AR:39:VAL:HG12	1:AR:42:ASP:H	1.82	0.44
1:AS:26:LEU:HD12	1:AS:36:ASN:O	2.17	0.44
1:AS:108:LEU:HA	1:AS:111:ILE:HG22	2.00	0.44
1:BF:42:ASP:O	1:BF:48:ARG:HD3	2.17	0.44
1:BR:60:VAL:HG22	1:BR:65:TYR:CE1	2.52	0.44
1:CE:11:ALA:HB3	1:CE:110:LEU:HD23	1.98	0.44
1:CJ:68:GLY:O	1:CJ:95:GLU:HA	2.18	0.44
1:CO:108:LEU:HA	1:CO:111:ILE:HG22	1.99	0.44
1:AB:87:PHE:CZ	1:AS:60:VAL:HG11	2.51	0.44
1:AE:68:GLY:O	1:AE:95:GLU:HA	2.18	0.44
1:AG:108:LEU:HA	1:AG:111:ILE:HG22	1.99	0.44
1:AL:114:GLN:NE2	1:CB:16:ILE:HG21	2.33	0.44
1:AO:11:ALA:HB3	1:AO:110:LEU:HD23	1.98	0.44
1:AR:125:TRP:O	1:CK:70:ASN:ND2	2.51	0.44
1:AV:108:LEU:HA	1:AV:111:ILE:HG22	2.00	0.44
1:AY:26:LEU:HD12	1:AY:36:ASN:O	2.18	0.44
1:BD:39:VAL:HG12	1:BD:42:ASP:H	1.82	0.44
1:BF:68:GLY:O	1:BF:95:GLU:HA	2.18	0.44
1:BN:108:LEU:HA	1:BN:111:ILE:HG22	2.00	0.44
1:BO:65:TYR:CD2	1:DL:46:ARG:HG2	2.52	0.44
1:BZ:26:LEU:HD12	1:BZ:36:ASN:O	2.18	0.44
1:CK:11:ALA:HB3	1:CK:110:LEU:HD23	1.98	0.44
1:CL:35:LEU:HD22	1:CM:131:ALA:H	1.83	0.44
1:CL:108:LEU:HA	1:CL:111:ILE:HG22	2.00	0.44
1:CP:42:ASP:O	1:CP:48:ARG:HD3	2.17	0.44
1:CW:11:ALA:HB3	1:CW:110:LEU:HD23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DD:26:LEU:HD12	1:DD:36:ASN:O	2.18	0.44
1:DJ:35:LEU:HD22	1:DK:131:ALA:H	1.83	0.44
1:AC:14:ALA:HB2	1:BP:16:ILE:HD12	1.98	0.44
1:AF:48:ARG:NH1	1:DD:127:LEU:HD22	2.32	0.44
1:AP:108:LEU:HA	1:AP:111:ILE:HG22	1.99	0.44
1:AV:26:LEU:HD12	1:AV:36:ASN:O	2.18	0.44
1:AW:42:ASP:O	1:AW:48:ARG:HD3	2.17	0.44
1:AX:39:VAL:HG12	1:AX:42:ASP:H	1.82	0.44
1:BD:74:PHE:CZ	1:CZ:111:ILE:HD13	2.52	0.44
1:BK:87:PHE:O	1:BL:67:LYS:NZ	2.41	0.44
1:BL:58:PRO:HB3	1:BL:66:SER:O	2.18	0.44
1:BP:39:VAL:HG12	1:BP:42:ASP:H	1.82	0.44
1:BU:60:VAL:HG22	1:BU:65:TYR:CE1	2.52	0.44
1:BZ:35:LEU:HD22	1:CA:131:ALA:H	1.83	0.44
1:CC:26:LEU:HD12	1:CC:36:ASN:O	2.17	0.44
1:CF:35:LEU:HD22	1:CG:131:ALA:H	1.83	0.44
1:CF:108:LEU:HA	1:CF:111:ILE:HG22	2.00	0.44
1:CG:68:GLY:O	1:CG:95:GLU:HA	2.18	0.44
1:CI:108:LEU:HA	1:CI:111:ILE:HG22	1.99	0.44
1:DI:39:VAL:HG12	1:DI:42:ASP:H	1.82	0.44
1:AD:26:LEU:HD12	1:AD:36:ASN:O	2.17	0.44
1:AG:35:LEU:HD22	1:AH:131:ALA:H	1.83	0.44
1:AM:26:LEU:HD12	1:AM:36:ASN:O	2.17	0.44
1:AS:35:LEU:HD22	1:AT:131:ALA:H	1.83	0.44
1:AT:67:LYS:HD3	1:AT:95:GLU:HB3	2.00	0.44
1:AU:39:VAL:HG12	1:AU:42:ASP:H	1.82	0.44
1:AZ:67:LYS:HD3	1:AZ:95:GLU:HB3	2.00	0.44
1:BK:26:LEU:HD12	1:BK:36:ASN:O	2.17	0.44
1:BL:68:GLY:O	1:BL:95:GLU:HA	2.18	0.44
1:BT:35:LEU:HD22	1:BU:131:ALA:H	1.83	0.44
1:BU:68:GLY:O	1:BU:95:GLU:HA	2.18	0.44
1:BV:11:ALA:HB3	1:BV:110:LEU:HD23	1.98	0.44
1:CF:26:LEU:HD12	1:CF:36:ASN:O	2.17	0.44
1:CN:39:VAL:HG12	1:CN:42:ASP:H	1.82	0.44
1:CW:39:VAL:HG12	1:CW:42:ASP:H	1.82	0.44
1:CZ:11:ALA:HB3	1:CZ:110:LEU:HD23	1.98	0.44
1:DA:26:LEU:HD12	1:DA:36:ASN:O	2.18	0.44
1:DD:35:LEU:HD22	1:DE:131:ALA:H	1.83	0.44
1:DE:60:VAL:HG22	1:DE:65:TYR:CE1	2.52	0.44
1:DE:68:GLY:O	1:DE:95:GLU:HA	2.18	0.44
1:AA:35:LEU:HD22	1:AB:131:ALA:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AK:68:GLY:O	1:AK:95:GLU:HA	2.18	0.44
1:AL:39:VAL:HG12	1:AL:42:ASP:H	1.82	0.44
1:AT:68:GLY:O	1:AT:95:GLU:HA	2.18	0.44
1:BC:98:PRO:HB2	1:BP:46:ARG:HG3	2.00	0.44
1:BG:111:ILE:CD1	1:DC:74:PHE:CZ	2.99	0.44
1:BJ:22:ILE:HG22	1:DF:7:ILE:O	2.17	0.44
1:BO:58:PRO:HB3	1:BO:66:SER:O	2.18	0.44
1:BQ:26:LEU:HD12	1:BQ:36:ASN:O	2.17	0.44
1:BX:58:PRO:HB2	1:CN:45:TYR:CE2	2.53	0.44
1:CA:58:PRO:HB3	1:CA:66:SER:O	2.18	0.44
1:CB:39:VAL:HG12	1:CB:42:ASP:H	1.82	0.44
1:CD:58:PRO:HB3	1:CD:66:SER:O	2.18	0.44
1:CL:26:LEU:HD12	1:CL:36:ASN:O	2.17	0.44
1:CR:35:LEU:HD22	1:CS:131:ALA:H	1.83	0.44
1:CR:108:LEU:HA	1:CR:111:ILE:HG22	2.00	0.44
1:CS:67:LYS:HD3	1:CS:95:GLU:HB3	2.00	0.44
1:CS:68:GLY:O	1:CS:95:GLU:HA	2.18	0.44
1:CT:30:THR:OG1	1:DB:33:ASN:OD1	2.33	0.44
1:CT:39:VAL:HG12	1:CT:42:ASP:H	1.82	0.44
1:AE:60:VAL:HG22	1:AE:65:TYR:CE1	2.52	0.44
1:AN:68:GLY:O	1:AN:95:GLU:HA	2.18	0.44
1:AU:18:GLY:HA2	1:CN:12:THR:H	1.83	0.44
1:AW:67:LYS:HD3	1:AW:95:GLU:HB3	2.00	0.44
1:BE:108:LEU:HA	1:BE:111:ILE:HG22	2.00	0.44
1:BG:22:ILE:HG22	1:DC:7:ILE:O	2.18	0.44
1:BI:68:GLY:O	1:BI:95:GLU:HA	2.18	0.44
1:BM:11:ALA:HB3	1:BM:110:LEU:HD23	1.98	0.44
1:BT:26:LEU:HD12	1:BT:36:ASN:O	2.17	0.44
1:BT:108:LEU:HA	1:BT:111:ILE:HG22	2.00	0.44
1:BX:67:LYS:HD3	1:BX:95:GLU:HB3	2.00	0.44
1:CG:58:PRO:HB3	1:CG:66:SER:O	2.18	0.44
1:CK:39:VAL:HG12	1:CK:42:ASP:H	1.82	0.44
1:CM:58:PRO:HB3	1:CM:66:SER:O	2.18	0.44
1:CP:60:VAL:HG22	1:CP:65:TYR:CE1	2.52	0.44
1:CR:26:LEU:HD12	1:CR:36:ASN:O	2.18	0.44
1:CV:67:LYS:HD3	1:CV:95:GLU:HB3	2.00	0.44
1:CV:68:GLY:O	1:CV:95:GLU:HA	2.18	0.44
1:DH:58:PRO:HB3	1:DH:66:SER:O	2.18	0.44
1:AA:26:LEU:HD12	1:AA:36:ASN:O	2.17	0.44
1:AN:26:LEU:O	1:CA:129:ALA:HB2	2.17	0.44
1:AO:46:ARG:HG2	1:CP:65:TYR:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AW:58:PRO:HB3	1:AW:66:SER:O	2.18	0.44
1:BD:130:LEU:HD21	1:CZ:55:SER:HB3	1.99	0.44
1:BI:58:PRO:HB3	1:BI:66:SER:O	2.18	0.44
1:BJ:39:VAL:HG12	1:BJ:42:ASP:H	1.83	0.44
1:BN:26:LEU:HD12	1:BN:36:ASN:O	2.18	0.44
1:BR:58:PRO:HB3	1:BR:66:SER:O	2.18	0.44
1:BW:26:LEU:HD12	1:BW:36:ASN:O	2.17	0.44
1:CA:67:LYS:HD3	1:CA:95:GLU:HB3	2.00	0.44
1:CC:108:LEU:HA	1:CC:111:ILE:HG22	2.00	0.44
1:CI:26:LEU:HD12	1:CI:36:ASN:O	2.18	0.44
1:CJ:58:PRO:HB3	1:CJ:66:SER:O	2.18	0.44
1:CS:58:PRO:HB3	1:CS:66:SER:O	2.18	0.44
1:DJ:26:LEU:HD12	1:DJ:36:ASN:O	2.18	0.44
1:AH:58:PRO:HB3	1:AH:66:SER:O	2.18	0.43
1:AK:58:PRO:HB3	1:AK:66:SER:O	2.18	0.43
1:AW:68:GLY:O	1:AW:95:GLU:HA	2.18	0.43
1:AZ:68:GLY:O	1:AZ:95:GLU:HA	2.18	0.43
1:BG:39:VAL:HG12	1:BG:42:ASP:H	1.82	0.43
1:BX:58:PRO:HB3	1:BX:66:SER:O	2.18	0.43
1:CO:35:LEU:HD22	1:CP:131:ALA:H	1.83	0.43
1:CY:58:PRO:HB3	1:CY:66:SER:O	2.18	0.43
1:DB:67:LYS:HD3	1:DB:95:GLU:HB3	2.00	0.43
1:DK:58:PRO:HB3	1:DK:66:SER:O	2.18	0.43
1:AA:99:ALA:HA	1:DH:46:ARG:NH2	2.33	0.43
1:AD:35:LEU:HD22	1:AE:131:ALA:H	1.83	0.43
1:AD:60:VAL:HG11	1:DE:87:PHE:HE2	1.82	0.43
1:AD:108:LEU:HA	1:AD:111:ILE:HG22	2.00	0.43
1:AF:39:VAL:HG12	1:AF:42:ASP:H	1.82	0.43
1:AN:58:PRO:HB3	1:AN:66:SER:O	2.18	0.43
1:AQ:58:PRO:HB3	1:AQ:66:SER:O	2.18	0.43
1:BB:108:LEU:HA	1:BB:111:ILE:HG22	2.00	0.43
1:BJ:16:ILE:HD13	1:DF:114:GLN:NE2	2.20	0.43
1:BM:129:ALA:HB1	1:DG:26:LEU:HB3	2.00	0.43
1:BR:68:GLY:O	1:BR:95:GLU:HA	2.18	0.43
1:BW:108:LEU:HA	1:BW:111:ILE:HG22	2.00	0.43
1:CA:58:PRO:HD2	1:CH:45:TYR:CE2	2.54	0.43
1:CQ:11:ALA:HB3	1:CQ:110:LEU:HD23	1.98	0.43
1:CU:26:LEU:HD12	1:CU:36:ASN:O	2.17	0.43
1:CU:35:LEU:HD22	1:CV:131:ALA:H	1.83	0.43
1:DB:68:GLY:O	1:DB:95:GLU:HA	2.18	0.43
1:DG:26:LEU:HD12	1:DG:36:ASN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DL:11:ALA:HB3	1:DL:110:LEU:HD23	1.98	0.43
1:AJ:35:LEU:HD22	1:AK:131:ALA:H	1.83	0.43
1:AO:16:ILE:HD13	1:CE:114:GLN:NE2	2.18	0.43
1:BE:26:LEU:HD12	1:BE:36:ASN:O	2.18	0.43
1:BH:26:LEU:HD12	1:BH:36:ASN:O	2.17	0.43
1:BK:35:LEU:HD22	1:BL:131:ALA:H	1.83	0.43
1:BM:109:ARG:O	1:DI:116:LEU:HD13	2.18	0.43
1:BQ:35:LEU:HD22	1:BR:131:ALA:H	1.83	0.43
1:CC:111:ILE:O	1:CC:115:LEU:HG	2.19	0.43
1:CN:7:ILE:HD12	1:CN:111:ILE:HG13	2.01	0.43
1:CP:68:GLY:O	1:CP:95:GLU:HA	2.18	0.43
1:CT:7:ILE:HD12	1:CT:111:ILE:HG13	2.01	0.43
1:CX:35:LEU:HD22	1:CY:131:ALA:H	1.83	0.43
1:DB:58:PRO:HB3	1:DB:66:SER:O	2.18	0.43
1:DH:68:GLY:O	1:DH:95:GLU:HA	2.18	0.43
1:AC:16:ILE:HD13	1:BP:114:GLN:NE2	2.21	0.43
1:AJ:108:LEU:HA	1:AJ:111:ILE:HG22	2.00	0.43
1:AM:53:PHE:CD1	1:AM:72:VAL:HG22	2.54	0.43
1:BA:39:VAL:HG12	1:BA:42:ASP:H	1.82	0.43
1:BE:53:PHE:CD1	1:BE:72:VAL:HG22	2.54	0.43
1:BH:111:ILE:O	1:BH:115:LEU:HG	2.19	0.43
1:BI:67:LYS:HD3	1:BI:95:GLU:HB3	2.00	0.43
1:BK:108:LEU:HA	1:BK:111:ILE:HG22	2.00	0.43
1:BM:90:VAL:CG1	1:DI:108:LEU:HD22	2.48	0.43
1:BO:65:TYR:HE2	1:DL:46:ARG:HA	1.83	0.43
1:BU:58:PRO:HB3	1:BU:66:SER:O	2.18	0.43
1:BU:67:LYS:HD3	1:BU:95:GLU:HB3	2.00	0.43
1:CM:68:GLY:O	1:CM:95:GLU:HA	2.18	0.43
1:CP:67:LYS:HD3	1:CP:95:GLU:HB3	2.00	0.43
1:DD:111:ILE:O	1:DD:115:LEU:HG	2.19	0.43
1:DG:53:PHE:CD1	1:DG:72:VAL:HG22	2.54	0.43
1:DG:108:LEU:HA	1:DG:111:ILE:HG22	1.99	0.43
1:AF:48:ARG:HH12	1:DD:127:LEU:CB	2.31	0.43
1:AV:53:PHE:CD1	1:AV:72:VAL:HG22	2.54	0.43
1:AY:53:PHE:CD1	1:AY:72:VAL:HG22	2.54	0.43
1:BB:35:LEU:HD22	1:BC:131:ALA:H	1.83	0.43
1:BC:58:PRO:HB3	1:BC:66:SER:O	2.18	0.43
1:BC:67:LYS:HD3	1:BC:95:GLU:HB3	2.00	0.43
1:BC:68:GLY:O	1:BC:95:GLU:HA	2.18	0.43
1:BD:7:ILE:HD12	1:BD:111:ILE:HG13	2.01	0.43
1:BF:67:LYS:HD3	1:BF:95:GLU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BS:7:ILE:HD12	1:BS:111:ILE:HG13	2.01	0.43
1:BV:39:VAL:HG12	1:BV:42:ASP:H	1.82	0.43
1:BX:68:GLY:O	1:BX:95:GLU:HA	2.18	0.43
1:CA:68:GLY:O	1:CA:95:GLU:HA	2.18	0.43
1:CP:58:PRO:HB3	1:CP:66:SER:O	2.18	0.43
1:CU:111:ILE:O	1:CU:115:LEU:HG	2.19	0.43
1:CY:68:GLY:O	1:CY:95:GLU:HA	2.18	0.43
1:DE:58:PRO:HB3	1:DE:66:SER:O	2.18	0.43
1:DH:67:LYS:HD3	1:DH:95:GLU:HB3	2.00	0.43
1:AB:68:GLY:O	1:AB:95:GLU:HA	2.18	0.43
1:AK:67:LYS:HD3	1:AK:95:GLU:HB3	2.00	0.43
1:AY:111:ILE:O	1:AY:115:LEU:HG	2.19	0.43
1:BB:53:PHE:CD1	1:BB:72:VAL:HG22	2.54	0.43
1:BK:53:PHE:CD1	1:BK:72:VAL:HG22	2.54	0.43
1:BL:67:LYS:HD3	1:BL:95:GLU:HB3	2.00	0.43
1:BM:124:PHE:CE2	1:DI:70:ASN:HB3	2.53	0.43
1:BW:35:LEU:HD22	1:BX:131:ALA:H	1.83	0.43
1:CE:7:ILE:HD12	1:CE:111:ILE:HG13	2.01	0.43
1:CG:67:LYS:HD3	1:CG:95:GLU:HB3	2.00	0.43
1:CK:7:ILE:HD12	1:CK:111:ILE:HG13	2.01	0.43
1:DA:53:PHE:CD1	1:DA:72:VAL:HG22	2.54	0.43
1:DI:7:ILE:HD12	1:DI:111:ILE:HG13	2.01	0.43
1:AC:22:ILE:HG22	1:BP:7:ILE:O	2.18	0.43
1:AM:35:LEU:HD22	1:AN:131:ALA:H	1.83	0.43
1:AM:111:ILE:O	1:AM:115:LEU:HG	2.19	0.43
1:AO:18:GLY:HA2	1:CE:12:THR:H	1.83	0.43
1:AP:53:PHE:CD1	1:AP:72:VAL:HG22	2.54	0.43
1:AQ:68:GLY:O	1:AQ:95:GLU:HA	2.18	0.43
1:BE:111:ILE:O	1:BE:115:LEU:HG	2.19	0.43
1:BF:58:PRO:HB3	1:BF:66:SER:O	2.18	0.43
1:BH:108:LEU:HA	1:BH:111:ILE:HG22	2.00	0.43
1:BJ:7:ILE:HD12	1:BJ:111:ILE:HG13	2.01	0.43
1:BK:111:ILE:O	1:BK:115:LEU:HG	2.19	0.43
1:BM:39:VAL:HG12	1:BM:42:ASP:H	1.82	0.43
1:BM:92:ILE:HG12	1:DI:92:ILE:HG12	2.00	0.43
1:BM:122:ASP:OD1	1:DI:109:ARG:NH1	2.40	0.43
1:BN:53:PHE:CD1	1:BN:72:VAL:HG22	2.54	0.43
1:BR:67:LYS:HD3	1:BR:95:GLU:HB3	2.00	0.43
1:BT:111:ILE:O	1:BT:115:LEU:HG	2.19	0.43
1:BZ:111:ILE:O	1:BZ:115:LEU:HG	2.19	0.43
1:CB:7:ILE:HD12	1:CB:111:ILE:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CH:7:ILE:HD12	1:CH:111:ILE:HG13	2.01	0.43
1:CX:108:LEU:HA	1:CX:111:ILE:HG22	2.00	0.43
1:DG:111:ILE:O	1:DG:115:LEU:HG	2.19	0.43
1:DJ:111:ILE:O	1:DJ:115:LEU:HG	2.19	0.43
1:AD:111:ILE:O	1:AD:115:LEU:HG	2.19	0.43
1:AH:67:LYS:HD3	1:AH:95:GLU:HB3	2.00	0.43
1:AH:68:GLY:O	1:AH:95:GLU:HA	2.18	0.43
1:AJ:111:ILE:O	1:AJ:115:LEU:HG	2.19	0.43
1:AQ:67:LYS:HD3	1:AQ:95:GLU:HB3	2.00	0.43
1:AT:58:PRO:HB3	1:AT:66:SER:O	2.18	0.43
1:AV:35:LEU:HD22	1:AW:131:ALA:H	1.83	0.43
1:AW:51:ALA:HA	1:AW:73:VAL:O	2.19	0.43
1:BA:114:GLN:NE2	1:CW:16:ILE:HG21	2.34	0.43
1:BO:67:LYS:HD3	1:BO:95:GLU:HB3	2.00	0.43
1:BT:53:PHE:CD1	1:BT:72:VAL:HG22	2.54	0.43
1:BV:7:ILE:HD12	1:BV:111:ILE:HG13	2.01	0.43
1:BZ:53:PHE:CD1	1:BZ:72:VAL:HG22	2.54	0.43
1:CV:58:PRO:HB3	1:CV:66:SER:O	2.18	0.43
1:CW:7:ILE:HD12	1:CW:111:ILE:HG13	2.01	0.43
1:CX:53:PHE:CD1	1:CX:72:VAL:HG22	2.54	0.43
1:DK:68:GLY:O	1:DK:95:GLU:HA	2.18	0.43
1:AA:111:ILE:O	1:AA:115:LEU:HG	2.19	0.43
1:AB:58:PRO:HB3	1:AB:66:SER:O	2.18	0.43
1:AB:67:LYS:HD3	1:AB:95:GLU:HB3	2.00	0.43
1:AE:51:ALA:HA	1:AE:73:VAL:O	2.19	0.43
1:AE:58:PRO:HB3	1:AE:66:SER:O	2.18	0.43
1:AI:17:THR:O	1:BY:12:THR:OG1	2.25	0.43
1:AN:67:LYS:HD3	1:AN:95:GLU:HB3	2.00	0.43
1:AP:35:LEU:HD22	1:AQ:131:ALA:H	1.83	0.43
1:AS:53:PHE:CD1	1:AS:72:VAL:HG22	2.54	0.43
1:AU:19:GLY:H	1:CN:11:ALA:HA	1.84	0.43
1:AY:108:LEU:HA	1:AY:111:ILE:HG22	2.00	0.43
1:AZ:58:PRO:HB3	1:AZ:66:SER:O	2.18	0.43
1:BA:19:GLY:O	1:CW:8:LYS:HD2	2.19	0.43
1:BB:26:LEU:HD12	1:BB:36:ASN:O	2.18	0.43
1:BD:14:ALA:HB2	1:CZ:16:ILE:HD12	2.01	0.43
1:BE:35:LEU:HD22	1:BF:131:ALA:H	1.83	0.43
1:BG:7:ILE:HD12	1:BG:111:ILE:HG13	2.01	0.43
1:BO:68:GLY:O	1:BO:95:GLU:HA	2.18	0.43
1:BQ:53:PHE:CD1	1:BQ:72:VAL:HG22	2.54	0.43
1:CD:68:GLY:O	1:CD:95:GLU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CL:53:PHE:CD1	1:CL:72:VAL:HG22	2.54	0.43
1:CQ:7:ILE:HD12	1:CQ:111:ILE:HG13	2.01	0.43
1:CR:111:ILE:O	1:CR:115:LEU:HG	2.19	0.43
1:CU:53:PHE:CD1	1:CU:72:VAL:HG22	2.54	0.43
1:DA:35:LEU:HD22	1:DB:131:ALA:H	1.83	0.43
1:DA:111:ILE:O	1:DA:115:LEU:HG	2.19	0.43
1:DE:67:LYS:HD3	1:DE:95:GLU:HB3	2.00	0.43
1:AA:53:PHE:CD1	1:AA:72:VAL:HG22	2.54	0.43
1:AD:53:PHE:CD1	1:AD:72:VAL:HG22	2.54	0.43
1:AH:45:TYR:HD2	1:CC:98:PRO:HB3	1.84	0.43
1:AI:100:LEU:HD13	1:BY:88:ASN:ND2	2.34	0.43
1:AM:26:LEU:O	1:CE:129:ALA:HB2	2.19	0.43
1:AM:28:GLY:HA3	1:CE:128:GLY:O	2.19	0.43
1:AR:53:PHE:CD1	1:AR:72:VAL:HG22	2.54	0.43
1:BF:48:ARG:HH22	1:BR:127:LEU:HD23	1.83	0.43
1:BH:53:PHE:CD1	1:BH:72:VAL:HG22	2.54	0.43
1:BK:26:LEU:HB3	1:DI:129:ALA:HB1	2.01	0.43
1:BL:51:ALA:HA	1:BL:73:VAL:O	2.19	0.43
1:BN:35:LEU:HD22	1:BO:131:ALA:H	1.83	0.43
1:BP:7:ILE:HD12	1:BP:111:ILE:HG13	2.01	0.43
1:BX:51:ALA:HA	1:BX:73:VAL:O	2.19	0.43
1:CA:51:ALA:HA	1:CA:73:VAL:O	2.19	0.43
1:CC:35:LEU:HD22	1:CD:131:ALA:H	1.83	0.43
1:CE:39:VAL:HG12	1:CE:42:ASP:H	1.82	0.43
1:CG:51:ALA:HA	1:CG:73:VAL:O	2.19	0.43
1:CJ:67:LYS:HD3	1:CJ:95:GLU:HB3	2.00	0.43
1:CK:53:PHE:CD1	1:CK:72:VAL:HG22	2.54	0.43
1:CY:67:LYS:HD3	1:CY:95:GLU:HB3	2.00	0.43
1:DG:35:LEU:HD22	1:DH:131:ALA:H	1.83	0.43
1:AE:67:LYS:HD3	1:AE:95:GLU:HB3	2.00	0.42
1:AF:7:ILE:O	1:BV:22:ILE:HG22	2.18	0.42
1:AG:53:PHE:CD1	1:AG:72:VAL:HG22	2.54	0.42
1:AI:7:ILE:HD12	1:AI:111:ILE:HG13	2.01	0.42
1:AI:53:PHE:CD1	1:AI:72:VAL:HG22	2.54	0.42
1:AJ:53:PHE:CD1	1:AJ:72:VAL:HG22	2.54	0.42
1:AL:8:LYS:HD2	1:CB:19:GLY:O	2.19	0.42
1:AP:111:ILE:O	1:AP:115:LEU:HG	2.19	0.42
1:BB:111:ILE:O	1:BB:115:LEU:HG	2.19	0.42
1:CD:67:LYS:HD3	1:CD:95:GLU:HB3	2.00	0.42
1:CH:53:PHE:CD1	1:CH:72:VAL:HG22	2.54	0.42
1:CI:35:LEU:HD22	1:CJ:131:ALA:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CI:111:ILE:O	1:CI:115:LEU:HG	2.19	0.42
1:CU:108:LEU:HA	1:CU:111:ILE:HG22	2.00	0.42
1:CV:51:ALA:HA	1:CV:73:VAL:O	2.19	0.42
1:CZ:53:PHE:CD1	1:CZ:72:VAL:HG22	2.54	0.42
1:DJ:53:PHE:CD1	1:DJ:72:VAL:HG22	2.54	0.42
1:AC:7:ILE:HD12	1:AC:111:ILE:HG13	2.01	0.42
1:AF:53:PHE:CD1	1:AF:72:VAL:HG22	2.54	0.42
1:AK:48:ARG:HH22	1:BX:127:LEU:HD23	1.84	0.42
1:AK:51:ALA:HA	1:AK:73:VAL:O	2.19	0.42
1:AN:51:ALA:HA	1:AN:73:VAL:O	2.19	0.42
1:AT:51:ALA:HA	1:AT:73:VAL:O	2.19	0.42
1:AV:111:ILE:O	1:AV:115:LEU:HG	2.19	0.42
1:BG:130:LEU:HD21	1:DC:55:SER:HB3	2.01	0.42
1:BJ:111:ILE:HD13	1:DF:74:PHE:CZ	2.54	0.42
1:BQ:111:ILE:O	1:BQ:115:LEU:HG	2.19	0.42
1:CC:53:PHE:CD1	1:CC:72:VAL:HG22	2.54	0.42
1:CM:67:LYS:HD3	1:CM:95:GLU:HB3	2.00	0.42
1:CT:46:ARG:HA	1:DB:65:TYR:HE2	1.84	0.42
1:DD:108:LEU:HA	1:DD:111:ILE:HG22	2.00	0.42
1:DF:7:ILE:HD12	1:DF:111:ILE:HG13	2.01	0.42
1:DF:39:VAL:HG12	1:DF:42:ASP:H	1.82	0.42
1:DK:67:LYS:HD3	1:DK:95:GLU:HB3	2.00	0.42
1:AC:53:PHE:CD1	1:AC:72:VAL:HG22	2.54	0.42
1:AH:51:ALA:HA	1:AH:73:VAL:O	2.19	0.42
1:AI:114:GLN:NE2	1:BY:16:ILE:HG21	2.34	0.42
1:AK:65:TYR:CE2	1:BY:46:ARG:HG2	2.54	0.42
1:AZ:51:ALA:HA	1:AZ:73:VAL:O	2.19	0.42
1:BA:7:ILE:HD12	1:BA:111:ILE:HG13	2.01	0.42
1:BD:53:PHE:CD1	1:BD:72:VAL:HG22	2.54	0.42
1:BG:53:PHE:CD1	1:BG:72:VAL:HG22	2.54	0.42
1:BP:53:PHE:CD1	1:BP:72:VAL:HG22	2.54	0.42
1:BW:53:PHE:CD1	1:BW:72:VAL:HG22	2.54	0.42
1:CM:51:ALA:HA	1:CM:73:VAL:O	2.19	0.42
1:CO:111:ILE:O	1:CO:115:LEU:HG	2.19	0.42
1:DD:53:PHE:CD1	1:DD:72:VAL:HG22	2.54	0.42
1:DI:53:PHE:CD1	1:DI:72:VAL:HG22	2.55	0.42
1:AC:125:TRP:HZ3	1:BP:70:ASN:O	2.03	0.42
1:BH:35:LEU:HD22	1:BI:131:ALA:H	1.83	0.42
1:CI:53:PHE:CD1	1:CI:72:VAL:HG22	2.54	0.42
1:CN:53:PHE:CD1	1:CN:72:VAL:HG22	2.54	0.42
1:DL:53:PHE:CD1	1:DL:72:VAL:HG22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AC:46:ARG:HG2	1:DH:65:TYR:CD2	2.54	0.42
1:AM:108:LEU:HA	1:AM:111:ILE:HG22	2.00	0.42
1:BN:111:ILE:O	1:BN:115:LEU:HG	2.19	0.42
1:CF:53:PHE:CD1	1:CF:72:VAL:HG22	2.54	0.42
1:CJ:51:ALA:HA	1:CJ:73:VAL:O	2.19	0.42
1:CL:111:ILE:O	1:CL:115:LEU:HG	2.19	0.42
1:CS:74:PHE:HB3	1:CS:90:VAL:HG13	2.02	0.42
1:CW:53:PHE:CD1	1:CW:72:VAL:HG22	2.55	0.42
1:DK:51:ALA:HA	1:DK:73:VAL:O	2.19	0.42
1:AB:74:PHE:HB3	1:AB:90:VAL:HG13	2.02	0.42
1:AR:7:ILE:HD12	1:AR:111:ILE:HG13	2.01	0.42
1:AU:16:ILE:HD12	1:CN:14:ALA:HB2	2.01	0.42
1:AY:35:LEU:HD22	1:AZ:131:ALA:H	1.83	0.42
1:BI:51:ALA:HA	1:BI:73:VAL:O	2.19	0.42
1:BI:74:PHE:HB3	1:BI:90:VAL:HG13	2.02	0.42
1:BR:51:ALA:HA	1:BR:73:VAL:O	2.19	0.42
1:BU:33:ASN:OD1	1:DI:30:THR:OG1	2.36	0.42
1:BW:111:ILE:O	1:BW:115:LEU:HG	2.19	0.42
1:CR:53:PHE:CD1	1:CR:72:VAL:HG22	2.54	0.42
1:DF:53:PHE:CD1	1:DF:72:VAL:HG22	2.54	0.42
1:DH:51:ALA:HA	1:DH:73:VAL:O	2.19	0.42
1:AF:7:ILE:HD12	1:AF:111:ILE:HG13	2.01	0.42
1:AI:16:ILE:HA	1:BY:14:ALA:HA	2.02	0.42
1:AQ:51:ALA:HA	1:AQ:73:VAL:O	2.19	0.42
1:AT:74:PHE:HB3	1:AT:90:VAL:HG13	2.02	0.42
1:AU:114:GLN:NE2	1:CN:16:ILE:HD13	2.23	0.42
1:BA:53:PHE:CD1	1:BA:72:VAL:HG22	2.54	0.42
1:BE:130:LEU:O	1:BS:26:LEU:HB3	2.19	0.42
1:BF:51:ALA:HA	1:BF:73:VAL:O	2.19	0.42
1:BS:53:PHE:CD1	1:BS:72:VAL:HG22	2.54	0.42
1:BU:51:ALA:HA	1:BU:73:VAL:O	2.19	0.42
1:CD:51:ALA:HA	1:CD:73:VAL:O	2.19	0.42
1:CT:53:PHE:CD1	1:CT:72:VAL:HG22	2.54	0.42
1:CX:111:ILE:O	1:CX:115:LEU:HG	2.19	0.42
1:AA:98:PRO:HB3	1:DH:45:TYR:HD2	1.83	0.42
1:AB:46:ARG:HA	1:AS:65:TYR:CE2	2.54	0.42
1:AI:16:ILE:HG21	1:BY:114:GLN:NE2	2.35	0.42
1:AL:7:ILE:HD12	1:AL:111:ILE:HG13	2.01	0.42
1:AL:109:ARG:NH2	1:CB:122:ASP:OD1	2.49	0.42
1:AO:53:PHE:CD1	1:AO:72:VAL:HG22	2.55	0.42
1:AS:111:ILE:O	1:AS:115:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AX:7:ILE:HD12	1:AX:111:ILE:HG13	2.01	0.42
1:BM:7:ILE:HD12	1:BM:111:ILE:HG13	2.01	0.42
1:BM:53:PHE:CD1	1:BM:72:VAL:HG22	2.54	0.42
1:BO:51:ALA:HA	1:BO:73:VAL:O	2.19	0.42
1:BX:74:PHE:HB3	1:BX:90:VAL:HG13	2.02	0.42
1:CF:111:ILE:O	1:CF:115:LEU:HG	2.19	0.42
1:CY:74:PHE:HB3	1:CY:90:VAL:HG13	2.02	0.42
1:DB:74:PHE:HB3	1:DB:90:VAL:HG13	2.02	0.42
1:AL:53:PHE:CD1	1:AL:72:VAL:HG22	2.54	0.42
1:AU:53:PHE:CD1	1:AU:72:VAL:HG22	2.54	0.42
1:BJ:53:PHE:CD1	1:BJ:72:VAL:HG22	2.54	0.42
1:CO:53:PHE:CD1	1:CO:72:VAL:HG22	2.54	0.42
1:CP:51:ALA:HA	1:CP:73:VAL:O	2.19	0.42
1:CU:87:PHE:O	1:CV:67:LYS:NZ	2.41	0.42
1:CZ:7:ILE:HD12	1:CZ:111:ILE:HG13	2.01	0.42
1:DB:51:ALA:HA	1:DB:73:VAL:O	2.19	0.42
1:AE:74:PHE:HB3	1:AE:90:VAL:HG13	2.02	0.42
1:AF:20:SER:O	1:BV:8:LYS:HA	2.20	0.42
1:AG:111:ILE:O	1:AG:115:LEU:HG	2.19	0.42
1:BO:74:PHE:HB3	1:BO:90:VAL:HG13	2.02	0.42
1:CE:53:PHE:CD1	1:CE:72:VAL:HG22	2.54	0.42
1:CQ:53:PHE:CD1	1:CQ:72:VAL:HG22	2.54	0.42
1:DE:51:ALA:HA	1:DE:73:VAL:O	2.19	0.42
1:AR:130:LEU:O	1:CK:35:LEU:HD22	2.20	0.41
1:AW:74:PHE:HB3	1:AW:90:VAL:HG13	2.02	0.41
1:BC:74:PHE:HB3	1:BC:90:VAL:HG13	2.02	0.41
1:CS:51:ALA:HA	1:CS:73:VAL:O	2.19	0.41
1:CY:51:ALA:HA	1:CY:73:VAL:O	2.19	0.41
1:DE:74:PHE:HB3	1:DE:90:VAL:HG13	2.02	0.41
1:AO:7:ILE:HD12	1:AO:111:ILE:HG13	2.01	0.41
1:BY:7:ILE:HD12	1:BY:111:ILE:HG13	2.01	0.41
1:CP:74:PHE:HB3	1:CP:90:VAL:HG13	2.02	0.41
1:DH:74:PHE:HB3	1:DH:90:VAL:HG13	2.02	0.41
1:DK:74:PHE:HB3	1:DK:90:VAL:HG13	2.02	0.41
1:AB:51:ALA:HA	1:AB:73:VAL:O	2.19	0.41
1:AC:19:GLY:O	1:BP:8:LYS:HD2	2.20	0.41
1:AI:74:PHE:CZ	1:BY:111:ILE:HD13	2.55	0.41
1:AU:111:ILE:HD13	1:CN:74:PHE:CZ	2.55	0.41
1:BY:53:PHE:CD1	1:BY:72:VAL:HG22	2.54	0.41
1:DC:53:PHE:CD1	1:DC:72:VAL:HG22	2.54	0.41
1:DL:7:ILE:HD12	1:DL:111:ILE:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AI:109:ARG:NE	1:BY:116:LEU:O	2.50	0.41
1:AJ:18:GLY:HA2	1:AK:12:THR:H	1.86	0.41
1:AM:18:GLY:HA2	1:AN:12:THR:H	1.86	0.41
1:AU:7:ILE:HD12	1:AU:111:ILE:HG13	2.01	0.41
1:AY:18:GLY:HA2	1:AZ:12:THR:H	1.86	0.41
1:BM:109:ARG:NE	1:DI:116:LEU:O	2.52	0.41
1:BV:53:PHE:CD1	1:BV:72:VAL:HG22	2.54	0.41
1:CD:74:PHE:HB3	1:CD:90:VAL:HG13	2.02	0.41
1:CI:18:GLY:HA2	1:CJ:12:THR:H	1.86	0.41
1:DC:7:ILE:HD12	1:DC:111:ILE:HG13	2.01	0.41
1:AL:46:ARG:HG3	1:CV:98:PRO:HB2	2.03	0.41
1:AU:16:ILE:HA	1:CN:14:ALA:HA	2.02	0.41
1:AX:14:ALA:HB3	1:CT:117:THR:HB	2.01	0.41
1:AX:53:PHE:CD1	1:AX:72:VAL:HG22	2.54	0.41
1:BH:18:GLY:HA2	1:BI:12:THR:H	1.86	0.41
1:BK:18:GLY:HA2	1:BL:12:THR:H	1.86	0.41
1:BL:74:PHE:HB3	1:BL:90:VAL:HG13	2.02	0.41
1:CX:18:GLY:HA2	1:CY:12:THR:H	1.86	0.41
1:AF:95:GLU:HB2	1:BV:89:SER:HB2	2.02	0.41
1:AG:57:VAL:HG21	1:CS:29:GLN:HG3	2.03	0.41
1:AH:74:PHE:HB3	1:AH:90:VAL:HG13	2.02	0.41
1:AJ:65:TYR:CD2	1:CV:46:ARG:HG3	2.55	0.41
1:AK:74:PHE:HB3	1:AK:90:VAL:HG13	2.02	0.41
1:AZ:10:GLY:H	1:AZ:107:ASP:CG	2.24	0.41
1:BC:10:GLY:H	1:BC:107:ASP:CG	2.24	0.41
1:BO:10:GLY:H	1:BO:107:ASP:CG	2.24	0.41
1:BU:10:GLY:H	1:BU:107:ASP:CG	2.24	0.41
1:CF:18:GLY:HA2	1:CG:12:THR:H	1.86	0.41
1:AB:10:GLY:H	1:AB:107:ASP:CG	2.24	0.41
1:AC:46:ARG:HA	1:DH:65:TYR:CE2	2.49	0.41
1:AF:111:ILE:HD13	1:BV:74:PHE:CZ	2.56	0.41
1:AI:46:ARG:HG2	1:CS:65:TYR:HD2	1.84	0.41
1:AK:10:GLY:H	1:AK:107:ASP:CG	2.24	0.41
1:AR:122:ASP:OD1	1:CK:109:ARG:NH2	2.52	0.41
1:AT:10:GLY:H	1:AT:107:ASP:CG	2.24	0.41
1:AX:122:ASP:OD1	1:CT:109:ARG:NH2	2.49	0.41
1:BC:51:ALA:HA	1:BC:73:VAL:O	2.19	0.41
1:CB:53:PHE:CD1	1:CB:72:VAL:HG22	2.54	0.41
1:CU:18:GLY:HA2	1:CV:12:THR:H	1.86	0.41
1:DA:18:GLY:HA2	1:DB:12:THR:H	1.86	0.41
1:DG:18:GLY:HA2	1:DH:12:THR:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AE:127:LEU:HD23	1:DE:48:ARG:HH22	1.85	0.41
1:AH:10:GLY:H	1:AH:107:ASP:CG	2.24	0.41
1:AP:18:GLY:HA2	1:AQ:12:THR:H	1.86	0.41
1:BQ:16:ILE:CD1	1:BR:114:GLN:HE21	2.26	0.41
1:CA:10:GLY:H	1:CA:107:ASP:CG	2.24	0.41
1:CM:74:PHE:HB3	1:CM:90:VAL:HG13	2.02	0.41
1:CO:18:GLY:HA2	1:CP:12:THR:H	1.86	0.41
1:CP:10:GLY:H	1:CP:107:ASP:CG	2.24	0.41
1:DH:10:GLY:H	1:DH:107:ASP:CG	2.24	0.41
1:DJ:18:GLY:HA2	1:DK:12:THR:H	1.86	0.41
1:AG:18:GLY:HA2	1:AH:12:THR:H	1.86	0.41
1:AO:122:ASP:OD1	1:CE:109:ARG:NH1	2.45	0.41
1:AQ:74:PHE:HB3	1:AQ:90:VAL:HG13	2.02	0.41
1:BD:19:GLY:O	1:CZ:8:LYS:HD2	2.21	0.41
1:BF:10:GLY:H	1:BF:107:ASP:CG	2.24	0.41
1:BG:16:ILE:HD13	1:DC:114:GLN:NE2	2.22	0.41
1:BM:12:THR:H	1:DI:18:GLY:HA2	1.86	0.41
1:BQ:18:GLY:HA2	1:BR:12:THR:H	1.86	0.41
1:BR:74:PHE:HB3	1:BR:90:VAL:HG13	2.02	0.41
1:CA:74:PHE:HB3	1:CA:90:VAL:HG13	2.02	0.41
1:CC:18:GLY:HA2	1:CD:12:THR:H	1.86	0.41
1:CG:74:PHE:HB3	1:CG:90:VAL:HG13	2.02	0.41
1:CL:130:LEU:O	1:CZ:26:LEU:HB3	2.20	0.41
1:CV:74:PHE:HB3	1:CV:90:VAL:HG13	2.02	0.41
1:DB:10:GLY:H	1:DB:107:ASP:CG	2.24	0.41
1:DD:18:GLY:HA2	1:DE:12:THR:H	1.86	0.41
1:DE:10:GLY:H	1:DE:107:ASP:CG	2.24	0.41
1:AC:6:SER:HA	1:BP:22:ILE:O	2.21	0.41
1:AD:18:GLY:HA2	1:AE:12:THR:H	1.86	0.41
1:AI:46:ARG:HA	1:CS:65:TYR:HE2	1.84	0.41
1:AS:18:GLY:HA2	1:AT:12:THR:H	1.86	0.41
1:AX:109:ARG:HD2	1:CT:125:TRP:HB3	2.03	0.41
1:BF:74:PHE:HB3	1:BF:90:VAL:HG13	2.02	0.41
1:CA:65:TYR:HE2	1:CH:46:ARG:CA	2.33	0.41
1:CD:10:GLY:H	1:CD:107:ASP:CG	2.24	0.41
1:AC:116:LEU:HG	1:BP:92:ILE:HG21	2.03	0.40
1:AL:26:LEU:HB3	1:CU:130:LEU:O	2.22	0.40
1:AL:46:ARG:HG2	1:CV:65:TYR:HD2	1.84	0.40
1:AR:55:SER:HB3	1:CK:130:LEU:HD21	2.01	0.40
1:AZ:74:PHE:HB3	1:AZ:90:VAL:HG13	2.02	0.40
1:CS:110:LEU:O	1:CS:114:GLN:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AN:74:PHE:HB3	1:AN:90:VAL:HG13	2.02	0.40
1:AR:122:ASP:OD1	1:CK:109:ARG:NH1	2.52	0.40
1:AU:74:PHE:CZ	1:CN:111:ILE:HD13	2.56	0.40
1:AW:10:GLY:H	1:AW:107:ASP:CG	2.24	0.40
1:BO:110:LEU:O	1:BO:114:GLN:HG3	2.22	0.40
1:CJ:74:PHE:HB3	1:CJ:90:VAL:HG13	2.02	0.40
1:CM:110:LEU:O	1:CM:114:GLN:HG3	2.22	0.40
1:AA:18:GLY:HA2	1:AB:12:THR:H	1.86	0.40
1:AK:26:LEU:O	1:BX:129:ALA:HB2	2.21	0.40
1:AT:48:ARG:HH22	1:AW:127:LEU:HD23	1.85	0.40
1:BB:18:GLY:HA2	1:BC:12:THR:H	1.86	0.40
1:BI:10:GLY:H	1:BI:107:ASP:CG	2.24	0.40
1:BN:18:GLY:HA2	1:BO:12:THR:H	1.86	0.40
1:BX:10:GLY:H	1:BX:107:ASP:CG	2.24	0.40
1:BX:110:LEU:O	1:BX:114:GLN:HG3	2.22	0.40
1:CG:10:GLY:H	1:CG:107:ASP:CG	2.24	0.40
1:CI:11:ALA:HA	1:CJ:18:GLY:HA2	2.04	0.40
1:CJ:10:GLY:H	1:CJ:107:ASP:CG	2.24	0.40
1:CU:11:ALA:HA	1:CV:18:GLY:HA2	2.04	0.40
1:CY:110:LEU:O	1:CY:114:GLN:HG3	2.22	0.40
1:DG:11:ALA:HA	1:DH:18:GLY:HA2	2.04	0.40
1:AF:92:ILE:HA	1:BV:91:ARG:O	2.22	0.40
1:AO:129:ALA:HB2	1:CC:26:LEU:O	2.21	0.40
1:AQ:10:GLY:H	1:AQ:107:ASP:CG	2.24	0.40
1:AT:85:THR:N	1:AV:63:GLY:O	2.47	0.40
1:AV:18:GLY:HA2	1:AW:12:THR:H	1.86	0.40
1:BA:26:LEU:HD13	1:BA:35:LEU:HD11	2.04	0.40
1:BC:65:TYR:HE2	1:BP:46:ARG:CA	2.32	0.40
1:BL:110:LEU:O	1:BL:114:GLN:HG3	2.22	0.40
1:BR:42:ASP:CB	1:BR:48:ARG:HG2	2.50	0.40
1:BU:110:LEU:O	1:BU:114:GLN:HG3	2.22	0.40
1:BW:11:ALA:HA	1:BX:18:GLY:HA2	2.04	0.40
1:CM:8:LYS:HB2	1:CM:114:GLN:NE2	2.32	0.40
1:CR:18:GLY:HA2	1:CS:12:THR:H	1.86	0.40
1:CX:31:VAL:HG13	1:CX:54:LYS:HE2	2.04	0.40
1:DA:31:VAL:HG13	1:DA:54:LYS:HE2	2.04	0.40
1:DE:110:LEU:O	1:DE:114:GLN:HG3	2.22	0.40
1:DG:31:VAL:HG13	1:DG:54:LYS:HE2	2.04	0.40
1:AJ:31:VAL:HG13	1:AJ:54:LYS:HE2	2.04	0.40
1:AN:10:GLY:H	1:AN:107:ASP:CG	2.24	0.40
1:AY:71:GLU:HG2	1:AY:93:ALA:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:122:ASP:OD1	1:CW:109:ARG:NH2	2.53	0.40
1:BB:71:GLU:HG2	1:BB:93:ALA:HB2	2.04	0.40
1:BB:87:PHE:O	1:BC:67:LYS:NZ	2.41	0.40
1:BC:42:ASP:CB	1:BC:48:ARG:HG2	2.50	0.40
1:BE:18:GLY:HA2	1:BF:12:THR:H	1.86	0.40
1:BL:10:GLY:H	1:BL:107:ASP:CG	2.24	0.40
1:BR:110:LEU:O	1:BR:114:GLN:HG3	2.22	0.40
1:BT:18:GLY:HA2	1:BU:12:THR:H	1.86	0.40
1:BZ:18:GLY:HA2	1:CA:12:THR:H	1.86	0.40
1:CC:11:ALA:HA	1:CD:18:GLY:HA2	2.04	0.40
1:CC:31:VAL:HG13	1:CC:54:LYS:HE2	2.04	0.40
1:CF:87:PHE:O	1:CG:67:LYS:NZ	2.41	0.40
1:CI:31:VAL:HG13	1:CI:54:LYS:HE2	2.04	0.40
1:CL:11:ALA:HA	1:CM:18:GLY:HA2	2.04	0.40
1:CL:18:GLY:HA2	1:CM:12:THR:H	1.86	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BS:17:THR:O	1:CH:12:THR:OG1[2_555]	2.03	0.17
1:AR:30:THR:OG1	1:CG:33:ASN:OD1[2_555]	2.04	0.16
1:AP:33:ASN:OD1	1:CG:30:THR:OG1[2_555]	2.13	0.07

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	AB	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	AC	129/131 (98%)	129 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AD	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	AE	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	AF	129/131 (98%)	129 (100%)	0	0	100	100
1	AG	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	AH	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	AI	129/131 (98%)	129 (100%)	0	0	100	100
1	AJ	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	AK	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	AL	129/131 (98%)	129 (100%)	0	0	100	100
1	AM	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	AN	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	AO	129/131 (98%)	129 (100%)	0	0	100	100
1	AP	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	AQ	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	AR	129/131 (98%)	129 (100%)	0	0	100	100
1	AS	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	AT	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	AU	129/131 (98%)	129 (100%)	0	0	100	100
1	AV	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	AW	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	AX	129/131 (98%)	129 (100%)	0	0	100	100
1	AY	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	AZ	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	BA	129/131 (98%)	129 (100%)	0	0	100	100
1	BB	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	BC	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	BD	129/131 (98%)	129 (100%)	0	0	100	100
1	BE	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	BF	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	BG	129/131 (98%)	129 (100%)	0	0	100	100
1	BH	129/131 (98%)	127 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BI	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	BJ	129/131 (98%)	129 (100%)	0	0	100	100
1	BK	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	BL	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	BM	129/131 (98%)	129 (100%)	0	0	100	100
1	BN	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	BO	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	BP	129/131 (98%)	129 (100%)	0	0	100	100
1	BQ	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	BR	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	BS	129/131 (98%)	129 (100%)	0	0	100	100
1	BT	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	BU	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	BV	129/131 (98%)	129 (100%)	0	0	100	100
1	BW	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	BX	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	BY	129/131 (98%)	129 (100%)	0	0	100	100
1	BZ	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	CA	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	CB	129/131 (98%)	129 (100%)	0	0	100	100
1	CC	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	CD	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	CE	129/131 (98%)	129 (100%)	0	0	100	100
1	CF	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	CG	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	CH	129/131 (98%)	129 (100%)	0	0	100	100
1	CI	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	CJ	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	CK	129/131 (98%)	129 (100%)	0	0	100	100
1	CL	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	CM	129/131 (98%)	128 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CN	129/131 (98%)	129 (100%)	0	0	100	100
1	CO	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	CP	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	CQ	129/131 (98%)	129 (100%)	0	0	100	100
1	CR	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	CS	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	CT	129/131 (98%)	129 (100%)	0	0	100	100
1	CU	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	CV	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	CW	129/131 (98%)	129 (100%)	0	0	100	100
1	CX	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	CY	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	CZ	129/131 (98%)	129 (100%)	0	0	100	100
1	DA	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	DB	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	DC	129/131 (98%)	129 (100%)	0	0	100	100
1	DD	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	DE	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	DF	129/131 (98%)	129 (100%)	0	0	100	100
1	DG	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	DH	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	DI	129/131 (98%)	129 (100%)	0	0	100	100
1	DJ	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	DK	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
1	DL	129/131 (98%)	129 (100%)	0	0	100	100
All	All	11610/11790 (98%)	11520 (99%)	90 (1%)	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 X-ray entries followed by that with respect to entries of similar

resolution.

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	AA	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	AB	108/108 (100%)	108 (100%)	0	100	100
1	AC	108/108 (100%)	108 (100%)	0	100	100
1	AD	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	AE	108/108 (100%)	108 (100%)	0	100	100
1	AF	108/108 (100%)	108 (100%)	0	100	100
1	AG	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	AH	108/108 (100%)	108 (100%)	0	100	100
1	AI	108/108 (100%)	108 (100%)	0	100	100
1	AJ	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	AK	108/108 (100%)	108 (100%)	0	100	100
1	AL	108/108 (100%)	108 (100%)	0	100	100
1	AM	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	AN	108/108 (100%)	108 (100%)	0	100	100
1	AO	108/108 (100%)	108 (100%)	0	100	100
1	AP	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	AQ	108/108 (100%)	108 (100%)	0	100	100
1	AR	108/108 (100%)	108 (100%)	0	100	100
1	AS	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	AT	108/108 (100%)	108 (100%)	0	100	100
1	AU	108/108 (100%)	108 (100%)	0	100	100
1	AV	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	AW	108/108 (100%)	108 (100%)	0	100	100
1	AX	108/108 (100%)	108 (100%)	0	100	100
1	AY	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	AZ	108/108 (100%)	108 (100%)	0	100	100
1	BA	108/108 (100%)	108 (100%)	0	100	100
1	BB	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	BC	108/108 (100%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BD	108/108 (100%)	108 (100%)	0	100	100
1	BE	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	BF	108/108 (100%)	108 (100%)	0	100	100
1	BG	108/108 (100%)	108 (100%)	0	100	100
1	BH	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	BI	108/108 (100%)	108 (100%)	0	100	100
1	BJ	108/108 (100%)	108 (100%)	0	100	100
1	BK	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	BL	108/108 (100%)	108 (100%)	0	100	100
1	BM	108/108 (100%)	108 (100%)	0	100	100
1	BN	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	BO	108/108 (100%)	108 (100%)	0	100	100
1	BP	108/108 (100%)	108 (100%)	0	100	100
1	BQ	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	BR	108/108 (100%)	108 (100%)	0	100	100
1	BS	108/108 (100%)	108 (100%)	0	100	100
1	BT	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	BU	108/108 (100%)	108 (100%)	0	100	100
1	BV	108/108 (100%)	108 (100%)	0	100	100
1	BW	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	BX	108/108 (100%)	108 (100%)	0	100	100
1	BY	108/108 (100%)	108 (100%)	0	100	100
1	BZ	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	CA	108/108 (100%)	108 (100%)	0	100	100
1	CB	108/108 (100%)	108 (100%)	0	100	100
1	CC	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	CD	108/108 (100%)	108 (100%)	0	100	100
1	CE	108/108 (100%)	108 (100%)	0	100	100
1	CF	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	CG	108/108 (100%)	108 (100%)	0	100	100
1	CH	108/108 (100%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CI	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	CJ	108/108 (100%)	108 (100%)	0	100	100
1	CK	108/108 (100%)	108 (100%)	0	100	100
1	CL	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	CM	108/108 (100%)	108 (100%)	0	100	100
1	CN	108/108 (100%)	108 (100%)	0	100	100
1	CO	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	CP	108/108 (100%)	108 (100%)	0	100	100
1	CQ	108/108 (100%)	108 (100%)	0	100	100
1	CR	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	CS	108/108 (100%)	108 (100%)	0	100	100
1	CT	108/108 (100%)	108 (100%)	0	100	100
1	CU	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	CV	108/108 (100%)	108 (100%)	0	100	100
1	CW	108/108 (100%)	108 (100%)	0	100	100
1	CX	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	CY	108/108 (100%)	108 (100%)	0	100	100
1	CZ	108/108 (100%)	108 (100%)	0	100	100
1	DA	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	DB	108/108 (100%)	108 (100%)	0	100	100
1	DC	108/108 (100%)	108 (100%)	0	100	100
1	DD	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	DE	108/108 (100%)	108 (100%)	0	100	100
1	DF	108/108 (100%)	108 (100%)	0	100	100
1	DG	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	DH	108/108 (100%)	108 (100%)	0	100	100
1	DI	108/108 (100%)	108 (100%)	0	100	100
1	DJ	108/108 (100%)	107 (99%)	1 (1%)	78	91
1	DK	108/108 (100%)	108 (100%)	0	100	100
1	DL	108/108 (100%)	108 (100%)	0	100	100
All	All	9720/9720 (100%)	9690 (100%)	30 (0%)	92	97

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	36	ASN
1	AD	36	ASN
1	AG	36	ASN
1	AJ	36	ASN
1	AM	36	ASN
1	AP	36	ASN
1	AS	36	ASN
1	AV	36	ASN
1	AY	36	ASN
1	BB	36	ASN
1	BE	36	ASN
1	BH	36	ASN
1	BK	36	ASN
1	BN	36	ASN
1	BQ	36	ASN
1	BT	36	ASN
1	BW	36	ASN
1	BZ	36	ASN
1	CC	36	ASN
1	CF	36	ASN
1	CI	36	ASN
1	CL	36	ASN
1	CO	36	ASN
1	CR	36	ASN
1	CU	36	ASN
1	CX	36	ASN
1	DA	36	ASN
1	DD	36	ASN
1	DG	36	ASN
1	DJ	36	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	AB	29	GLN
1	AB	36	ASN
1	AE	29	GLN
1	AE	36	ASN
1	AH	29	GLN
1	AH	36	ASN
1	AK	29	GLN

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Mol	Chain	Res	Type
1	AK	36	ASN
1	AN	29	GLN
1	AN	36	ASN
1	AQ	29	GLN
1	AQ	36	ASN
1	AT	29	GLN
1	AT	36	ASN
1	AW	29	GLN
1	AW	36	ASN
1	AZ	29	GLN
1	AZ	36	ASN
1	BC	29	GLN
1	BC	36	ASN
1	BF	29	GLN
1	BF	36	ASN
1	BI	29	GLN
1	BI	36	ASN
1	BL	29	GLN
1	BL	36	ASN
1	BO	29	GLN
1	BO	36	ASN
1	BR	29	GLN
1	BR	36	ASN
1	BU	29	GLN
1	BU	36	ASN
1	BX	29	GLN
1	BX	36	ASN
1	CA	29	GLN
1	CA	36	ASN
1	CD	29	GLN
1	CD	36	ASN
1	CG	29	GLN
1	CG	36	ASN
1	CJ	29	GLN
1	CJ	36	ASN
1	CM	29	GLN
1	CM	36	ASN
1	CP	29	GLN
1	CP	36	ASN
1	CS	29	GLN
1	CS	36	ASN
1	CV	29	GLN

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Mol	Chain	Res	Type
1	CV	36	ASN
1	CY	29	GLN
1	CY	36	ASN
1	DA	36	ASN
1	DB	29	GLN
1	DB	36	ASN
1	DE	29	GLN
1	DE	36	ASN
1	DH	29	GLN
1	DH	36	ASN
1	DK	29	GLN
1	DK	36	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	131/131 (100%)	0.21	4 (3%)	49	45	64, 111, 139, 160	0
1	AB	131/131 (100%)	0.02	2 (1%)	73	70	64, 109, 138, 177	0
1	AC	131/131 (100%)	0.37	9 (6%)	16	18	64, 110, 142, 191	0
1	AD	131/131 (100%)	0.14	5 (3%)	40	37	64, 111, 139, 160	0
1	AE	131/131 (100%)	0.08	3 (2%)	60	56	64, 109, 138, 177	0
1	AF	131/131 (100%)	0.08	6 (4%)	32	30	64, 110, 142, 191	0
1	AG	131/131 (100%)	0.15	6 (4%)	32	30	64, 111, 139, 160	0
1	AH	131/131 (100%)	0.14	4 (3%)	49	45	64, 109, 138, 177	0
1	AI	131/131 (100%)	0.40	9 (6%)	16	18	64, 110, 142, 191	0
1	AJ	131/131 (100%)	0.11	3 (2%)	60	56	64, 111, 139, 160	0
1	AK	131/131 (100%)	0.07	3 (2%)	60	56	64, 109, 138, 177	0
1	AL	131/131 (100%)	0.11	1 (0%)	86	82	64, 110, 142, 191	0
1	AM	131/131 (100%)	0.07	1 (0%)	86	82	64, 111, 139, 160	0
1	AN	131/131 (100%)	0.17	3 (2%)	60	56	64, 109, 138, 177	0
1	AO	131/131 (100%)	0.26	5 (3%)	40	37	64, 110, 142, 191	0
1	AP	131/131 (100%)	-0.09	2 (1%)	73	70	64, 111, 139, 160	0
1	AQ	131/131 (100%)	-0.05	3 (2%)	60	56	64, 109, 138, 177	0
1	AR	131/131 (100%)	0.15	4 (3%)	49	45	64, 110, 142, 191	0
1	AS	131/131 (100%)	0.01	1 (0%)	86	82	64, 111, 139, 160	0
1	AT	131/131 (100%)	0.12	3 (2%)	60	56	64, 109, 138, 177	0
1	AU	131/131 (100%)	0.39	11 (8%)	11	13	64, 110, 142, 191	0
1	AV	131/131 (100%)	0.04	1 (0%)	86	82	64, 111, 139, 160	0
1	AW	131/131 (100%)	-0.01	4 (3%)	49	45	64, 109, 138, 177	0
1	AX	131/131 (100%)	0.03	5 (3%)	40	37	64, 110, 142, 191	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AY	131/131 (100%)	-0.02	2 (1%) 73 70	64, 111, 139, 160	0
1	AZ	131/131 (100%)	-0.01	3 (2%) 60 56	64, 109, 138, 177	0
1	BA	131/131 (100%)	0.08	7 (5%) 26 25	64, 110, 142, 191	0
1	BB	131/131 (100%)	0.11	2 (1%) 73 70	64, 111, 139, 160	0
1	BC	131/131 (100%)	0.12	1 (0%) 86 82	64, 109, 138, 177	0
1	BD	131/131 (100%)	-0.01	3 (2%) 60 56	64, 110, 142, 191	0
1	BE	131/131 (100%)	0.31	9 (6%) 16 18	64, 111, 139, 160	0
1	BF	131/131 (100%)	0.26	7 (5%) 26 25	64, 109, 138, 177	0
1	BG	131/131 (100%)	0.16	8 (6%) 21 21	64, 110, 142, 191	0
1	BH	131/131 (100%)	0.30	12 (9%) 9 10	64, 111, 139, 160	0
1	BI	131/131 (100%)	0.02	3 (2%) 60 56	64, 109, 138, 177	0
1	BJ	131/131 (100%)	0.25	10 (7%) 13 15	64, 110, 142, 191	0
1	BK	131/131 (100%)	0.11	9 (6%) 16 18	64, 111, 139, 160	0
1	BL	131/131 (100%)	0.19	3 (2%) 60 56	64, 109, 138, 177	0
1	BM	131/131 (100%)	0.30	12 (9%) 9 10	64, 110, 142, 191	0
1	BN	131/131 (100%)	0.11	3 (2%) 60 56	64, 111, 139, 160	0
1	BO	131/131 (100%)	-0.04	5 (3%) 40 37	64, 109, 138, 177	0
1	BP	131/131 (100%)	0.32	9 (6%) 16 18	64, 110, 142, 191	0
1	BQ	131/131 (100%)	0.16	8 (6%) 21 21	64, 111, 139, 160	0
1	BR	131/131 (100%)	0.03	3 (2%) 60 56	64, 109, 138, 177	0
1	BS	131/131 (100%)	0.17	5 (3%) 40 37	64, 110, 142, 191	0
1	BT	131/131 (100%)	0.08	5 (3%) 40 37	64, 111, 139, 160	0
1	BU	131/131 (100%)	-0.01	2 (1%) 73 70	64, 109, 138, 177	0
1	BV	131/131 (100%)	0.22	11 (8%) 11 13	64, 110, 142, 191	0
1	BW	131/131 (100%)	0.18	5 (3%) 40 37	64, 111, 139, 160	0
1	BX	131/131 (100%)	0.08	3 (2%) 60 56	64, 109, 138, 177	0
1	BY	131/131 (100%)	0.15	2 (1%) 73 70	64, 110, 142, 191	0
1	BZ	131/131 (100%)	0.08	7 (5%) 26 25	64, 111, 139, 160	0
1	CA	131/131 (100%)	0.15	4 (3%) 49 45	64, 109, 138, 177	0
1	CB	131/131 (100%)	0.20	5 (3%) 40 37	64, 110, 142, 191	0
1	CC	131/131 (100%)	0.18	4 (3%) 49 45	64, 111, 139, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	CD	131/131 (100%)	0.01	4 (3%)	49	45	64, 109, 138, 177	0
1	CE	131/131 (100%)	0.13	8 (6%)	21	21	64, 110, 142, 191	0
1	CF	131/131 (100%)	0.30	6 (4%)	32	30	64, 111, 139, 160	0
1	CG	131/131 (100%)	0.08	6 (4%)	32	30	64, 109, 138, 177	0
1	CH	131/131 (100%)	0.15	5 (3%)	40	37	64, 110, 142, 191	0
1	CI	131/131 (100%)	0.09	7 (5%)	26	25	64, 111, 139, 160	0
1	CJ	131/131 (100%)	-0.06	2 (1%)	73	70	64, 109, 138, 177	0
1	CK	131/131 (100%)	0.14	8 (6%)	21	21	64, 110, 142, 191	0
1	CL	131/131 (100%)	0.25	10 (7%)	13	15	64, 111, 139, 160	0
1	CM	131/131 (100%)	0.09	4 (3%)	49	45	64, 109, 138, 177	0
1	CN	131/131 (100%)	0.04	1 (0%)	86	82	64, 110, 142, 191	0
1	CO	131/131 (100%)	-0.05	2 (1%)	73	70	64, 111, 139, 160	0
1	CP	131/131 (100%)	-0.01	3 (2%)	60	56	64, 109, 138, 177	0
1	CQ	131/131 (100%)	0.01	3 (2%)	60	56	64, 110, 142, 191	0
1	CR	131/131 (100%)	0.10	6 (4%)	32	30	64, 111, 139, 160	0
1	CS	131/131 (100%)	0.10	5 (3%)	40	37	64, 109, 138, 177	0
1	CT	131/131 (100%)	0.32	16 (12%)	4	6	64, 110, 142, 191	0
1	CU	131/131 (100%)	-0.04	4 (3%)	49	45	64, 111, 139, 160	0
1	CV	131/131 (100%)	0.09	5 (3%)	40	37	64, 109, 138, 177	0
1	CW	131/131 (100%)	0.47	17 (12%)	3	5	64, 110, 142, 191	0
1	CX	131/131 (100%)	-0.01	4 (3%)	49	45	64, 111, 139, 160	0
1	CY	131/131 (100%)	-0.09	1 (0%)	86	82	64, 109, 138, 177	0
1	CZ	131/131 (100%)	0.13	4 (3%)	49	45	64, 110, 142, 191	0
1	DA	131/131 (100%)	-0.04	3 (2%)	60	56	64, 111, 139, 160	0
1	DB	131/131 (100%)	0.09	8 (6%)	21	21	64, 109, 138, 177	0
1	DC	131/131 (100%)	0.25	12 (9%)	9	10	64, 110, 142, 191	0
1	DD	131/131 (100%)	0.37	10 (7%)	13	15	64, 111, 139, 160	0
1	DE	131/131 (100%)	0.10	3 (2%)	60	56	64, 109, 138, 177	0
1	DF	131/131 (100%)	0.27	10 (7%)	13	15	64, 110, 142, 191	0
1	DG	131/131 (100%)	-0.00	3 (2%)	60	56	64, 111, 139, 160	0
1	DH	131/131 (100%)	0.04	4 (3%)	49	45	64, 109, 138, 177	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	DI	131/131 (100%)	0.17	6 (4%) 32 30	64, 110, 142, 191	0
1	DJ	131/131 (100%)	-0.01	3 (2%) 60 56	64, 111, 139, 160	0
1	DK	131/131 (100%)	-0.00	2 (1%) 73 70	64, 109, 138, 177	0
1	DL	131/131 (100%)	0.03	3 (2%) 60 56	64, 110, 142, 191	0
All	All	11790/11790 (100%)	0.12	468 (3%) 38 35	64, 110, 141, 191	0

All (468) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BH	65	TYR	6.2
1	CT	88	ASN	5.8
1	CW	24	PHE	5.5
1	AU	54	LYS	5.4
1	BH	62	ASN	5.2
1	AY	65	TYR	4.7
1	BM	131	ALA	4.6
1	AU	55	SER	4.4
1	AU	53	PHE	4.4
1	CS	88	ASN	4.4
1	BY	61	VAL	4.4
1	BQ	62	ASN	4.3
1	CT	64	ASN	4.3
1	CF	65	TYR	4.2
1	AF	53	PHE	4.1
1	CW	23	THR	4.0
1	CS	60	VAL	4.0
1	BA	53	PHE	3.8
1	DI	53	PHE	3.8
1	AI	53	PHE	3.8
1	CL	65	TYR	3.8
1	DD	65	TYR	3.8
1	CW	22	ILE	3.7
1	BH	61	VAL	3.7
1	DC	74	PHE	3.7
1	AG	65	TYR	3.7
1	AO	53	PHE	3.6
1	AX	92	ILE	3.6
1	CE	61	VAL	3.6
1	BE	53	PHE	3.6
1	AN	74	PHE	3.6
1	CT	76	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	BK	65	TYR	3.6
1	BV	53	PHE	3.5
1	CE	88	ASN	3.5
1	AC	65	TYR	3.5
1	AU	35	LEU	3.5
1	DF	53	PHE	3.5
1	BH	88	ASN	3.5
1	CT	60	VAL	3.5
1	BH	60	VAL	3.5
1	DC	94	LEU	3.5
1	BQ	78	MET	3.5
1	BJ	62	ASN	3.5
1	CF	53	PHE	3.5
1	BF	53	PHE	3.4
1	AC	24	PHE	3.4
1	CS	76	ILE	3.4
1	BP	88	ASN	3.4
1	AH	53	PHE	3.4
1	CT	92	ILE	3.4
1	BH	53	PHE	3.4
1	DC	53	PHE	3.4
1	DB	79	SER	3.4
1	BV	92	ILE	3.4
1	CH	74	PHE	3.3
1	DE	125	TRP	3.3
1	CL	88	ASN	3.3
1	CX	62	ASN	3.3
1	BM	60	VAL	3.3
1	AA	65	TYR	3.3
1	CW	53	PHE	3.2
1	AQ	60	VAL	3.2
1	CW	115	LEU	3.2
1	AS	65	TYR	3.2
1	CD	60	VAL	3.2
1	CL	67	LYS	3.2
1	AF	92	ILE	3.2
1	AI	35	LEU	3.2
1	BY	60	VAL	3.2
1	BO	85	THR	3.2
1	CQ	53	PHE	3.2
1	AD	88	ASN	3.2
1	DB	65	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	CT	65	TYR	3.1
1	DJ	65	TYR	3.1
1	DB	78	MET	3.1
1	DB	55	SER	3.1
1	CW	35	LEU	3.1
1	DE	131	ALA	3.1
1	CC	65	TYR	3.1
1	CG	94	LEU	3.1
1	BH	64	ASN	3.0
1	BL	24	PHE	3.0
1	CL	96	ILE	3.0
1	CR	65	TYR	3.0
1	DB	88	ASN	3.0
1	BR	85	THR	3.0
1	DF	131	ALA	3.0
1	CL	66	SER	3.0
1	CS	74	PHE	3.0
1	BF	131	ALA	3.0
1	BH	16	ILE	3.0
1	BG	53	PHE	3.0
1	BI	74	PHE	3.0
1	CW	54	LYS	3.0
1	AT	88	ASN	3.0
1	CZ	53	PHE	3.0
1	DH	74	PHE	3.0
1	DC	86	VAL	2.9
1	AO	92	ILE	2.9
1	BS	65	TYR	2.9
1	BO	87	PHE	2.9
1	CD	74	PHE	2.9
1	BA	131	ALA	2.9
1	CV	131	ALA	2.9
1	AU	52	THR	2.9
1	AZ	85	THR	2.9
1	CE	53	PHE	2.9
1	CA	65	TYR	2.9
1	DC	51	ALA	2.9
1	AV	92	ILE	2.9
1	CJ	74	PHE	2.9
1	CW	65	TYR	2.9
1	AF	90	VAL	2.8
1	BJ	74	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	CW	8	LYS	2.8
1	CK	85	THR	2.8
1	CZ	24	PHE	2.8
1	AU	131	ALA	2.8
1	DD	63	GLY	2.8
1	DF	35	LEU	2.8
1	BG	74	PHE	2.8
1	CE	60	VAL	2.8
1	BP	129	ALA	2.8
1	BZ	65	TYR	2.8
1	CW	40	SER	2.8
1	AC	94	LEU	2.8
1	BR	24	PHE	2.8
1	BK	63	GLY	2.8
1	AC	53	PHE	2.8
1	CK	62	ASN	2.8
1	CZ	92	ILE	2.8
1	BP	89	SER	2.8
1	DG	88	ASN	2.8
1	BA	109	ARG	2.8
1	BE	8	LYS	2.8
1	BM	129	ALA	2.8
1	BZ	108	LEU	2.8
1	BX	60	VAL	2.8
1	BQ	67	LYS	2.7
1	AD	87	PHE	2.7
1	AD	27	THR	2.7
1	BJ	85	THR	2.7
1	BG	62	ASN	2.7
1	BH	63	GLY	2.7
1	CP	53	PHE	2.7
1	BJ	61	VAL	2.7
1	BQ	77	PRO	2.7
1	AW	88	ASN	2.7
1	CF	24	PHE	2.7
1	CK	53	PHE	2.7
1	AH	92	ILE	2.7
1	DA	65	TYR	2.7
1	AO	94	LEU	2.7
1	AI	40	SER	2.7
1	DB	60	VAL	2.7
1	AK	80	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	AT	78	MET	2.7
1	BA	40	SER	2.7
1	CW	121	TYR	2.7
1	BE	24	PHE	2.7
1	CB	53	PHE	2.7
1	DH	24	PHE	2.7
1	CO	65	TYR	2.6
1	AR	65	TYR	2.6
1	BZ	24	PHE	2.6
1	BG	92	ILE	2.6
1	BM	65	TYR	2.6
1	CJ	92	ILE	2.6
1	CU	65	TYR	2.6
1	DC	92	ILE	2.6
1	BJ	53	PHE	2.6
1	CR	94	LEU	2.6
1	DD	94	LEU	2.6
1	BP	74	PHE	2.6
1	CI	92	ILE	2.6
1	AF	129	ALA	2.6
1	AR	60	VAL	2.6
1	DA	24	PHE	2.6
1	DD	60	VAL	2.6
1	DF	65	TYR	2.6
1	AK	88	ASN	2.6
1	BN	64	ASN	2.6
1	CL	97	HIS	2.6
1	BT	92	ILE	2.6
1	CX	65	TYR	2.6
1	BN	65	TYR	2.6
1	DE	126	THR	2.6
1	BD	53	PHE	2.6
1	CW	92	ILE	2.6
1	BG	24	PHE	2.5
1	AC	96	ILE	2.5
1	AN	100	LEU	2.5
1	DI	74	PHE	2.5
1	AR	131	ALA	2.5
1	DC	85	THR	2.5
1	BW	86	VAL	2.5
1	CU	24	PHE	2.5
1	BG	90	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	CG	79	SER	2.5
1	BM	61	VAL	2.5
1	CA	60	VAL	2.5
1	CV	24	PHE	2.5
1	BF	71	GLU	2.5
1	BG	78	MET	2.5
1	CV	88	ASN	2.5
1	BK	92	ILE	2.5
1	CT	61	VAL	2.5
1	CF	1	SER	2.5
1	DD	21	ASP	2.5
1	AX	53	PHE	2.5
1	BM	53	PHE	2.5
1	DB	85	THR	2.5
1	BG	72	VAL	2.5
1	CR	63	GLY	2.5
1	DF	74	PHE	2.5
1	AP	53	PHE	2.5
1	CI	74	PHE	2.5
1	CL	74	PHE	2.5
1	AI	37	VAL	2.5
1	BP	53	PHE	2.5
1	BH	92	ILE	2.5
1	AE	55	SER	2.5
1	CM	78	MET	2.4
1	BE	26	LEU	2.4
1	CB	60	VAL	2.4
1	BW	121	TYR	2.4
1	CQ	74	PHE	2.4
1	BP	92	ILE	2.4
1	BV	90	VAL	2.4
1	BP	65	TYR	2.4
1	AI	2	ILE	2.4
1	CK	92	ILE	2.4
1	AD	86	VAL	2.4
1	DF	37	VAL	2.4
1	BQ	65	TYR	2.4
1	CT	53	PHE	2.4
1	AG	88	ASN	2.4
1	AG	92	ILE	2.4
1	BA	130	LEU	2.4
1	CT	72	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	CK	125	TRP	2.4
1	CF	54	LYS	2.4
1	CT	40	SER	2.4
1	AG	76	ILE	2.4
1	BO	76	ILE	2.4
1	AA	53	PHE	2.4
1	DK	74	PHE	2.4
1	BX	51	ALA	2.4
1	BW	78	MET	2.4
1	CM	88	ASN	2.4
1	BB	96	ILE	2.4
1	CK	94	LEU	2.4
1	DG	94	LEU	2.4
1	AT	24	PHE	2.4
1	BJ	59	THR	2.4
1	CH	24	PHE	2.4
1	BV	72	VAL	2.4
1	AJ	88	ASN	2.4
1	BF	65	TYR	2.4
1	BZ	45	TYR	2.4
1	CI	35	LEU	2.4
1	CM	94	LEU	2.4
1	AQ	24	PHE	2.4
1	CM	24	PHE	2.4
1	AX	72	VAL	2.4
1	CW	72	VAL	2.4
1	AE	74	PHE	2.4
1	BE	74	PHE	2.4
1	BK	62	ASN	2.4
1	BZ	16	ILE	2.4
1	CC	94	LEU	2.3
1	AI	23	THR	2.3
1	AJ	60	VAL	2.3
1	CR	53	PHE	2.3
1	AP	62	ASN	2.3
1	AO	51	ALA	2.3
1	BK	14	ALA	2.3
1	BM	35	LEU	2.3
1	BQ	45	TYR	2.3
1	CB	129	ALA	2.3
1	CF	100	LEU	2.3
1	AU	130	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	BA	2	ILE	2.3
1	AW	74	PHE	2.3
1	BF	74	PHE	2.3
1	BJ	60	VAL	2.3
1	CY	78	MET	2.3
1	CG	88	ASN	2.3
1	AU	92	ILE	2.3
1	AC	54	LYS	2.3
1	DJ	110	LEU	2.3
1	BE	45	TYR	2.3
1	BJ	24	PHE	2.3
1	BS	61	VAL	2.3
1	CP	74	PHE	2.3
1	AG	53	PHE	2.3
1	DF	60	VAL	2.3
1	BM	64	ASN	2.3
1	BS	59	THR	2.3
1	CB	88	ASN	2.3
1	CH	49	ARG	2.3
1	CR	96	ILE	2.3
1	AE	87	PHE	2.3
1	AN	65	TYR	2.3
1	BM	24	PHE	2.3
1	CN	53	PHE	2.3
1	DB	84	GLU	2.3
1	CT	59	THR	2.3
1	DI	35	LEU	2.3
1	CI	53	PHE	2.3
1	BW	80	LEU	2.2
1	CH	130	LEU	2.2
1	BO	86	VAL	2.2
1	DL	53	PHE	2.2
1	BE	38	SER	2.2
1	AO	70	ASN	2.2
1	BO	88	ASN	2.2
1	CA	85	THR	2.2
1	CP	24	PHE	2.2
1	CZ	74	PHE	2.2
1	DH	125	TRP	2.2
1	AH	74	PHE	2.2
1	AU	27	THR	2.2
1	AW	92	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	BK	53	PHE	2.2
1	BM	74	PHE	2.2
1	CE	74	PHE	2.2
1	DD	53	PHE	2.2
1	BM	37	VAL	2.2
1	CC	45	TYR	2.2
1	CD	63	GLY	2.2
1	DC	129	ALA	2.2
1	AU	62	ASN	2.2
1	BP	60	VAL	2.2
1	CB	16	ILE	2.2
1	AZ	83	GLY	2.2
1	AX	35	LEU	2.2
1	AA	24	PHE	2.2
1	DL	61	VAL	2.2
1	AC	58	PRO	2.2
1	AG	45	TYR	2.2
1	DG	65	TYR	2.2
1	CW	94	LEU	2.2
1	CK	74	PHE	2.2
1	CC	67	LYS	2.2
1	CE	24	PHE	2.2
1	AC	22	ILE	2.2
1	AI	51	ALA	2.2
1	AA	26	LEU	2.2
1	AU	94	LEU	2.2
1	AW	24	PHE	2.2
1	BQ	61	VAL	2.2
1	DD	69	LYS	2.2
1	CL	64	ASN	2.2
1	CG	16	ILE	2.2
1	DD	111	ILE	2.2
1	BE	51	ALA	2.2
1	AK	77	PRO	2.2
1	BP	62	ASN	2.2
1	DD	70	ASN	2.2
1	BU	53	PHE	2.2
1	CU	92	ILE	2.2
1	CW	61	VAL	2.2
1	DC	72	VAL	2.2
1	AF	88	ASN	2.2
1	BE	63	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	CT	62	ASN	2.2
1	CE	131	ALA	2.1
1	DI	51	ALA	2.1
1	AF	74	PHE	2.1
1	AJ	65	TYR	2.1
1	BL	85	THR	2.1
1	AR	92	ILE	2.1
1	CE	86	VAL	2.1
1	DC	35	LEU	2.1
1	BV	62	ASN	2.1
1	CD	65	TYR	2.1
1	AI	24	PHE	2.1
1	AL	53	PHE	2.1
1	BM	29	GLN	2.1
1	CV	60	VAL	2.1
1	BJ	94	LEU	2.1
1	AZ	24	PHE	2.1
1	BT	88	ASN	2.1
1	BV	74	PHE	2.1
1	BX	53	PHE	2.1
1	DF	85	THR	2.1
1	BF	76	ILE	2.1
1	BV	40	SER	2.1
1	DC	18	GLY	2.1
1	BV	54	LYS	2.1
1	BW	65	TYR	2.1
1	BD	90	VAL	2.1
1	CG	85	THR	2.1
1	DK	33	ASN	2.1
1	BI	115	LEU	2.1
1	BZ	110	LEU	2.1
1	CV	74	PHE	2.1
1	DI	71	GLU	2.1
1	DC	52	THR	2.1
1	AD	77	PRO	2.1
1	CT	74	PHE	2.1
1	AX	80	LEU	2.1
1	BV	94	LEU	2.1
1	CX	63	GLY	2.1
1	BS	64	ASN	2.1
1	CO	53	PHE	2.1
1	CW	62	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	BK	121	TYR	2.1
1	CS	77	PRO	2.1
1	CH	131	ALA	2.1
1	AB	46	ARG	2.1
1	AY	92	ILE	2.1
1	BD	92	ILE	2.1
1	CK	72	VAL	2.1
1	CL	61	VAL	2.1
1	CI	115	LEU	2.1
1	AI	74	PHE	2.1
1	BB	53	PHE	2.1
1	BI	53	PHE	2.1
1	BT	74	PHE	2.1
1	AM	65	TYR	2.1
1	CT	90	VAL	2.1
1	DF	25	ALA	2.1
1	BS	92	ILE	2.1
1	DF	130	LEU	2.1
1	CT	87	PHE	2.1
1	DD	62	ASN	2.1
1	BK	61	VAL	2.1
1	CL	60	VAL	2.1
1	CT	86	VAL	2.1
1	CW	55	SER	2.1
1	BF	24	PHE	2.0
1	BU	125	TRP	2.0
1	BC	37	VAL	2.0
1	BJ	65	TYR	2.0
1	BH	85	THR	2.0
1	BZ	113	ALA	2.0
1	CG	60	VAL	2.0
1	DI	92	ILE	2.0
1	BH	37	VAL	2.0
1	BL	63	GLY	2.0
1	BN	8	LYS	2.0
1	DJ	74	PHE	2.0
1	AQ	121	TYR	2.0
1	BR	86	VAL	2.0
1	BV	65	TYR	2.0
1	DL	94	LEU	2.0
1	BK	74	PHE	2.0
1	BQ	74	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	AH	72	VAL	2.0
1	CU	45	TYR	2.0
1	CR	92	ILE	2.0
1	BT	53	PHE	2.0
1	CX	74	PHE	2.0
1	DH	98	PRO	2.0
1	BA	92	ILE	2.0
1	BT	94	LEU	2.0
1	AB	74	PHE	2.0
1	AC	74	PHE	2.0
1	CA	74	PHE	2.0
1	CQ	54	LYS	2.0
1	BV	35	LEU	2.0
1	CI	60	VAL	2.0
1	CI	90	VAL	2.0
1	DA	94	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.